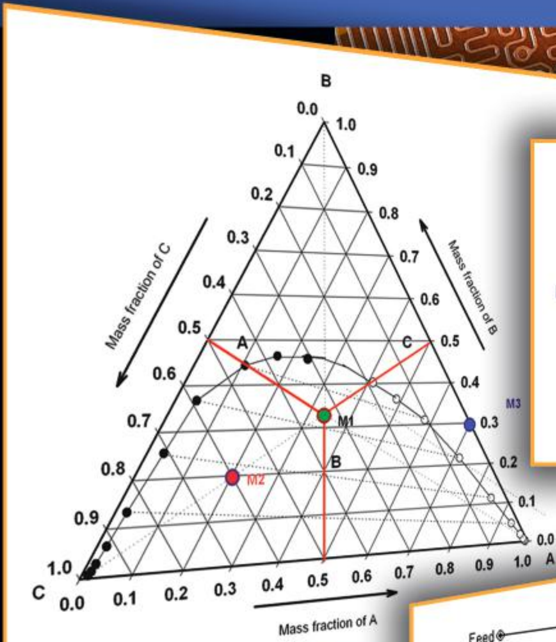
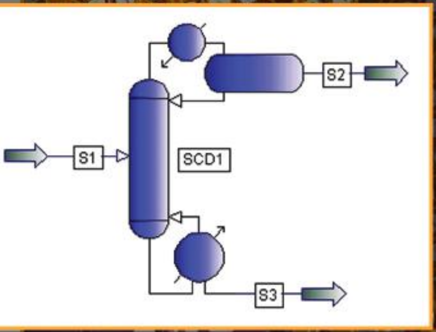
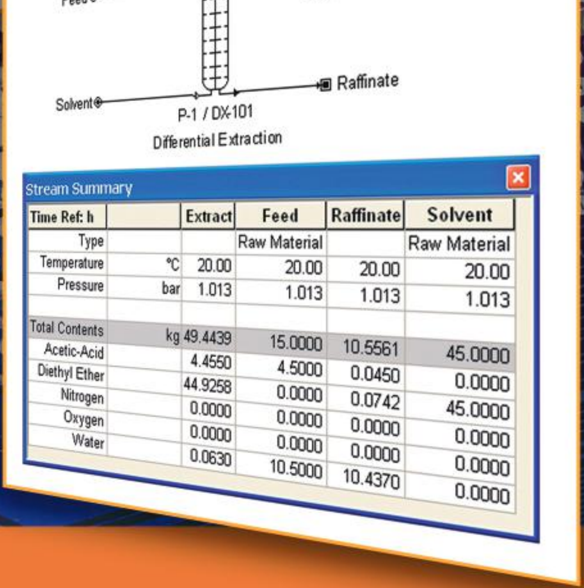
Computer Methods in Chemical Engineering







Stream Summary

Time Ref: h		Extract	Feed	Raffinate	Solvent
Type			Raw Material		Raw Material
Temperature	°C	20.00	20.00	20.00	20.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	49.4439	15.0000	10.5561	45.0000
Acetic-Acid		4.4550	4.5000	0.0450	0.0000
Diethyl Ether		44.9258	0.0000	0.0742	45.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		0.0630	10.5000	10.4370	0.0000

Nayef Ghasem

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To Prof. Önder Özbelge

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Preface

Purpose of the Book

In industry, complicated problems are often not solved by hand for two reasons: human error and time constraints. There are many different simulation programs used in industry, depending on field, application, and desired simulation products. When software is used to its full capabilities, it is a very powerful tool for a chemical engineer in a variety of fields, including oil and gas production, refining, chemical and petrochemical processes, environmental studies, and power generation. Although most of the software packages are user friendly, considerable effort must be expended to master these softwares.

Software packages, such as PRO/II, Hysys/Unisim, Aspen Plus, and Design Pro, have been developed to perform rigorous solutions of most unit operations in chemical engineering. However, as a design engineer, one always needs to know the fundamental theory and methods of calculation to enable one to make decisions about the validity of these black box packages to verify the results. Most software packages are interactive process simulation programs. They are user-friendly and powerful programs that can be used to solve various kinds of chemical engineering processes. However, various conditions and choices have to be provided in order to solve a problem; good knowledge about the process is needed to be used effectively. The objective of this book is to introduce chemical engineering students to the most commonly used simulation softwares and the theory in order to cover core chemical engineering courses. The book is very useful in covering the application parts in various core chemical engineering courses such as chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, computer applications in chemical engineering, and also in graduation projects and in industrial applications.

Each chapter in *Computer Methods in Chemical Engineering* contains a theoretical description of process units followed by numerous examples solved by hand calculations and simulation with the four software packages, Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer, through step-by-step instructions. The book is perfect for students and professionals and gives them the tools to solve real problems involving mainly thermodynamics and fluid phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid–liquid extraction.

Course Objective

Students should be able to:

1. Obtain a feel for what chemical engineers do.
2. Find out the functions of the basic chemical engineering unit operations.
3. Learn the theoretical background of the main unit operations that face chemical engineers.
4. Become skilled at how to simulate the basic chemical processes using software packages such as PRO/II, Hysys, Unisim, Aspen Plus, and SuperPro Designer.
5. Gain knowledge of how to size chemical process units manually and with software packages.
6. Fit experimental data, solve linear and non linear algebraic equations, and solve ordinary differential equations using the Polymath software package.

Course Intended Outcomes

Relation of the covered subjects to the program outcomes (Accreditation Board for Engineering and Technology [ABET] criteria).

By completing the subjects covered in this book, one should be able to:

1. Know the features of PRO/II, Hysys, Unisim, Aspen Plus, and SuperPro Designer software packages (k).
2. Verify hand calculations with available software packages used to simulate pipes, pumps, compressors, heaters, air coolers, and shell and tube heat exchangers (c, e, k).
3. Design and simulate multi-component distillation columns using rigorous and shortcut distillation methods (c, e, k).
4. Calculate reactor sizing and compare hand calculations with simulated results for conversion, equilibrium, plug flow reactors and continuous stirred tank reactors (c, e, k).
5. Know how to design gas absorbers used to remove unwanted gases from certain gas streams, manually and with available software (c, e, k).

6. Be trained in how to use and design liquid–liquid extraction columns (c, e, k).
7. Connect different unit operations in a process flow diagram (k).
8. Familiarize yourself with tray sizing utility for distillation columns and absorbers (c, e, k).
9. Work in teams, including a beginning ability to work in multidisciplinary teams (d).
10. Communicate effectively through presentations and class participation (g).

Acknowledgments

The author would like to thank Allison Shatkin, acquiring editor for this book, Jessica Vakili, the project coordinator, and Robert Sims, the project editor, for their help and cooperation. The author would also like to thank the engineers from Simsci PRO/II and SuperPro Designer for their help and cooperation, and Honeywell for providing the free educational license of Unisim. The comments and suggestions of the reviewers were highly appreciated.

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Nayef Ghasem is an associate professor of chemical engineering at the United Arab Emirates University, where he teaches chemical process principles and computer applications in chemical engineering as undergraduate courses along with other courses in chemical engineering. He has published primarily in the areas of modeling and simulation, bifurcation theory, polymer reaction engineering, and advanced control of polyethylene and polystyrene polymerization processes. He has also authored *Principles of Chemical Engineering Processes* (CRC Press, 2009) and *Simulation of Unit Operations with HYSYS* (Umpress, 2006). Dr. Ghasem is a member of the Institute of Chemical Engineers (IChemE) and a member of the American Chemical Society (ACS).

1

Thermodynamics and Fluid-Phase Equilibria

At the end of this chapter you should be able to

1. Estimate the vapor pressure of pure components.
2. Determine boiling point and dew point of a mixture.
3. Calculate relative volatility.
4. Estimate the molar volume using equation of state (EOS).
5. Plot the effect of temperature on density.
6. Use Hysys, Aspen, PRO/II, and SuperPro softwares to estimate physical properties.

1.1 Introduction

Phase-equilibrium thermodynamics deals with the relationships that govern the distribution of a substance between gas and liquid phases. When a species is transferred from one phase to another, the rate of transfer generally decreases with time until the second phase is saturated with the species, holding as much as it can hold at the prevailing process conditions. When concentrations of all species in each phase cease to change, the phases are said to be at phase equilibrium. When two phases are brought into contact, a redistribution of the components of each phase occurs through evaporation, condensation, dissolution, and/or precipitation until a state of equilibrium is reached in which the temperatures and pressures of both phases are the same, and the compositions of each phase no longer change with time. The volatility of a species is the degree to which the species tends to be transferred from the liquid phase to the vapor phase. The vapor pressure of a species is a measure of its volatility. Estimation of vapor pressure can be carried out by empirical correlation.

When a liquid is heated slowly at constant pressure, the temperature at which the first vapor bubble forms is called the bubble-point temperature. When the vapor is cooled slowly at constant pressure, the temperature at which the first liquid droplet forms is the dew point temperature.

1.2 Boiling Point Calculations

When heating a liquid consists of two or more components, the bubble point is the point where the first bubble of vapor is formed. Given that vapor will probably have a different composition in the liquid, the bubble point and the dew point at different compositions which provide useful data when designing distillation systems. For single-component mixtures the bubble point and the dew point are the same and are referred to as the boiling point. At the bubble point, the following relationship holds:

$$\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} K_i x_i = 1.0 \tag{1.1}$$

where

$$K_i = \frac{y_i}{x_i} \tag{1.2}$$

K is the distribution coefficient or K factor, defined as the ratio of mole fraction in the vapor phase y_i to the mole fraction in the liquid phase x_i at equilibrium. When Raoult's law and Dalton's law hold for the mixture, the K factor is defined as the ratio of the vapor pressure to the total pressure of the system [2]:

$$K_i = \frac{P_{\mathrm{v},i}}{P} \tag{1.3}$$

1.3 Dew Point Calculation

The dew point is the temperature at which a given parcel of air must be cooled, at constant barometric pressure, for water vapor to condense into water. The condensed water is called dew. Dew point is a saturation point. The basic equation for the dew point is as follows:

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \frac{y_i}{K_i} = 1.0 \tag{1.4}$$

1.4 Vapor Pressure Correlations

One of the most successful correlations is called Antoine equation, which uses three coefficients, A, B, and C, which depend on the substance being analyzed. Antoine equation is as follows:

$$\log(P_\mathrm{v}) = A - \frac{B}{T + C} \tag{1.5}$$

If Raoult's law and Dalton's law hold, values of K_i can be calculated from the vapor pressure (P_v) and the total pressure (P) of the system

$$K_i = \frac{P_\mathrm{v}}{P} \tag{1.6}$$

1.5 Relative Volatility

The K factors are strongly temperature dependent because of the change in vapor pressure, but the relative volatility of K for two components change only moderately with temperature. The ratio of K factors is the same as the relative volatility (α_{ij}) of the components

$$\alpha_{ij} = \frac{y_i/x_i}{y_j/x_j} = \frac{K_i}{K_j} \tag{1.7}$$

when Raoult's law applies,

$$\alpha_{ij} = \frac{P_{\mathrm{v},i}}{P_{\mathrm{v},j}} \tag{1.8}$$

Example 1.1: Bubble Point

Find the bubble-point temperature for a mixture of 35 mol% n-hexane, 30% n-heptane, 25% n-octane, and 10% n-nonane at 1.5 atm total pressure.

SOLUTION

HAND CALCULATION

Assume the temperature, calculate the vapor pressure using Antoine equation, and then calculate the summation of y_i; if the summation is 1, then temperature is

TABLE 1.1

Bubble-Point Calculation Assumed at $T = 110°C$

Component	x_i	P_v (110°C), atm	$K_i = P_v/1.5$	$y_i = K_i x_i$
n-Hexane	0.35	3.11	2.074	0.726
n-Heptane	0.30	1.385	0.923	0.277
n-Octane	0.25	0.623	0.417	0.104
n-Nonane	0.10	0.292	0.1945	0.020
				$\sum K_i x_i = 1.127$

the boiling point temperature, and if not, consider other temperatures (Tables 1.1 and 1.2).

At 110°C the summation of $\sum K_i x_i = 1.127$ and at $T = 100°C$ $\sum K_i x_i = 0.862$; by interpolation at $\sum K_i x_i = 1.0$, the bubble point is 105.2°C.

HYSYS CALCULATIONS

In a new case in Hysys, add all components involved in the mixture, select *Antoine* as the fluid package, and then enter the simulation environment. Click on *stream* in the object pallet, then click on any place in the PFD, double click on the stream and enter molar compositions of each component. In the conditions page set the vapor/phase fraction = 0; the calculated temperature (which is the boiling point temperature at the given pressure 1.5 atm) is 105.5°C as shown in Figure 1.1.

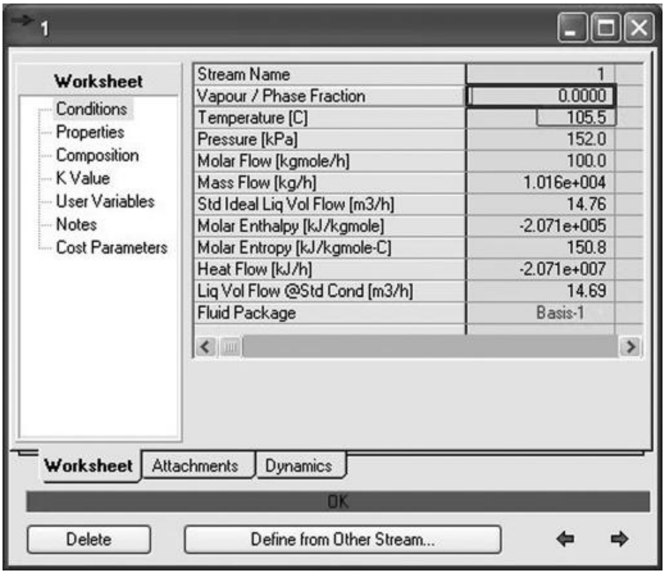
PRO/II CALCULATION

To open Provision, go to the *Start* menu, click on *All Programs*, *Simsci*, and then *PROII*. A screen will appear, click *OK* at the bottom to continue. Next, click on *File* and then *New*. This will bring you to the basic simulation environment from which you have to begin each time you use Provision. It is called the PFD screen. Enter the components that you will be using and your EOS. First click on the *Component Selection button* on the top toolbar (Benzene ring icon). From the popup menu you can either type in the names of your desired components or you can select them from a list already inside Provision. After you select all species click *OK*, then *OK* to return to the PFD. Next click on the *Thermodynamics Data* button, select Peng–Robinson EOS, add all components involved in the mixture. Click on *Streams* in the object pallet, then click anywhere in the PFD. Double click the stream S1 and specify the pressure as 1.5 atm (Figure 1.2). For the second specification select "Bubble Point." Using the Peng–Robinson EOS, the calculated bubble point is 106.67°C (Figure 1.3).

TABLE 1.2

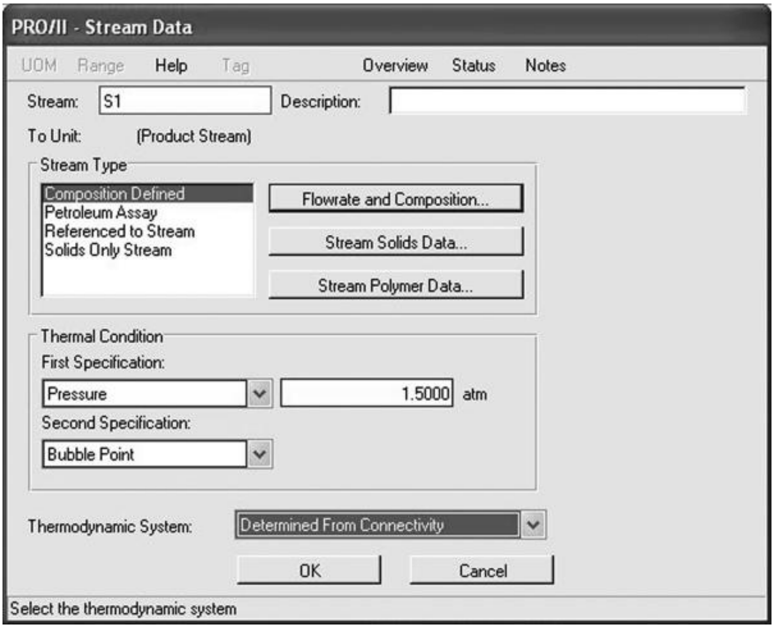
Bubble-Point Calculation at Assumed $T = 100°C$

Component	x_i	P_v (100°C), atm	$K_i = P_v/1.5$	$y_i = K_i x_i$
n-Hexane	0.35	2.42	1.61	0.565
n-Heptane	0.30	1.036	0.69	0.207
n-Octane	0.25	0.454	0.303	0.076
n-Nonane	0.10	0.205	0.137	0.0137
				$\sum K_i x_i = 0.862$



Stream Name	1
Vapour / Phase Fraction	0.0000
Temperature [C]	105.5
Pressure [kPa]	152.0
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	1.016e+004
Std Ideal Liq Vol Flow [m3/h]	14.76
Molar Enthalpy [kJ/kgmole]	-2.071e+005
Molar Entropy [kJ/kgmole-C]	150.8
Heat Flow [kJ/h]	-2.071e+007
Liq Vol Flow @Std Cond [m3/h]	14.69
Fluid Package	Basis-1

FIGURE 1.1
Bubble-point temperature (105.5°C).



Stream: S1

Description:

To Unit: (Product Stream)

Stream Type: Composition Defined

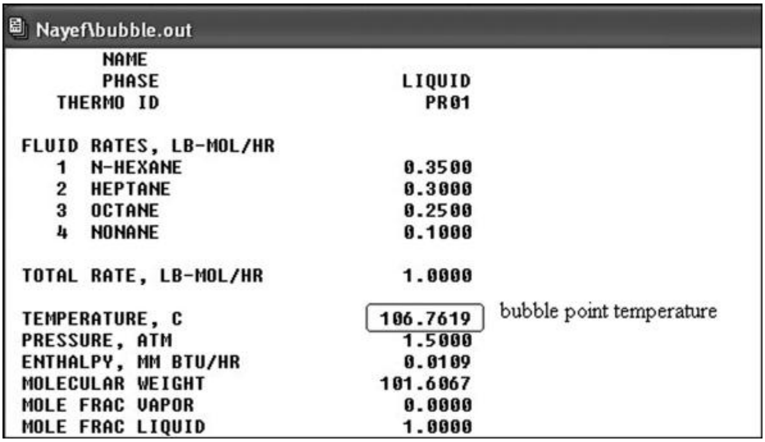
First Specification: Pressure 1.5000 atm

Second Specification: Bubble Point

Thermodynamic System: Determined From Connectivity

Select the thermodynamic system

FIGURE 1.2
Stream specifications at bubble-point conditions.



Nayef\bubble.out

```
       NAME
       PHASE                     LIQUID
   THERMO ID                       PR01

FLUID RATES, LB-MOL/HR
   1  N-HEXANE                   0.3500
   2  HEPTANE                    0.3000
   3  OCTANE                     0.2500
   4  NONANE                     0.1000

TOTAL RATE, LB-MOL/HR            1.0000

TEMPERATURE, C                 106.7619
PRESSURE, ATM                    1.5000
ENTHALPY, MM BTU/HR              0.0109
MOLECULAR WEIGHT               101.6067
MOLE FRAC VAPOR                  0.0000
MOLE FRAC LIQUID                 1.0000
```

bubble point temperature

FIGURE 1.3
Bubble-point calculation using PRO/II.

ASPEN CALCULATIONS

The easy way to estimate the bubble-point temperature with Aspen is to build a simple mixing process with feed stream S1 and exit stream S2. The property estimation method is Peng–Robinson. Double click on S1 and fill in pressure and composition. Since the bubble-point temperature is to be determined, the vapor-to-phase ratio is set to 0. The system is ready to run. The bubble-point temperature is 379.9 (106.7°C) (Figure 1.4).

SUPERPRO CALCULATIONS

In SuperPro the feed pressure and temperature should be defined and there is no option of setting the feed at its boiling or dew point unless the value is provided in the form of temperature or pressure.

Example 1.2: Dew Point Calculation

Find the dew-point temperature for a mixture of 35 mol% *n*-hexane, 30% *n*-heptane, 25% *n*-octane, and 10% *n*-nonane at 1.5 atm total pressure.

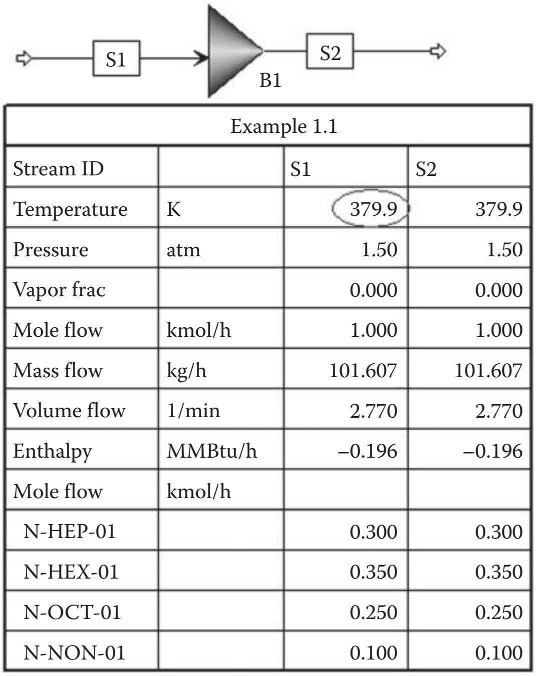
SOLUTION

HAND CALCULATIONS

Assume the temperature, calculate the vapor pressure using Antoine equation, and then calculate summation of x_i; if the summation is 1, then temperature is the dew-point temperature, and if not, consider other temperatures. To make use of the previous assumed temperature, assume $T = 110°C$ (Table 1.3).

The assumed temperature should be increased, and hence assume $T = 130°C$ (Table 1.4).

By interpolation, the dew point is 127.27°C.



Example 1.1			
Stream ID		S1	S2
Temperature	K	379.9	379.9
Pressure	atm	1.50	1.50
Vapor frac		0.000	0.000
Mole flow	kmol/h	1.000	1.000
Mass flow	kg/h	101.607	101.607
Volume flow	1/min	2.770	2.770
Enthalpy	MMBtu/h	–0.196	–0.196
Mole flow	kmol/h		
N-HEP-01		0.300	0.300
N-HEX-01		0.350	0.350
N-OCT-01		0.250	0.250
N-NON-01		0.100	0.100

FIGURE 1.4
Bubble point of the hydrocarbon mixture calculated with Aspen.

TABLE 1.3
Dew-Point Calculation at Assumed $T = 110°\text{C}$

Component	y_i	P_v(110°C), atm	$K_i = P_v/1.5$	$x_i = y_i/K_i$
n-Hexane	0.35	3.11	2.074	0.169
n-Heptane	0.30	1.385	0.923	0.325
n-Octane	0.25	0.623	0.417	0.600
n-Nonane	0.10	0.292	0.1945	0.514
				$\Sigma y_i/K_i = 1.608$

TABLE 1.4
Dew-Point Calculation at Assumed $T = 130°\text{C}$

Component	y_i	P_v(130°C), atm	$K_i = P_v/1.5$	$x_i = y_i/K_i$
n-Hexane	0.35	4.94	3.29	0.106
n-Heptane	0.30	2.329	1.553	0.193
n-Octane	0.25	1.12	0.747	0.335
n-Nonane	0.10	0.556	0.371	0.27
				$\Sigma y_i/K_i = 0.94$

HYSYS CALCULATION

The dew-point temperature can be determined by setting the vapor/phase fraction = 1; the calculated temperature is the dew-point temperature (T_{dp} = 126.3°C) (Figure 1.5).

PRO/II CALCULATION

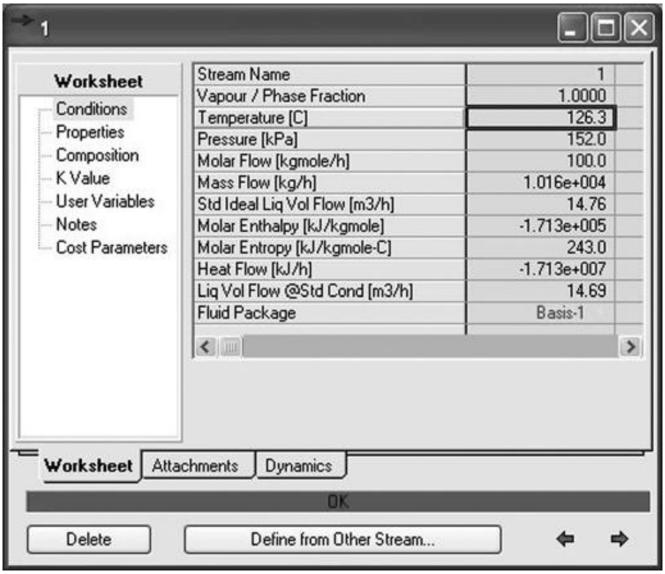
In a new case in Pro/II, add all components involved, for the fluid package select the Peng–Robinson EOS, click on *stream* in the object pallet, and then click and drag in the PFD area. Double click on the stream and specify pressure as 1.5 atm, as a second specification, select *Dew Point* from the pull-down menu (Figure 1.6). Double click on flow rate and specify the molar composition of all streams. For total flow rate you can enter any value, for example, 1 kgmol/h (Figure 1.7).

ASPEN CALCULATION

The property estimation method is Peng–Robinson. Double click on S1 and fill in pressure and composition. Since the dew-point temperature is to be determined, the vapor-to-phase ratio is set to 1. The system is ready to run. The bubble-point temperature is 399 K (127°C) (Figure 1.8).

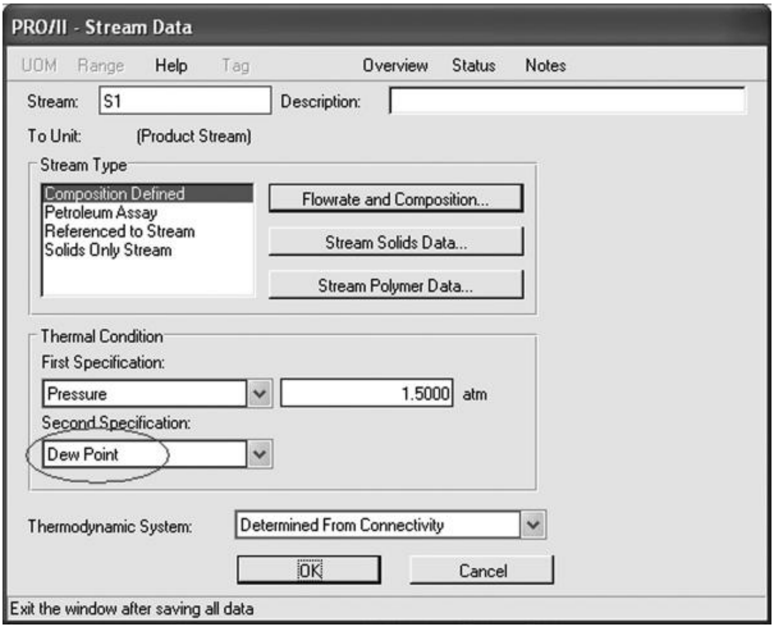
Example 1.3: Vapor Pressure of Gas Mixture

Find the vapor pressure of the pure components and the mixture of 35 mol% *n*-hexane, 30% *n*-heptane, 25% *n*-octane, and 10% *n*-nonane at 130°C.



Stream Name	1
Vapour / Phase Fraction	1.0000
Temperature [C]	126.3
Pressure [kPa]	152.0
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	1.016e+004
Std Ideal Liq Vol Flow [m3/h]	14.76
Molar Enthalpy [kJ/kgmole]	-1.713e+005
Molar Entropy [kJ/kgmole-C]	243.0
Heat Flow [kJ/h]	-1.713e+007
Liq Vol Flow @Std Cond [m3/h]	14.69
Fluid Package	Basis-1

FIGURE 1.5
Dew-point temperature (126.3°C) calculated with Hysys.



Stream: S1

Description:

To Unit: (Product Stream)

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Thermal Condition

First Specification: Pressure 1.5000 atm

Second Specification: Dew Point

Thermodynamic System: Determined From Connectivity

Exit the window after saving all data

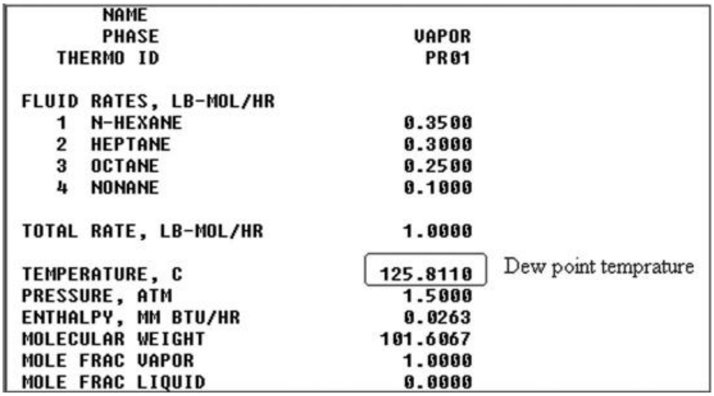
FIGURE 1.6
Dew-point selection as a second specification.

SOLUTION

Hand Calculation

Using Antoine equation, for *n*-hexane,

$$\log(P_v, \text{mmHg}) = A - \frac{B}{(T + C)} = 6.87 - \frac{1168.72}{(130 + 224.21)} = 3722 \text{ mmHg } (496.2 \text{kPa})$$



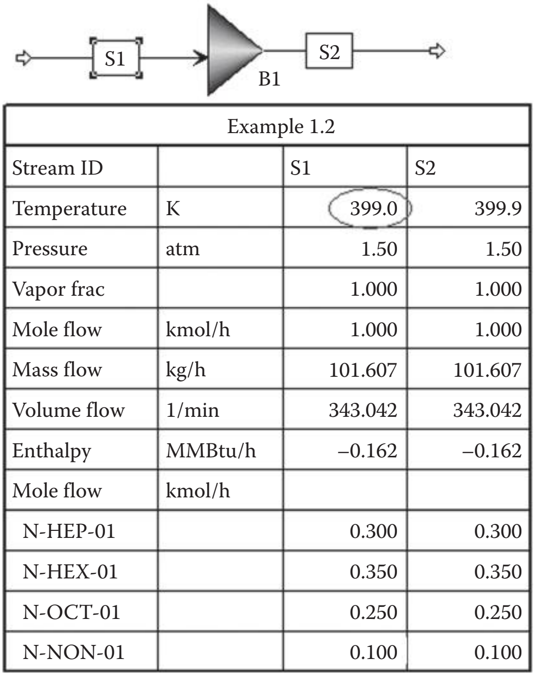
```
         NAME
         PHASE                          VAPOR
     THERMO ID                          PR01

   FLUID RATES, LB-MOL/HR
      1  N-HEXANE                      0.3500
      2  HEPTANE                       0.3000
      3  OCTANE                        0.2500
      4  NONANE                        0.1000

   TOTAL RATE, LB-MOL/HR               1.0000

   TEMPERATURE, C                    125.8110
   PRESSURE, ATM                       1.5000
   ENTHALPY, MM BTU/HR                 0.0263
   MOLECULAR WEIGHT                  101.6067
   MOLE FRAC VAPOR                     1.0000
   MOLE FRAC LIQUID                    0.0000
```

FIGURE 1.7
Dew-point temperature using PRO/II.



Example 1.2			
Stream ID		S1	S2
Temperature	K	399.0	399.9
Pressure	atm	1.50	1.50
Vapor frac		1.000	1.000
Mole flow	kmol/h	1.000	1.000
Mass flow	kg/h	101.607	101.607
Volume flow	1/min	343.042	343.042
Enthalpy	MMBtu/h	–0.162	–0.162
Mole flow	kmol/h		
N-HEP-01		0.300	0.300
N-HEX-01		0.350	0.350
N-OCT-01		0.250	0.250
N-NON-01		0.100	0.100

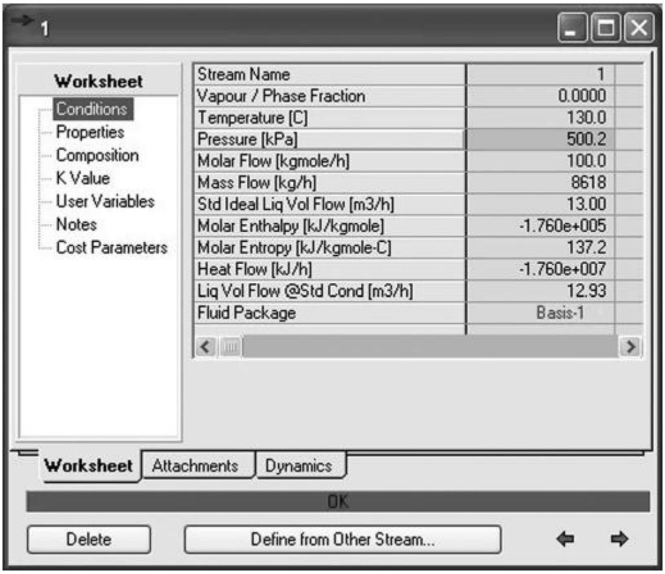
FIGURE 1.8
Dew-point temperature (126°C) calculated with Aspen.

HYSYS CALCULATIONS

1. Create the stream with the composition required; select Antoine equation for the fluid package.
2. Set the vapor fraction to 0 and the temperature to the desired temperature where you want to find out the vapor pressure. Then HYSYS will calculate the pressure; the calculated pressure is the vapor pressure (or more precisely the bubble-point pressure = the vapor pressure) at the specified temperature—similarly, if you want to calculate the dew point, set the vapor fraction to 1. The result depends on many parameters, for example, selection of EOS, components in a mixture. Using Antoine equation, the vapor pressure of pure *n*-hexane at 130°C is 500.2 kPa (Figure 1.9), and the vapor pressure of pure *n*-heptane, *n*-octane, and *n*-nonane is 236 kPa, 113.4 kPa, and 56.33 kPa, respectively. The vapor pressure using Peng–Robinson EOS at 130 is 496 kPa, the same as that obtained by Antoine equation (Figure 1.10). For the gas mixture at 130°C, the vapor pressure is 280 kPa (Figure 1.11).

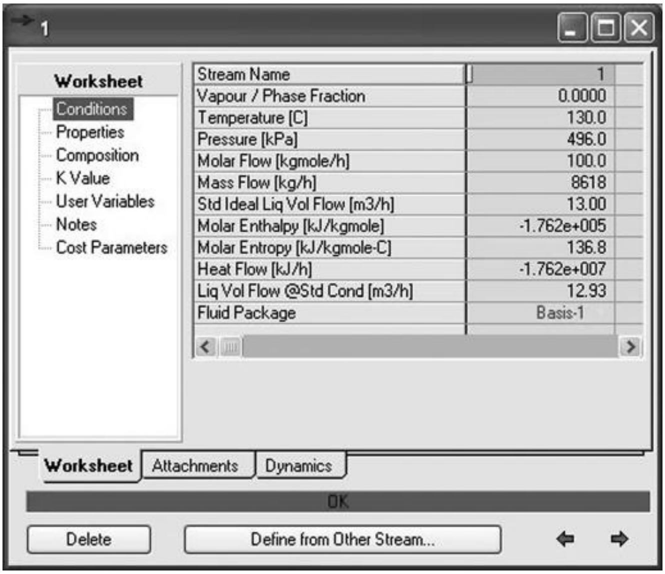
PRO/II CALCULATION

The vapor pressure of pure *n*-hexane using PRO/II is estimated by specifying the temperature at which vapor pressure is to be calculated (in this case 130°C), and the second specification is the bubble point as shown in Figure 1.12. The



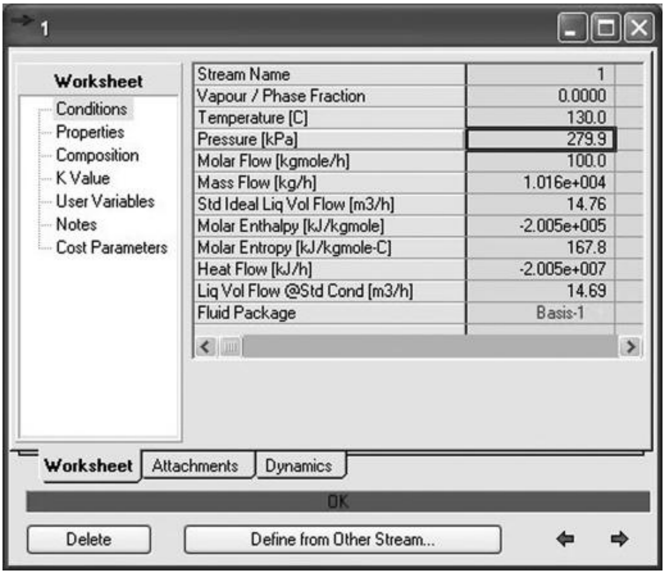
Stream Name	1
Vapour / Phase Fraction	0.0000
Temperature [C]	130.0
Pressure [kPa]	500.2
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	8618
Std Ideal Liq Vol Flow [m3/h]	13.00
Molar Enthalpy [kJ/kgmole]	-1.760e+005
Molar Entropy [kJ/kgmole-C]	137.2
Heat Flow [kJ/h]	-1.760e+007
Liq Vol Flow @Std Cond [m3/h]	12.93
Fluid Package	Basis-1

FIGURE 1.9
Vapor pressure of pure *n*-hexane using Antoine equation.



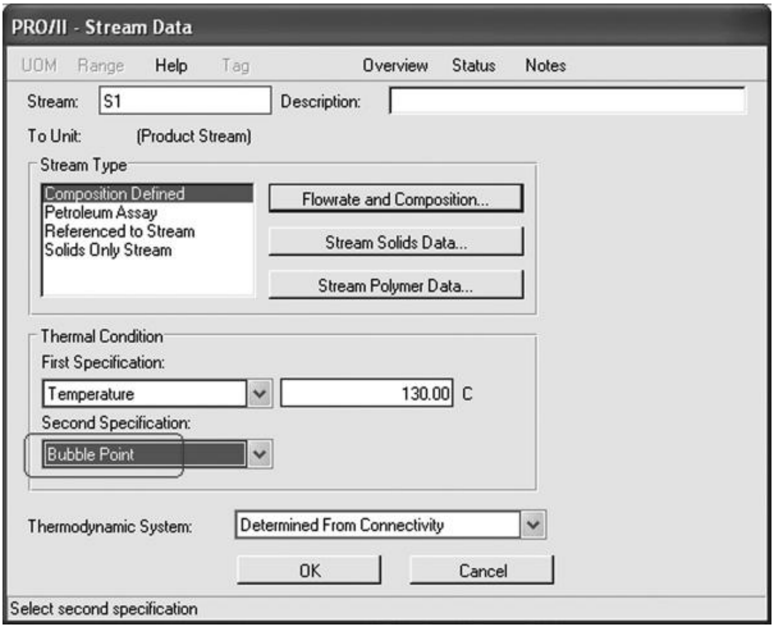
Stream Name	1
Vapour / Phase Fraction	0.0000
Temperature [C]	130.0
Pressure [kPa]	496.0
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	8618
Std Ideal Liq Vol Flow [m3/h]	13.00
Molar Enthalpy [kJ/kgmole]	-1.762e+005
Molar Entropy [kJ/kgmole-C]	136.8
Heat Flow [kJ/h]	-1.762e+007
Liq Vol Flow @Std Cond [m3/h]	12.93
Fluid Package	Basis-1

FIGURE 1.10
Vapor pressure of pure *n*-hexane using Peng–Robinson.



Stream Name	1
Vapour / Phase Fraction	0.0000
Temperature [C]	130.0
Pressure [kPa]	279.9
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	1.016e+004
Std Ideal Liq Vol Flow [m3/h]	14.76
Molar Enthalpy [kJ/kgmole]	-2.005e+005
Molar Entropy [kJ/kgmole-C]	167.8
Heat Flow [kJ/h]	-2.005e+007
Liq Vol Flow @Std Cond [m3/h]	14.69
Fluid Package	Basis-1

FIGURE 1.11
Vapor pressure of mixture at 130°C.



Stream: S1 Description:

To Unit: (Product Stream)

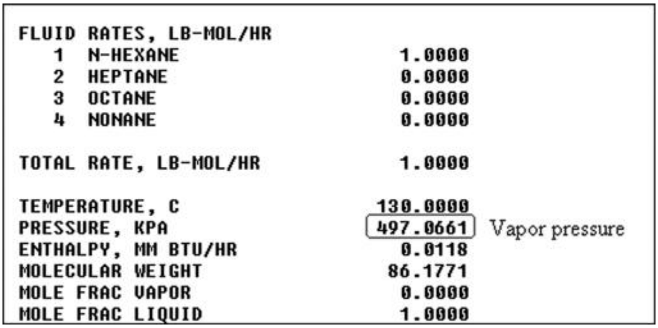
First Specification: Temperature 130.00 C

Second Specification: Bubble Point

Thermodynamic System: Determined From Connectivity

Select second specification

FIGURE 1.12
Vapor pressure calculations at a specified temperature.



```
FLUID RATES, LB-MOL/HR
   1  N-HEXANE                      1.0000
   2  HEPTANE                       0.0000
   3  OCTANE                        0.0000
   4  NONANE                        0.0000

TOTAL RATE, LB-MOL/HR               1.0000

TEMPERATURE, C                    130.0000
PRESSURE, KPA                     497.0661
ENTHALPY, MM BTU/HR                 0.0118
MOLECULAR WEIGHT                   86.1771
MOLE FRAC VAPOR                     0.0000
MOLE FRAC LIQUID                    1.0000
```

FIGURE 1.13
Vapor pressure of pure *n*-hexane at 130°C using PRO/II.

determined vapor pressure of pure *n*-hexane is 497 kPa and the mixture vapor pressure is 268 as shown in Figures 1.13 and 1.14, respectively.

ASPEN CALCULATIONS

To calculate the vapor pressure of pure *n*-hexane at 130°C, set the vapor fraction to 0. The vapor pressure of pure *n*-hexane is 4.91 atm (Figure 1.15).

To calculate the vapor pressure of gas mixture at 130°C, set the vapor fraction to 0. The vapor pressure is 2.64 atm (Figure 1.16).

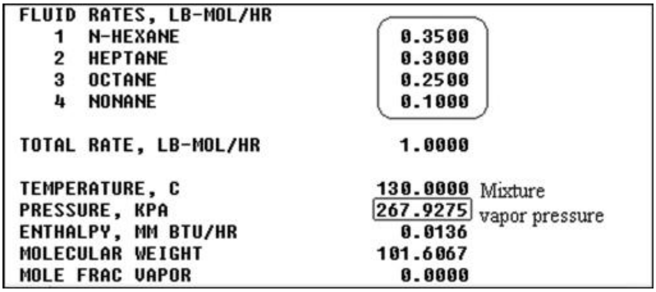
SUPERPRO CALCULATIONS

The vapor pressure of pure *n*-hexane is determined from the pure component property window in SuperPro. To calculate the vapor pressure of a pure gas mixture at 130°C, the following equation is extracted from the SuperPro physical property menu, at $T = 130°C$ (303 K), the vapor pressure of pure *n*-hexane is calculated from the following equation at 130°C:

Log P (mmHg) = 6.88–1171.17/ (T–48.8)

P = 3745.23 mmHg (4.93 atm)

The result is close to that obtained from Hysys and Aspen Plus.

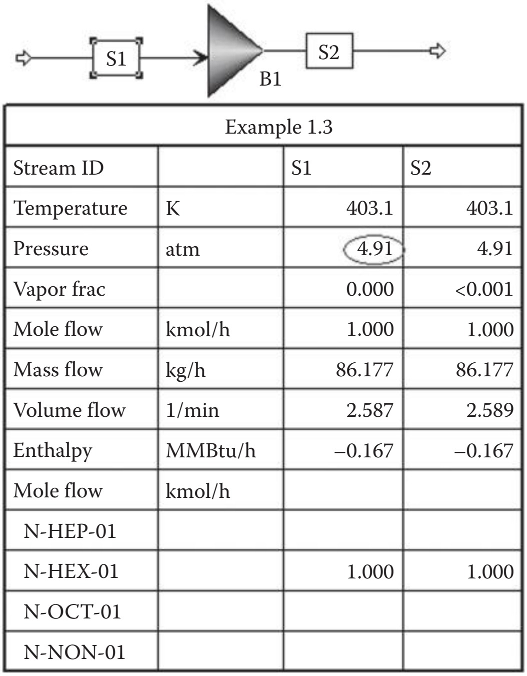


```
FLUID RATES, LB-MOL/HR
   1  N-HEXANE                      0.3500
   2  HEPTANE                       0.3000
   3  OCTANE                        0.2500
   4  NONANE                        0.1000

TOTAL RATE, LB-MOL/HR               1.0000

TEMPERATURE, C                    130.0000
PRESSURE, KPA                     267.9275
ENTHALPY, MM BTU/HR                 0.0136
MOLECULAR WEIGHT                  101.6067
MOLE FRAC VAPOR                     0.0000
```

FIGURE 1.14
Mixture vapor pressure at 130°C.



Example 1.3			
Stream ID		S1	S2
Temperature	K	403.1	403.1
Pressure	atm	4.91	4.91
Vapor frac		0.000	<0.001
Mole flow	kmol/h	1.000	1.000
Mass flow	kg/h	86.177	86.177
Volume flow	1/min	2.587	2.589
Enthalpy	MMBtu/h	–0.167	–0.167
Mole flow	kmol/h		
N-HEP-01			
N-HEX-01		1.000	1.000
N-OCT-01			
N-NON-01			

FIGURE 1.15
Vapor pressure of pure component generated with Aspen.

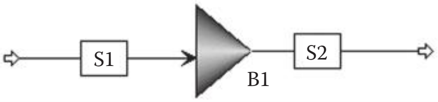
1.6 Equations of State

An expression is required for gases that relate specific volume to temperature and pressure.

An EOS relates molar quantity and volume of a gas to temperature and pressure. EOS is used to predict p, V, n, and T for real gases, pure components, or mixtures. The simplest example of an EOS is the ideal gas law [3]. EOS is formulated by collecting experimental data and calculating the coefficients in a proposed equation by statistical fitting. Numerous EOSs have been proposed in the literature, the equations involving two or more coefficients. Cubic EOSs such as Redlich–Kwong, Soave–Redlich–Kwong, and Peng–Robinson can have an accuracy of 1–2% over a large range of conditions of many compounds.

In solving for n or V, one must solve a cubic equation that might have more than one real root. For example, Peng–Robinson EOS can easily be solved for p if V and T are given [4].

$$p = \frac{RT}{V - b} - \frac{a}{V(V + b) + b(V - b)} \tag{1.9}$$



Example 1.3			
Stream ID		S1	S2
Temperature	K	403.1	403.1
Pressure	atm	2.64	2.64
Vapor frac		0.000	<0.001
Mole flow	kmol/h	1.000	1.000
Mass flow	kg/h	101.607	101.607
Volume flow	1/min	2.886	2.895
Enthalpy	MMBtu/h	–0.190	–0.190
Mole flow	kmol/h		
N-HEP-01		0.300	0.300
N-HEX-01		0.350	0.350
N-OCT-01		0.250	0.250
N-NON-01		0.100	0.100

FIGURE 1.16
Vapor pressure of gas mixture.

The constants *a*, *b* are determined as follows:

$$a = 0.45724\left(\frac{R^2T_c^2}{p_c}\right)\left[1 + m(1 - T_r^{1/2})\right] \tag{1.10}$$

$$b = 0.07780\left(\frac{RT_c}{p_c}\right) \tag{1.11}$$

$$m = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{1.12}$$

$$T_r = \frac{T}{T_c} \tag{1.13}$$

ω = acentric factor, where T_c and p_c are critical temperature and critical pressure, respectively. *V* is the specific volume.

Example 1.4: Specific Molar Volume of *N*-Hexane

Estimate the specific molar volume of *n*-hexane at 1 atm and 25°C.

SOLUTION

HAND CALCULATION, POLYMATH

The equations can be easily solved using the polymath program as shown in Figure 1.17 (for more details on Polymath software, see Appendix A).

HYSYS SIMULATION

The molar volume of pure *n*-hexane at 1 atm and 25°C is calculated using Hysys and Peng–Robinson EOS. The result is shown in Figure 1.18.

PRO/II SIMULATION

Set the stream conditions with pure *n*-hexane. Physical properties were determined with Peng–Robinson. The specific molar volume is the inverse of the molar density (mass density divided by molecular weight of *n*-hexane) is found from the generated text report as shown in Figure 1.19.

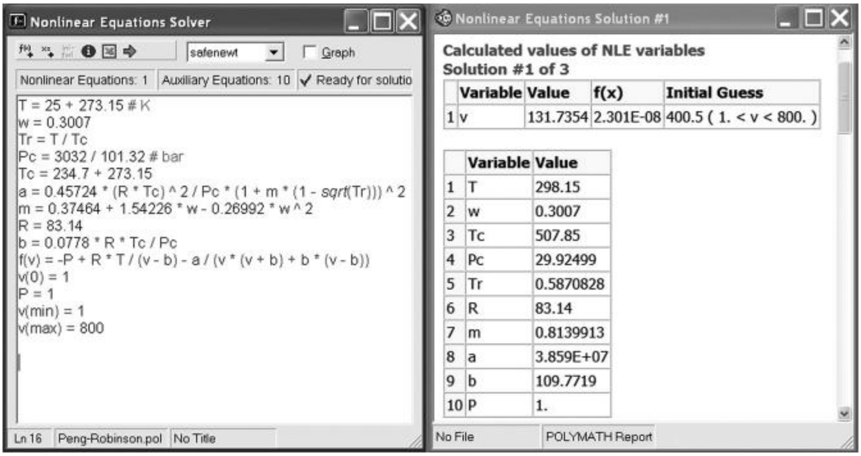
ASPEN CALCULATIONS

Using Aspen plus the result is shown in Figure 1.20, which is almost the same as that obtained by PRO/II.

SUPERPRO CALCULATION

Using the SuperPro designer, select pure component and then select *n*-hexane. At $T = 25°C$ and pressure = 1 atm, the density of pure *n*-hexane is determined using the following equation obtained from the pure component property windows:

Density (g/L) = 924.33 – 0.8999 T (K)
Density (g/L) = 924.33 – 0.8999 (298) = 656 g/L or 656 kg/m^3



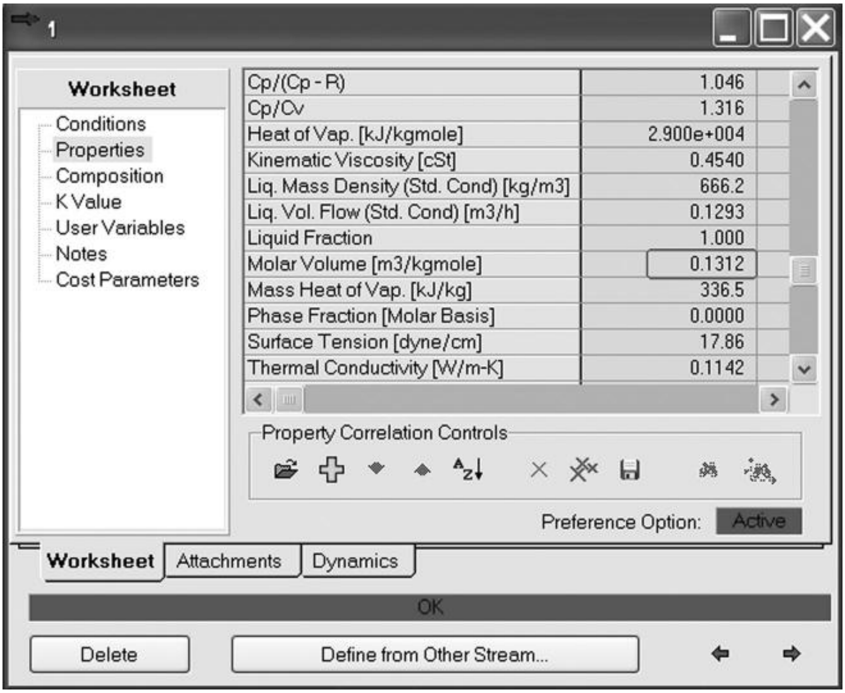
```
T = 25 + 273.15 # K
w = 0.3007
Tr = T / Tc
Pc = 3032 / 101.32 # bar
Tc = 234.7 + 273.15
a = 0.45724 * (R * Tc) ^ 2 / Pc * (1 + m * (1 - sqrt(Tr))) ^ 2
m = 0.37464 + 1.54226 * w - 0.26992 * w ^ 2
R = 83.14
b = 0.0778 * R * Tc / Pc
f(v) = -P + R * T / (v - b) - a / (v * (v + b) + b * (v - b))
v(0) = 1
P = 1
v(min) = 1
v(max) = 800
```

Calculated values of NLE variables
Solution #1 of 3

	Variable	Value	f(x)	Initial Guess
1	v	131.7354	2.301E-08	400.5 (1. < v < 800.)

	Variable	Value
1	T	298.15
2	w	0.3007
3	Tc	507.85
4	Pc	29.92499
5	Tr	0.5870828
6	R	83.14
7	m	0.8139913
8	a	3.859E+07
9	b	109.7719
10	P	1.

FIGURE 1.17
Polymath programs for specific volume calculation.



Cp/(Cp - R)	1.046
Cp/Cv	1.316
Heat of Vap. [kJ/kgmole]	2.900e+004
Kinematic Viscosity [cSt]	0.4540
Liq. Mass Density (Std. Cond) [kg/m3]	666.2
Liq. Vol. Flow (Std. Cond) [m3/h]	0.1293
Liquid Fraction	1.000
Molar Volume [m3/kgmole]	0.1312
Mass Heat of Vap. [kJ/kg]	336.5
Phase Fraction [Molar Basis]	0.0000
Surface Tension [dyne/cm]	17.86
Thermal Conductivity [W/m-K]	0.1142

FIGURE 1.18
Molar volume determined by Hysys.

1.7 Physical Properties

Many correlations are available in the literature to measure physical properties such as density, viscosity, and specific heat as a function of temperature.

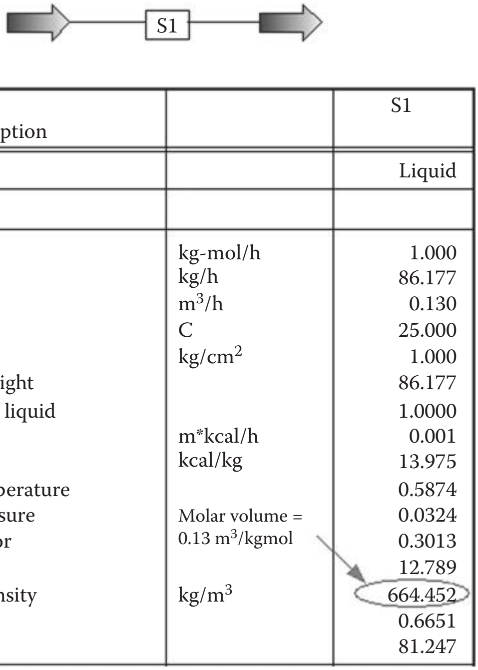
1.7.1 Liquid Density

For saturated-liquid molar volume, the Gunn and Ymada method is used [1].

$$\frac{V}{V_{sc}} = V_r^0\left(1 - \omega\Gamma\right) \tag{1.14}$$

where V is the liquid specific volume and V_{sc} is the scaling parameter that is defined in terms of the volume at $T_r = 0.6$

$$V_{sc} = \frac{V_{0.6}}{0.3862 - 0.0866} \tag{1.15}$$



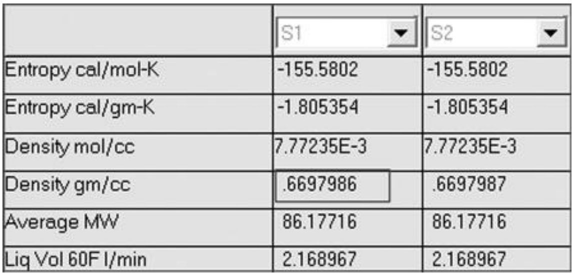
Stream name Stream description		S1
Phase		Liquid
Dry stream		
Rate	kg-mol/h	1.000
	kg/h	86.177
Std. liq. rate	m^3/h	0.130
Temperature	C	25.000
Pressure	kg/cm^2	1.000
Molecular weight		86.177
Mole fraction liquid		1.0000
Enthalpy	m*kcal/h	0.001
	kcal/kg	13.975
Reduced temperature		0.5874
Reduced pressure	Molar volume =	0.0324
Acentric factor	$0.13\ m^3/kgmol$	0.3013
UOP K factor		12.789
Std. liquid density	kg/m^3	664.452
Sp. gravity		0.6651
API gravity		81.247

FIGURE 1.19
Saturated liquid density and molar volume.

where $V_{0.6}$ is the saturated-liquid molar volume at a reduced temperature of 0.6. If $V_{0.6}$ is not available, then approximately V_{sc} can be estimated by

$$V_{sc} = \frac{RT_c}{P_c}(0.2920 - 0.0967\omega) \tag{1.16}$$

In most cases, V_{sc} is close to V_c. However, if the saturated-liquid molar volume is available at any temperature, V_{sc} can be eliminated as shown later in



	S1	S2
Entropy cal/mol-K	-155.5802	-155.5802
Entropy cal/gm-K	-1.805354	-1.805354
Density mol/cc	7.77235E-3	7.77235E-3
Density gm/cc	.6697986	.6697987
Average MW	86.17716	86.17716
Liq Vol 60F l/min	2.168967	2.168967

FIGURE 1.20
Density of pure *n*-hexane at 25°C and 1 atm.

Equation 1.17. In Equation 1.17, $V_r^{(0)}$ and Γ are functions of reduced temperature and ω is the acentric factor.

For $0.2 \le T_r \le 0.8$

$$V_r^{(0)} = 0.33593 - 0.33953\,T_r + 1.51941T_r^2 - 2.02512T_r^3 + 1.11422T_r^4 \quad (1.17)$$

For $0.8 < T_r < 1.0$

$$V_r^{(0)} = 1 + 1.3(1 - T_r)^{1/2}\log(1 - T_r) - 0.50879(1 - T_r) - 0.91534(1 - T_r)^2 \quad (1.18)$$

For $0.2 \le T_r < 1.0$

$$\Gamma = 0.29607 - 0.09045T_r - 0.04842T_r^2 \quad (1.19)$$

where, $T_r = T/T_c$.

In the absence of experimental data, one may assume volume or mass additivity to calculate mixture densities from those of pure components.

$$\bar{\rho} = \sum_{i=1}^{n} x_i\rho_i \quad (1.20)$$

$$\frac{1}{\bar{\rho}} = \sum_{i=1}^{n} \frac{x_i}{\rho_i} \quad (1.21)$$

Equation 1.21 is more accurate than Equation 1.20.

Example 1.5: Estimation of Density of Benzene

Estimate the density of benzene as a function of temperature at 1 atm pressure and 25°C.

SOLUTION

HAND CALCULATIONS, POLYMATH

The set of equation in Section 1.5 is solved using polymath nonlinear equations solver as shown in Table 1.5, the density of liquid benzene at 70°C is shown in Figure 1.21.

HYSYS SIMULATION

Generate a material stream, then use:

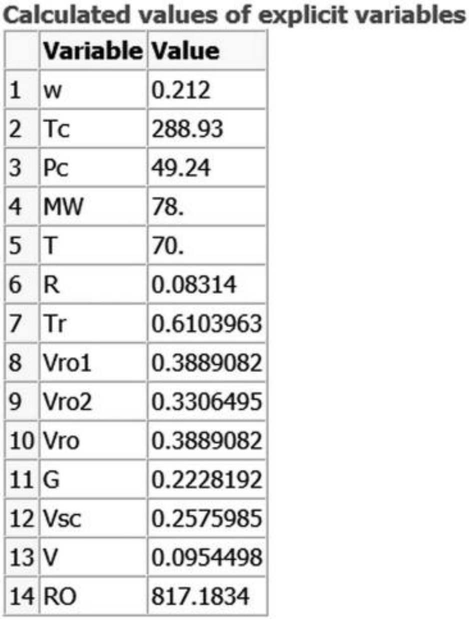
Tools >> Utilities >> Property Table

Then click *Add Utility* as shown in Figure 1.22 and then click on *View Utility*. Click on *Select Stream* to select stream 1, and fill in the popup menu as shown in

TABLE 1.5

Polymath Program of Example 1.5

```
# Density of liquid benzene
w = 0.212
Tc = 288.93#C
Pc = 49.24#bar
MW = 78#g/mol
T = 70#C
R = 0.08314#L.atm/mol.K
Tr = (T + 273)/(Tc + 273)
Vro1 = 0.33593 – 0.33953*Tr + 1.51941*(Tr^2)
 -2.0251*(Tr^3) + 1.11422*(Tr^4)
Vro2 = 1 + 1.3*(1 Tr)^0.5*log(1 – Tr) – 0.50879*(1 – Tr)-0.91534*(1 – Tr)^2
Vro= If (Tr <= 0.8) Then (Vro1) Else (Vro2)
G = 0.29607 – 0.09045*Tr – 0.04842*(Tr^2)
Vsc = (R*(Tc + 273)/Pc)*(0.292 – 0.0967*w)
# Vro = 0.33593 – 0.33953*Tr + 1.51941*(Tr^2)
 -2.0251*(Tr^3) + 1.11422*(Tr^4)
V = Vsc*Vro*(1 – w*G)*1
RO = MW/V # kg/m^3
```



Calculated values of explicit variables

	Variable	Value
1	w	0.212
2	Tc	288.93
3	Pc	49.24
4	MW	78.
5	T	70.
6	R	0.08314
7	Tr	0.6103963
8	Vro1	0.3889082
9	Vro2	0.3306495
10	Vro	0.3889082
11	G	0.2228192
12	Vsc	0.2575985
13	V	0.0954498
14	RO	817.1834

FIGURE 1.21
Liquid density at 70°C is 817.1834 kg/m^3.

Figure 1.23. Click on *Calculate*. From the performance page select press *Plot*. The change in mass density as a function of temperature is shown in Figure 1.24.

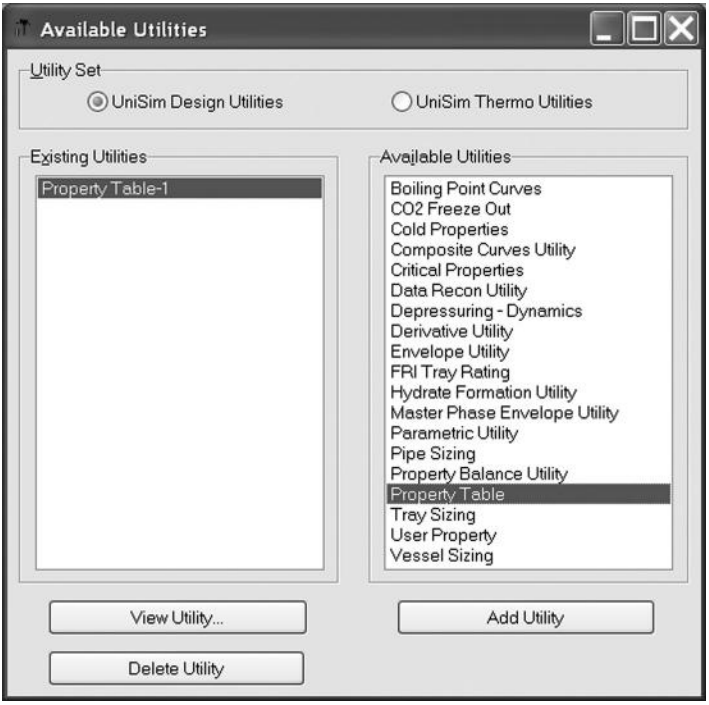
PRO/II SIMULATION

With PRO/II it is easy to find the physical properties of components such as density, viscosity, and surface tension as a function of temperature. After opening PRO/II, click on *Launch TDB* (Thermo Data Manager). Under *Data Bank Type* click on *SIMSCI*. Select benzene from the list of components. Click on *TempDep* in the toolbar, and then select *Density*, followed by *liquid* (Figure 1.25). Click on *Plot* and export the generated data to Excel as shown in Figure 1.26. Other physical properties can be found in the same way.

ASPEN PLUS SIMULATION

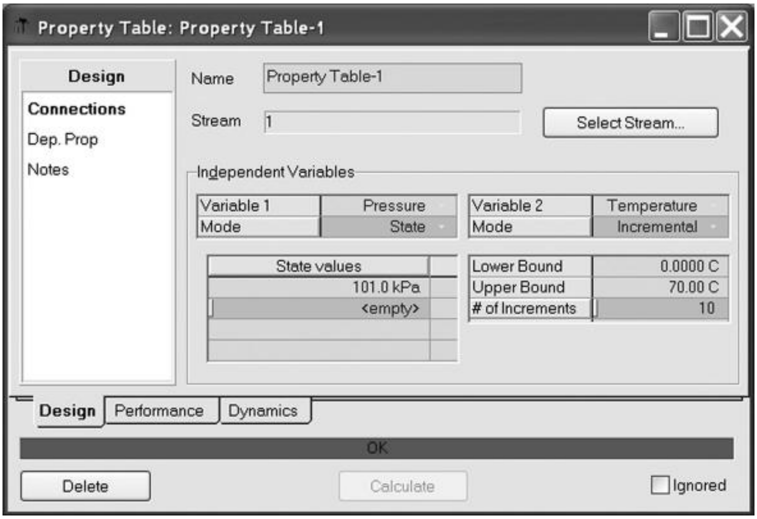
When opening Aspen Plus, select *create new simulation* using *Template*. For this example, choose *General with Metric Units* as the Application Type and *Property Analysis* as the Run Type (Figure 1.27).

Since we are not generating a flow sheet, simply click on *Next* to proceed into the *Property Table Generation System*. Enter the title *Density* into the Title area by simply clicking on the box and typing it. Click on *Next* to continue. Enter all components; for this example benzene is the only component. A base method



Utility Set
● UniSim Design Utilities ○ UniSim Thermo Utilities

FIGURE 1.22
Property table.



Property Table: Property Table-1

Name: Property Table-1

Stream: 1

Variable 1	Pressure
Mode	State

Variable 2	Temperature
Mode	Incremental

State values
101.0 kPa
<empty>

Lower Bound	0.0000 C
Upper Bound	70.00 C
# of Increments	10

OK

FIGURE 1.23
Property calculation menu.

must be chosen, click on the arrow pointing downward in the Base method box and from the list of options, choose NRTL. Click on *Next* to continue. A popup screen appears as a reminder that you must name a table to be generated. Click on *OK* to continue. At this screen a new property set will need to be specified. To do this, click on *New* at the bottom of the screen. Here a name for the new property set can be entered in the ID box. Aspen defaults to *PT–1*. The Select type must

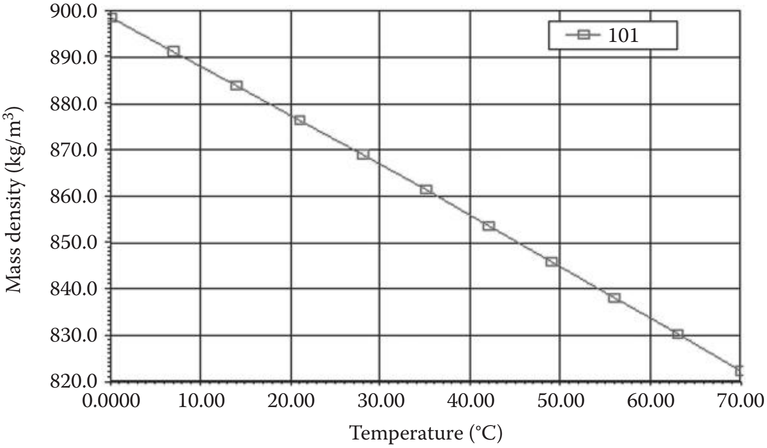
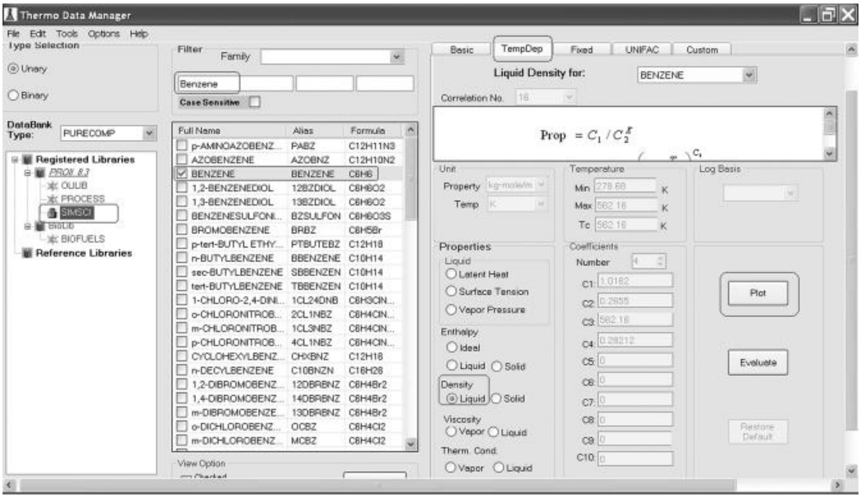


FIGURE 1.24
Plot of mass density versus temperature.



◉ Unary
○ Binary

Benzene
Case Sensitive ☐

DataBank Type: PURECOMP

Full Name	Alias	Formula
☐ p-AMINOAZOBENZ...	PABZ	C12H11N3
☐ AZOBENZENE	AZOBNZ	C12H10N2
☑ BENZENE	BENZENE	C6H6
☐ 1,2-BENZENEDIOL	12BZDIOL	C6H6O2
☐ 1,3-BENZENEDIOL	13BZDIOL	C6H6O2
☐ BENZENESULFONI...	BZSULFON	C6H6O3S
☐ BROMOBENZENE	BRBZ	C6H5Br
☐ p-tert-BUTYL ETHY...	PTBUTEBZ	C12H18
☐ n-BUTYLBENZENE	BBENZENE	C10H14
☐ sec-BUTYLBENZENE	SBBENZEN	C10H14
☐ tert-BUTYLBENZENE	TBBENZEN	C10H14
☐ 1-CHLORO-2,4-DINI...	1CL24DNB	C6H3ClN...
☐ o-CHLORONITROB...	2CL1NBZ	C6H4ClN...
☐ m-CHLORONITROB...	1CL3NBZ	C6H4ClN...
☐ p-CHLORONITROB...	4CL1NBZ	C6H4ClN...
☐ CYCLOHEXYLBENZ...	CHXBNZ	C12H16
☐ n-DECYLBENZENE	C10BNZN	C16H26
☐ 1,2-DIBROMOBENZ...	12DBRBNZ	C6H4Br2
☐ 1,4-DIBROMOBENZ...	14DBRBNZ	C6H4Br2
☐ m-DIBROMOBENZE...	13DBRBNZ	C6H4Br2
☐ o-DICHLOROBENZ...	OCBZ	C6H4Cl2
☐ m-DICHLOROBENZ...	MCBZ	C6H4Cl2

Liquid Density for: BENZENE

Correlation No. 16

$$\text{Prop} = C_1 / C_2^{x}$$

Unit
Property kg-mole/m
Temp K

Temperature
Min 278.68 K
Max 562.16 K
Tc 562.16 K

Properties
Liquid
○ Latent Heat
○ Surface Tension
○ Vapor Pressure
Enthalpy
○ Ideal
○ Liquid ○ Solid
Density
◉ Liquid ○ Solid
Viscosity
○ Vapor ○ Liquid
Therm. Cond.
○ Vapor ○ Liquid

Coefficients
Number 4
C1: 1.0182
C2: 0.2655
C3: 562.16
C4: 0.28212
C5: 0
C6: 0
C7: 0
C8: 0
C9: 0
C10: 0

FIGURE 1.25
Property selection window.

also be chosen. For this example, choose *GENERIC* from the pull-down menu. Click on *OK* to continue. For Aspen to calculate any properties, a flow rate must be specified. For pure component properties, the flow entered does not affect the properties. Since the flow rate is not given, a basis of an arbitrary flow of 1 kmol/h is possible (Figure 1.28).

Choose the variables (Temperature for this example) with which the physical properties will vary. For example, to find density as a function of temperature at

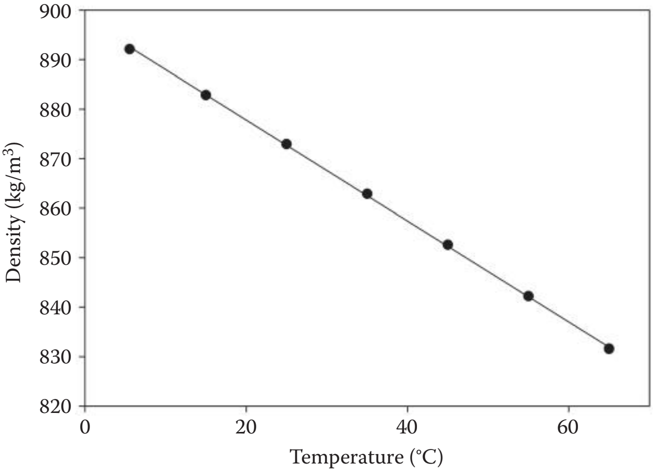
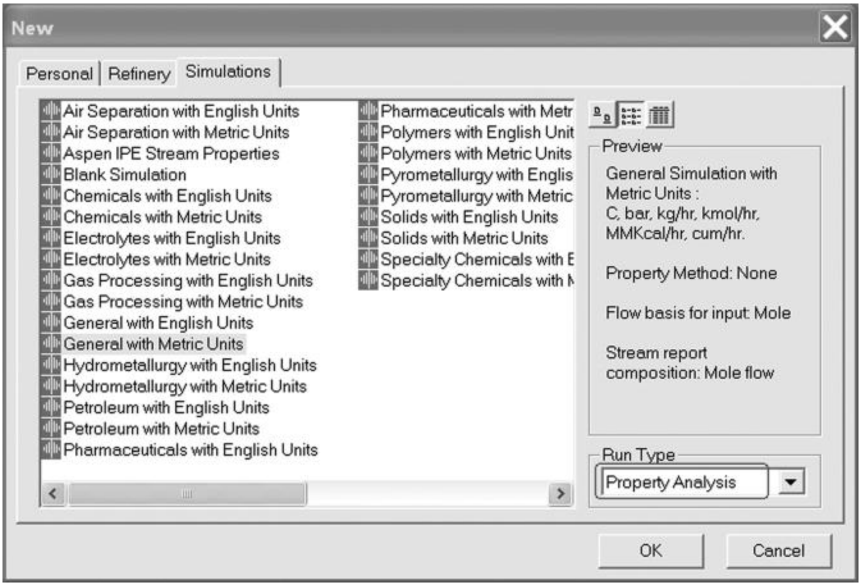


FIGURE 1.26
Liquid density of benzene versus temperature.



Air Separation with English Units
Air Separation with Metric Units
Aspen IPE Stream Properties
Blank Simulation
Chemicals with English Units
Chemicals with Metric Units
Electrolytes with English Units
Electrolytes with Metric Units
Gas Processing with English Units
Gas Processing with Metric Units
General with English Units
General with Metric Units
Hydrometallurgy with English Units
Hydrometallurgy with Metric Units
Petroleum with English Units
Petroleum with Metric Units
Pharmaceuticals with English Units
Pharmaceuticals with Metr
Polymers with English Unit
Polymers with Metric Units
Pyrometallurgy with Englis
Pyrometallurgy with Metric
Solids with English Units
Solids with Metric Units
Specialty Chemicals with E
Specialty Chemicals with M

Preview

General Simulation with Metric Units : C, bar, kg/hr, kmol/hr, MMKcal/hr, cum/hr.

Property Method: None

Flow basis for input: Mole

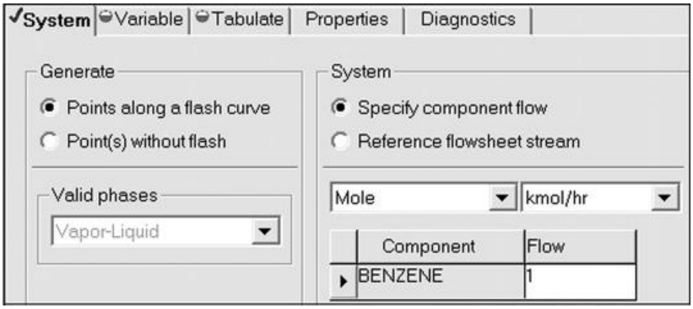
Stream report composition: Mole flow

Run Type: Property Analysis

FIGURE 1.27
Selection of property selection.

1 atm pressure, the variable would be temperature. Before we can continue to calculate the physical properties, we need to vary our temperature over a range, and so highlight temperature by clicking on the box in front of where Temperature was originally chosen. Once you have done so, an arrow should appear next to Temperature and the box should be highlighted. Then click on the *Range/List* at the bottom of the screen (Figure 1.29).

Now the lower and upper values of the desired range are entered. We want properties from 0°C to 100°C, and therefore enter a lower limit of 0 and an upper of 100 in the Lower and Upper fields, respectively, by clicking and typing in the appropriate box. The temperature increment must also be specified. Click on the



Generate
● Points along a flash curve
○ Point(s) without flash

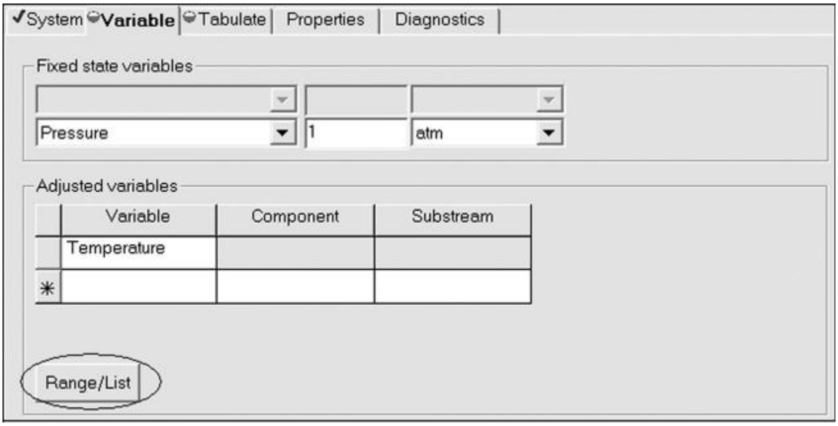
Valid phases: Vapor-Liquid

System
● Specify component flow
○ Reference flowsheet stream

Mole | kmol/hr

Component	Flow
BENZENE	1

FIGURE 1.28
Property analysis data browser.



Fixed state variables

Pressure 1 atm

Adjusted variables

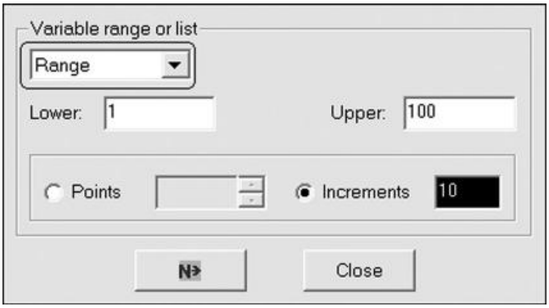
	Variable	Component	Substream
	Temperature		
*			

FIGURE 1.29
Selecting of adjusted variable.

circle next to Increments to highlight it, and then enter 10 in the box (Figure 1.30). Click on *Next* to continue. The previous screen will now appear. Click on *Next* again.

A property set contains each property that you want to be calculated (e.g., density at a specific temperature and pressure). Aspen has several built-in property sets; however, in order to generate a new one a name for the new set must be specified. Right click in the box labeled *Available Property Sets*; choose *New* when it appears (Figure 1.31).

Specify the properties to be generated. By clicking on the arrow pointing downward in the Physical properties box, a list will appear. Each symbol is defined at the bottom of the screen. For this example, density, heat capacity, and vapor pressure are chosen for a pure component. You may want to type in symbols for the property you want such as RHO for density. You can also do a search for properties by clicking on the search button. A phase must be specified. To do this click



Variable range or list

Range

Lower: 1

Upper: 100

○ Points

● Increments 10

FIGURE 1.30
Variable range.

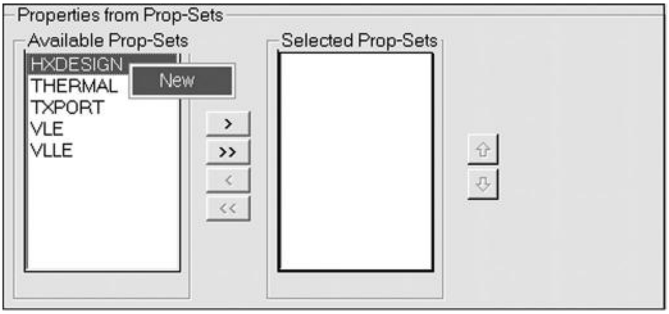


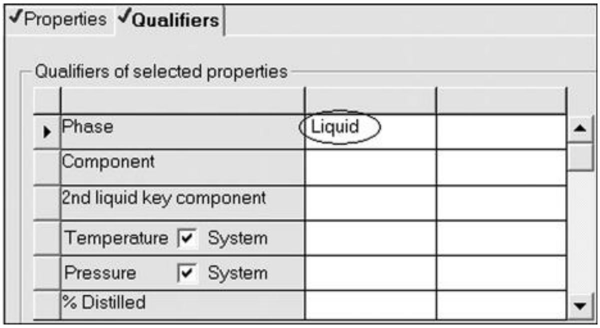
FIGURE 1.31
Selection of desired property.

on the *Qualifiers* tab. Click on the field labeled Phase. Now click on the arrow pointing downward that appears in the second column and choose liquid from the list (Figure 1.32). Click on *Next* to continue.

To open the generated table in Excel, first right click on the circled area to highlight the entire table and bring up a menu (Figure 1.33). Choose Copy from the menu that appears. To open the generated table in Excel, first right click on the circled area to highlight the entire table and bring up a menu. Choose Copy from the screen. In the Excel file click on Paste. The property table generated in Aspen should appear similar to what is displayed in the Excel file.

SUPERPRO DESIGNER

With SuperPro it is much easier to plot physical properties (Density in this case) versus adjustable variable (Temperature). Select the components involved (Benzene), double click on components name and click on the Physical (T-dependent) button. Click on *Plot any T Dependent Property* as shown in Figure 1.34. Then click on *Show Graph*. The graph should appear as that in Figure 1.35.



Phase	Liquid	
Component		
2nd liquid key component		
Temperature ☑ System		
Pressure ☑ System		
% Distilled		

FIGURE 1.32
Phase selection page.

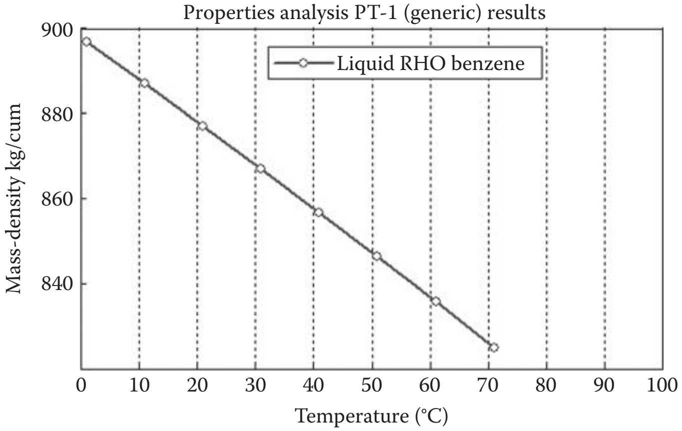
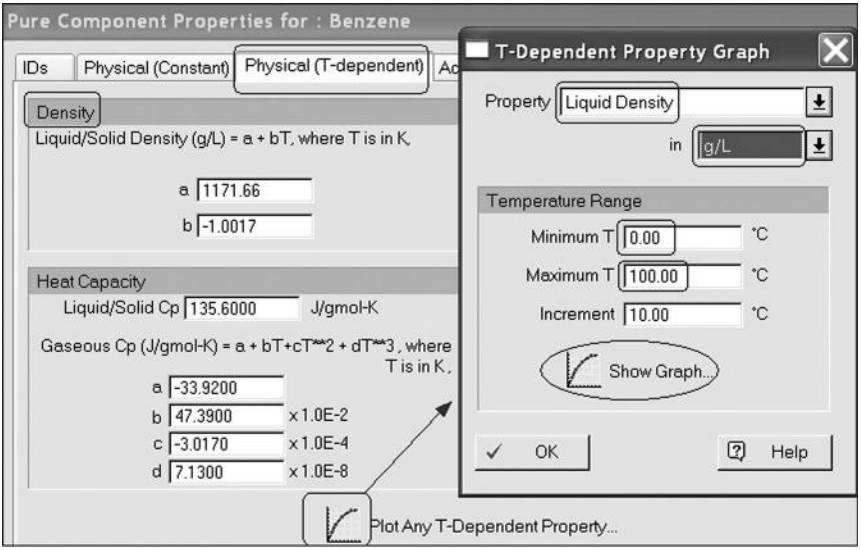


FIGURE 1.33
Density versus temperature.

Example 1.6: Estimate Density of Liquid Mixture

The density of 50 wt% H_2SO_4 in water at 25°C and 1 atm is 1.39 g/cm^3. Estimate the density of the liquid mixture using the following densities of pure H_2SO_4 and water, and compare it with the experimentally obtained value.

Density of H_2SO_4 at 25°C = 1.834 g/cm^3
Density of H_2O at 25°C = 0.998 g/cm^3



Liquid/Solid Density (g/L) = a + bT, where T is in K.
a 1171.66
b -1.0017

Liquid/Solid Cp 135.6000 J/gmol-K
Gaseous Cp (J/gmol-K) = a + bT+cT**2 + dT**3 , where T is in K.
a -33.9200
b 47.3900 x1.0E-2
c -3.0170 x1.0E-4
d 7.1300 x1.0E-8

Property Liquid Density
in g/L
Minimum T 0.00 °C
Maximum T 100.00 °C
Increment 10.00 °C

FIGURE 1.34
Plot of any temperature-dependent property (density in this case).

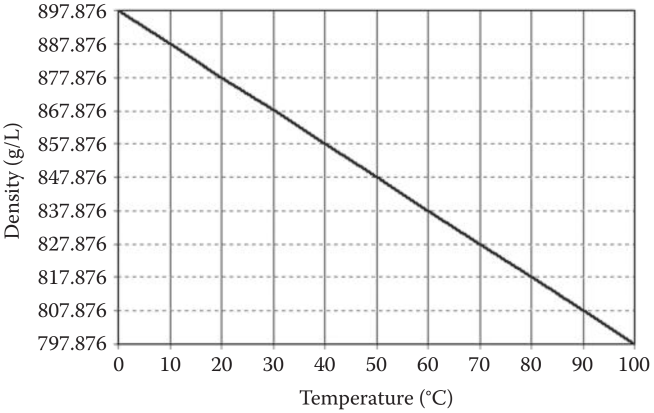


FIGURE 1.35
Plot of density versus temperature.

SOLUTION

Hand Calculations

The density of liquid mixture (method 1)

$$\bar{\rho} = \sum_{i=1}^{n} x_i \rho_i = 0.5 \times 0.998 + 0.5 \times 1.834 = 1.42 \ g/cm^3$$

The density of liquid mixture (method 2)

$$\frac{1}{\bar{\rho}} = \sum_{i=1}^{n} \frac{x_i}{\rho_i} = \frac{0.5}{0.998} + \frac{0.5}{1.834} \rightarrow \bar{\rho} = 1.29 \ g/cm^3$$

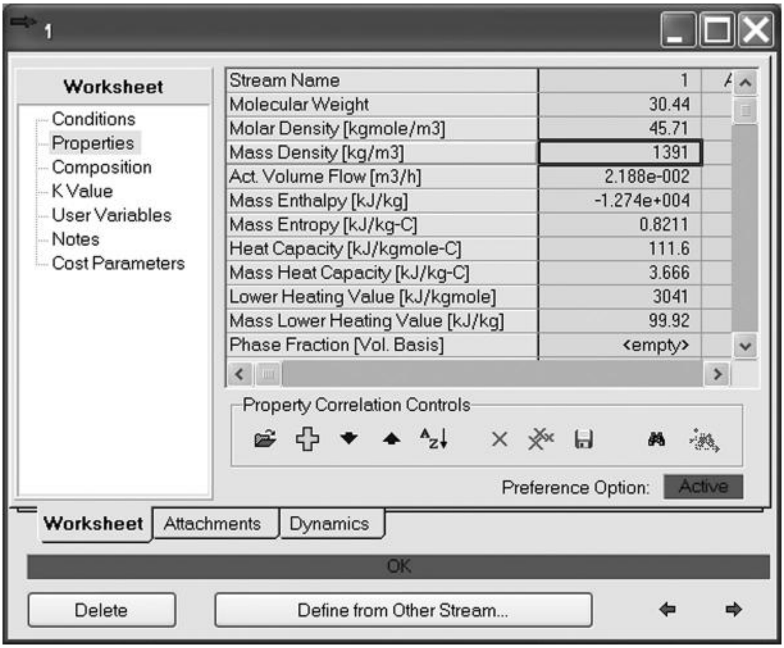
The percent error using the first and second equation is 7.3% and 1.5%, respectively.

Hysys Simulation

In a new case in Hysys, add the two components (H_2SO_4 and water) and select PRSV for the property estimation. Select the material stream, specify the temperature as 25°C, and set the pressure to 1 atm. The basis of assumption is 1 kmol/h of mixture. The result is shown in Figure 1.36.

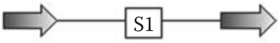
PRO/II Simulation

In a new case in Provision and then add the two components involved in the mixture (H_2SO_4 and water). Select PRSV for the property estimation method. Select a material stream, and specify its temperature as 25°C, and the pressure to 1 atm.



Stream Name	1
Molecular Weight	30.44
Molar Density [kgmole/m3]	45.71
Mass Density [kg/m3]	1391
Act. Volume Flow [m3/h]	2.188e-002
Mass Enthalpy [kJ/kg]	-1.274e+004
Mass Entropy [kJ/kg-C]	0.8211
Heat Capacity [kJ/kgmole-C]	111.6
Mass Heat Capacity [kJ/kg-C]	3.666
Lower Heating Value [kJ/kgmole]	3041
Mass Lower Heating Value [kJ/kg]	99.92
Phase Fraction [Vol. Basis]	<empty>

FIGURE 1.36
Density of liquid mixture using Unisim.



Stream name Stream description		S1
Phase		Liquid
Dry stream		
Rate	kg-mol/h	1.000
	kg/h	30.439
Std. liq. rate	m^3/h	0.024
Temperature	C	25.000
Pressure	kg/cm^2	1.000
Molecular weight		30.439
Mole fraction liquid		1.0000
Enthalpy	m*kcal/h	0.001
	kcal/kg	16.717
Reduced temperature		0.4320
Reduced pressure		0.0050
Acentric factor		0.2052
UOP K factor		7.183
Std. liquid density	kg/m^3	1294.329
Sp. gravity		1.2956
API gravity		–22.285

FIGURE 1.37
Liquid density of liquid mixture using PRO/II.

The basis of assumption is 1 kmol/h of mixture. The simulated result is shown in Figure 1.37.

Aspen Simulation

In a new case in Aspen Plus, add the two components (H_2SO_4 and water) and select PRSV for property estimation. Select a material stream, specify the temperature as 25°C, and set the pressure to 1 atm. The basis of assumption is 1 kmol/h of mixture. The Aspen simulated density of the liquid mixture is shown in Figure 1.38.

Example 1.7: Use of Henry's Law

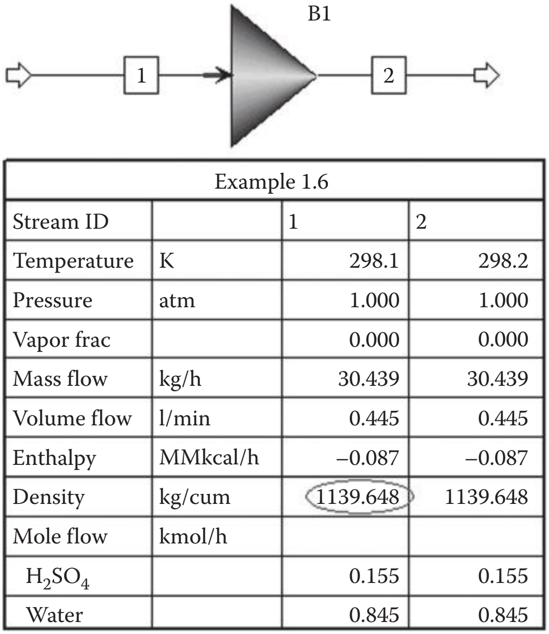
A gas containing 1.00 mol% of ethane and the remaining being nitrogen is contacted with water at 20.0°C and 20.0 atm. Estimate the mole fraction of dissolved ethane.

SOLUTION

Hand Calculations

Hydrocarbons are relatively insoluble in water, and so the solution of ethane is likely to be very dilute. We should therefore assume that Henry's law applies [5], and look up Henry's constant for ethane in water:

$$y_A P = x_A H_A(T) \rightarrow x_A = \frac{y_A P}{H_A(T)} = \frac{(0.100)(20.0\,\text{atm})}{2.63 \times 10^4\,\text{atm}} = 7.60 \times 10^{-6}\,\frac{\text{mol C}_2\text{H}_6}{\text{mol}}$$



Example 1.6			
Stream ID		1	2
Temperature	K	298.1	298.2
Pressure	atm	1.000	1.000
Vapor frac		0.000	0.000
Mass flow	kg/h	30.439	30.439
Volume flow	l/min	0.445	0.445
Enthalpy	MMkcal/h	–0.087	–0.087
Density	kg/cum	1139.648	1139.648
Mole flow	kmol/h		
H_2SO_4		0.155	0.155
Water		0.845	0.845

FIGURE 1.38
Calculated density of 50% H_2SO_4 in water using Aspen Plus.

HYSYS SIMULATION

In a new case in Hysys, add the components ethane and water, and select the appropriate fluid package (NRTL). Enter the simulation environment and mix the two streams as shown in Figure 1.39. The Workbook is used to display the stream summary table below the process flow sheet. Click on *Workbook* in the toolbar; once the workbook appears, click on *Setup* in the Workbook menu, and then click on *Add* to add the required variables from the list of variables. Once all information required is added to the workbook, right click anywhere in the PFD area and select *Add Workbook Table*.

PRO/II SIMULATION

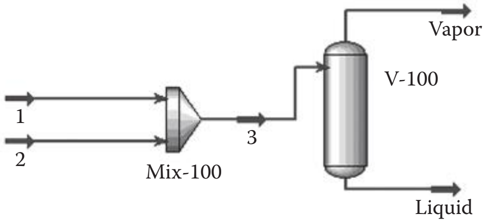
In a new case in Provision, add the components ethane, nitrogen, and water, and select NRTL as the appropriate fluid package. Connect two feed streams to a mixer and the outlet stream to a flash unit. The result is shown in Figure 1.40.

ASPEN PLUS SIMULATION

In a new case in Aspen Plus, add the components ethane, nitrogen, and water, and select Peng–Robinson as the appropriate fluid package. Connect two feed streams to a mixer and the outlet stream to a flash unit. The result is shown in Figure 1.41.

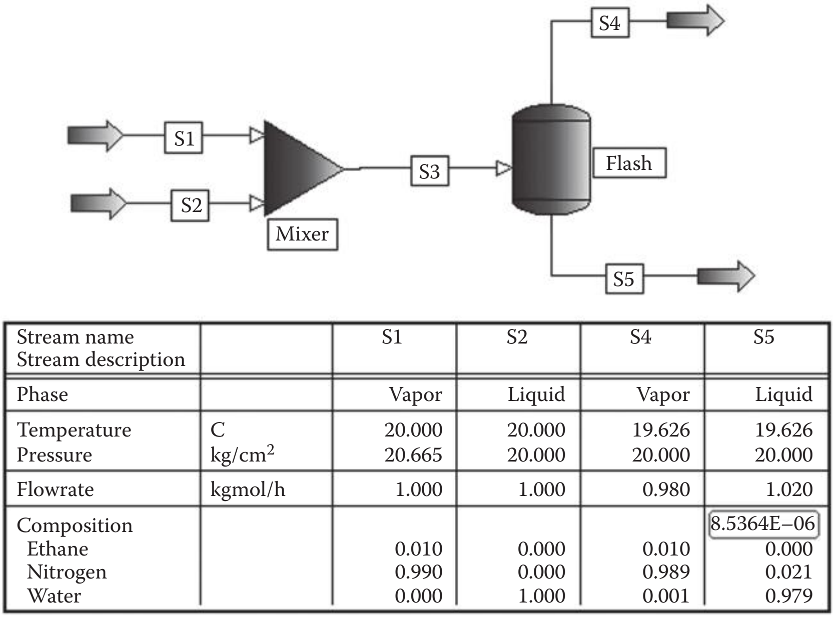
Example 1.8: Raoult's Law for Hydrocarbon Mixtures

An equimolar liquid mixture of benzene and toluene is in equilibrium with its vapor at 30.0°C. What is the system pressure and the composition of the vapor?



		Streams				
		1	2	3	Vapor	Liquid
Temperature	C	20.00	25.00	23.02	23.02	23.02
Pressure	kPa	2026	2026	2026	2026	2026
Mass flow	kg/h	28.03	18.02	46.05	28.03	18.02
Comp mass frac (H_2O)		0.0000	1.0000	0.3912	0.0009	0.9983

FIGURE 1.39
Fraction dissolved ethane in water at 20°C and 20 atm.



Stream name Stream description		S1	S2	S4	S5
Phase		Vapor	Liquid	Vapor	Liquid
Temperature	C	20.000	20.000	19.626	19.626
Pressure	kg/cm^2	20.665	20.000	20.000	20.000
Flowrate	kgmol/h	1.000	1.000	0.980	1.020
Composition					8.5364E–06
Ethane		0.010	0.000	0.010	0.000
Nitrogen		0.990	0.000	0.989	0.021
Water		0.000	1.000	0.001	0.979

FIGURE 1.40
Mole fraction of ethane in water at 20°C and 20 atm.

SOLUTION

HAND CALCULATIONS

Assuming Raoult's law applies [5], the vapor pressure of benzene, p_B^*

$$\log(p_B^*) = 6.906 - \frac{1211}{T + 220.8} \xrightarrow{T=30°C} p_B^* = 119 \text{ mmHg}$$

Vapor pressure of toluene, p_T^*

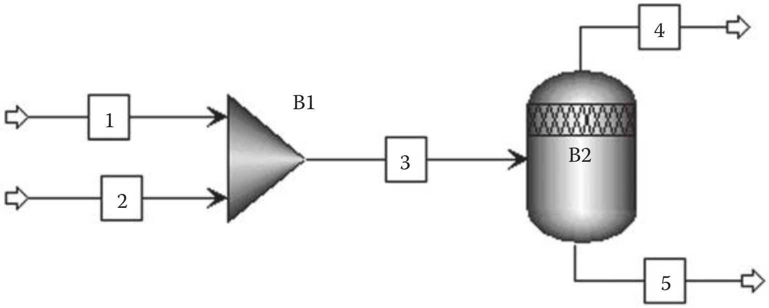
$$\log(p_T^*) = 6.9533 - \frac{1343.9}{T + 219.38} \xrightarrow{T=30°C} p_T^* = 36.7 \text{ mmHg}$$

Partial pressure of benzene, p_B

$$p_B = y_B P = x_B p_A^*(T) = 0.5(119) = 59.5 \text{ mmHg}$$

Partial pressure of benzene, p_T

$$p_T = y_T P = x_T p_A^*(T) = 0.5(36.7) = 18.4 \text{ mmHg}$$



Example 1.7						
Stream ID		1	2	3	4	5
Temperature	K	293.1	293.1	292.7	292.7	292.7
Pressure	atm	20.00	20.00	20.00	20.00	20.00
Vapor frac		1.000	0.000	0.501	1.000	0.000
Mole flow	kmol/h	1.000	1.000	2.000	1.001	0.999
Mass flow	kg/h	28.034	18.015	46.049	28.053	17.996
Volume flow	l/min	19.864	0.301	20.152	19.851	0.300
Enthalpy	MMBtu/h	−0.001	−0.273	−0.274	−0.001	−0.273
Mole frac						
Ethane		0.010		0.005	0.010	135 PPB
Nitrogen		0.990		0.495	0.989	1 PPM
Water			1.000	0.500	0.001	1.000

FIGURE 1.41
Ethane mole fractions in liquid water at 20°C and 20 atm.

Total pressure, P

$$P = 59.5 + 18.4 = 77.9 \text{ mmHg}$$

Mole fraction of benzene in the vapor phase, y_B

$$y_B = \frac{p_B}{P} = 0.764$$

Mole fraction of toluene in the vapor phase, y_T

$$y_T = \frac{p_T}{P} = 0.236$$

Hysys Simulation

In a new case in Hysys, add benzene and toluene components and select the appropriate fluid package. Peng–Robinson EOS is a proper fluid package for hydrocarbons. The process flow sheet is shown in Figure 1.42.

PRO/II Simulation

In a new case in Provision add benzene and toluene components, select Peng–Robinson EOS as a proper fluid package for hydrocarbons. Select a flash unit and connect two feed streams and two product streams. The process flow sheet is shown in Figure 1.43.

Aspen Plus Simulation

In a new case in Aspen Plus, add benzene and toluene components and select the appropriate fluid package. Select Peng–Robinson EOS as a proper fluid package for hydrocarbons. The process flow sheet is shown in Figure 1.44.

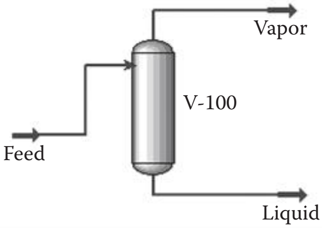
PROBLEMS

1.1 Dew Point Calculation

Calculate the temperature and composition of a liquid in equilibrium with a gas mixture containing 10.0 mol% benzene, 10.0 mol% toluene, and balance nitrogen (considered noncondensable) at 1 atm.

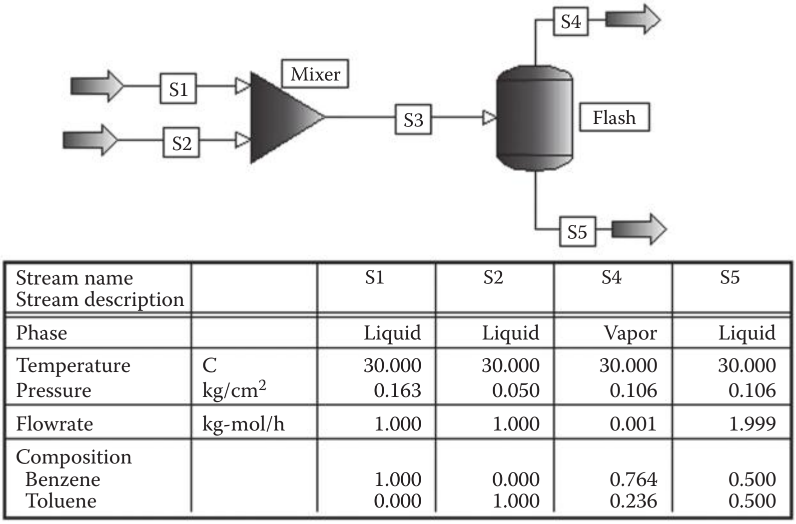
1.2 Compressibility Factors

Fifty cubic meters per hour of methane flow through a pipeline at 40.0 bar absolute and 300.0 K. Estimate the mass flow rate.



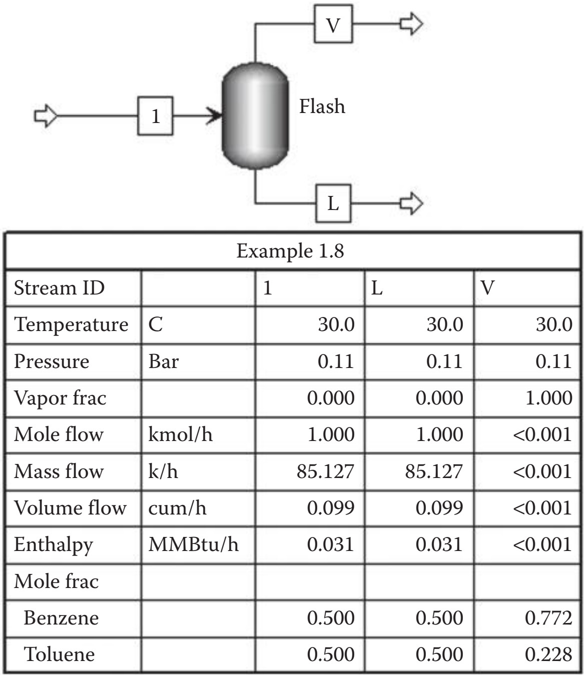
Streams				
		Feed	Vapor	Liquid
Temperature	C	30.00	30.00	30.00
Pressure	kPa	10.94	10.94	10.94
Molar flow	kgmol/h	1.000	0.0000	1.000
Comp mole frac (Benzene)		0.500	0.759	0.500
Comp mole frac (Toluene)		0.500	0.241	0.500

FIGURE 1.42
Mole fractions of benzene and toluene in equilibrium calculated using Hysys.



Stream name Stream description		S1	S2	S4	S5
Phase		Liquid	Liquid	Vapor	Liquid
Temperature	C	30.000	30.000	30.000	30.000
Pressure	kg/cm^2	0.163	0.050	0.106	0.106
Flowrate	kg-mol/h	1.000	1.000	0.001	1.999
Composition					
Benzene		1.000	0.000	0.764	0.500
Toluene		0.000	1.000	0.236	0.500

FIGURE 1.43
Mole fraction of benzene in vapor phase at equilibrium calculated using PRO/II.



Example 1.8

Stream ID		1	L	V
Temperature	C	30.0	30.0	30.0
Pressure	Bar	0.11	0.11	0.11
Vapor frac		0.000	0.000	1.000
Mole flow	kmol/h	1.000	1.000	<0.001
Mass flow	k/h	85.127	85.127	<0.001
Volume flow	cum/h	0.099	0.099	<0.001
Enthalpy	MMBtu/h	0.031	0.031	<0.001
Mole frac				
Benzene		0.500	0.500	0.772
Toluene		0.500	0.500	0.228

FIGURE 1.44
Benzene mole fractions in vapor phase at equilibrium calculated using Aspen.

1.3 Use of Raoult's Law

A liquid mixture contains 40% (mole percent) benzene and the remaining is toluene is in equilibrium with its vapor at 30.0°C. What are the system pressure and the composition of the vapor? Use Unisim, PRO/II, and Aspen Plus.

1.4 Use of Raoult's Law

A liquid mixture contains equimolar of benzene and toluene is in equilibrium with its vapor at 0.12 atm. What is the system temperature and the composition of the vapor? Use Unisim, PRO/II, and Aspen Plus.

1.5 Use of Henry's Law

A gas containing 1.00 mol% of ethane and the remaining methane is contacted with water at 20.0°C and 20.0 atm. Estimate the mole fraction of dissolved ethane and methane Hysys, PRO/II, and Aspen Plus.

1.6 Use of Henry's Law

A gas containing 15.00 mol% of CO_2 and the balance is methane is contacted with water at 20.0°C and 20.0 atm. Estimate the mole fraction of dissolved CO_2 in water using Hysys, PRO/II, and Aspen Plus.

1.7 Dew Point Calculation

Find the dew-point temperature for a mixture of 45 mol% *n*-hexane, 30% *n*-heptane, 15% *n*-octane, and 10% *n*-nonane at 2 atm total pressure.

1.8 Bubble-Point Calculation

Find the bubble-point temperature for a mixture of 45 mol% *n*-hexane, 30% *n*-heptane, 15% *n*-octane, and 10% *n*-nonane at 5 atm total pressure.

1.9 Vapor Pressure of Gas Mixture

Find the vapor pressure for the binary mixture of 50 mol% *n*-hexane and 50% *n*-heptane at 120°C.

1.10 Vapor Pressure of Gas Mixture

Find the vapor pressure for the pure components and for the mixture of 35 mol% *n*-hexane, 30% *n*-heptane, and 35% *n*-octane at 150°C.

References

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2

Fluid Flow in Pipes, Pumps, and Compressors

At the end of this chapter you should be able to

1. Fully understand the type of flow regime in pipes, pumps, and compressors.
2. Perform hand calculations and verify their results with Hysys, Provision, and Aspen simulation software.
3. Determine pressure drop in pipeline, inlet pipe flow rate, and pipe length.
4. Determine the useful power input needed to overcome the friction losses in a pipeline. Calculate brake kW for pumps and compressors.

2.1 Flow in Pipes

In this section a brief summary of the most general form of Bernoulli's equation for steady incompressible flows is introduced. Bernoulli's equation is composed of kinetic energy, potential energy, and internal energy. The energy equation is written between the inlet at point 1 and the exit of the pipeline at point 2 (Figure 2.1). The process flow diagram (PFD) represents sudden contraction (the exit of the first tank to the inlet of pipe 1), two 90° elbows, and sudden expansion (the exit of pipe 4 and the inlet of the second tank).

The energy equation for incompressible fluids [1,2]:

$$\frac{P_1}{\rho} + gz_1 + \frac{V_1^2}{2} = \frac{P_2}{\rho} + gz_2 + \frac{V_2^2}{2} + W_s + \Sigma F \tag{2.1}$$

where P_1 is the pressure at point 1 and P_2 is the pressure at point 2, ρ is the average fluid density, z_1 is the height at point 1, z_2 is the height at point 2, V_1 is the inlet velocity, V_2 is the exit velocity, W_s is the shaft work, and the summation of friction losses is ΣF. The friction loss is due to pipe skin friction,

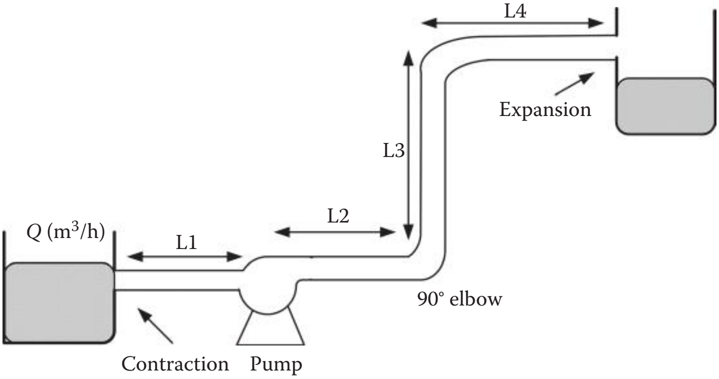


FIGURE 2.1
PFD of the piping system.

expansion losses, contraction losses, and fitting losses [3]. The summation of friction loss can be calculated using

$$\sum F = f\frac{L}{D}\frac{V_2^2}{2} + (K_{\text{exp}} + K_{\text{c}} + K_{\text{f}})\frac{V^2}{2} \tag{2.2}$$

where K_{exp} is the expansion loss, K_{c} is the contraction loss, and K_{f} is the fitting losses. Fitting losses include losses due to elbows (K_{e}), tees (K_{T}), and Globe valves (K_{G}).

Expansion loss (K_{exp}) is determined using

$$K_{\text{exp}} = \left(1 - \frac{A_1}{A_2}\right)^2 \tag{2.3}$$

where A_1 and A_2 are the cross-sectional areas at the inlet and the exit, respectively. The contraction loss (K_{c}) is calculated using

$$K_{\text{c}} = 0.55\left(1 - \frac{A_2}{A_1}\right) \tag{2.4}$$

For turbulent flow, $K_{\text{e}} = 0.75$ (for 90° elbow), $K_{\text{T}} = 1.0$ (Tee), $K_{\text{G}} = 6.0$ (Globe valve), $K_{\text{C}} = 2.0$ (check valve). For a horizontal pipe with the same inlet and exit diameter and incompressible fluid, $V_1 = V_2$. To calculate the pressure drop between the inlet and the exit of a horizontal pipe, first calculate the average velocity and then use Reynolds number to determine the flow regime (i.e., laminar, transient, or turbulent). The average velocity can be expressed in terms of the flow rate as

$$V = \frac{Q}{A_c} = \frac{Q}{\pi D^2/4} \tag{2.5}$$

where V is the average velocity, A_c is the pipe's inner cross-sectional area, Q is the inlet fluid volumetric flow rate, and D is the pipe inner diameter. Reynolds number, Re, from which the flow regime can be calculated is expressed as

$$\text{Re} = \frac{\rho V D}{\mu} \tag{2.6}$$

2.1.1 Laminar Flow

In fully developed laminar flow (Re < 4000) in a circular horizontal pipe, the pressure loss and the head loss are given by

$$\frac{\Delta P}{\rho} = \frac{P_1 - P_2}{\rho} = \Delta P_L = f\frac{L}{D}\frac{V^2}{2} \tag{2.7}$$

The friction factor

$$f = \frac{64}{\text{Re}} \tag{2.8}$$

Under laminar flow conditions, the friction factor, f, is directly proportional to viscosity and inversely proportional to the velocity, pipe diameter, and fluid density. The friction factor is independent of pipe roughness in laminar flow because the disturbances caused by surface roughness are quickly damped by viscosity [4]. The pressure drop in laminar flow for a circular horizontal pipe is

$$\Delta P_L = \frac{32\mu L V}{D^2} \tag{2.9}$$

When the flow rate and the average velocity are held constant, the head loss becomes proportional to viscosity. The head loss, h_L, is related to the pressure loss by

$$h_L = \frac{\Delta P_L}{\rho g} = \frac{32\mu L V}{\rho g D^2} \tag{2.10}$$

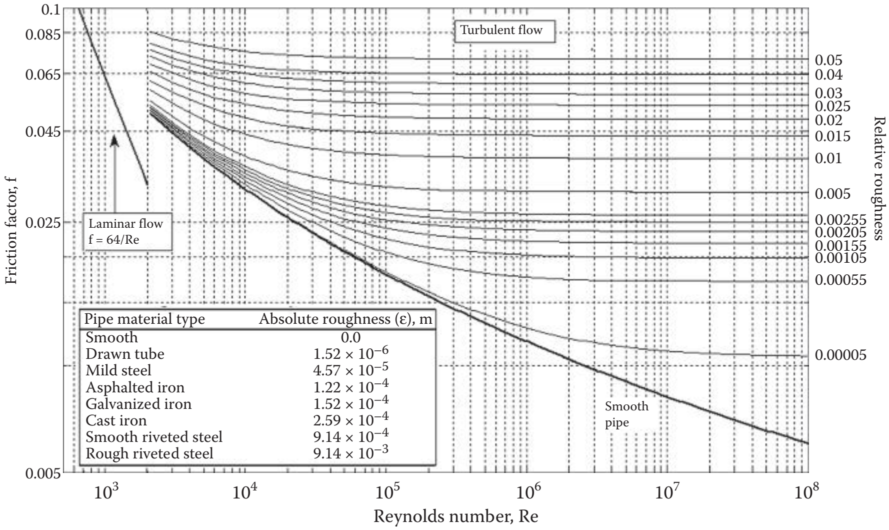
2.1.2 Turbulent Flow

When the flow is turbulent, the relationship becomes more complex and is best shown by the graph because the friction factor is a function of both Reynolds number and roughness [5,6]. The degree of roughness is designated as the ratio of the sand grain diameter to the pipe diameter (ε/D). The relationship between the friction factor and Reynolds number can be determined for every relative roughness. From these relationships, it is apparent that for rough pipes, the roughness is important in determining the magnitude of the friction factor. At high Reynolds number the friction factor depends entirely on roughness and the friction factor can be obtained from the rough pipe law. In fully developed turbulent flow (Re > 4000) in a circular pipe, the pressure drop for turbulent flow is

$$\Delta P = \Delta P_{\mathrm{L}} = f\frac{L}{D}\frac{\rho V^2}{2} \tag{2.11}$$

The friction factor, *f*, can be found from the Moody diagram (Figure 2.2) which is based on the Colebrook equation in the turbulent regime [7].

$$\frac{1}{\sqrt{f}} = -2\log\left(\frac{\varepsilon/D}{3.7} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right) \tag{2.12}$$



Pipe material type	Absolute roughness (ε), m
Smooth	0.0
Drawn tube	1.52×10^{-6}
Mild steel	4.57×10^{-5}
Asphalted iron	1.22×10^{-4}
Galvanized iron	1.52×10^{-4}
Cast iron	2.59×10^{-4}
Smooth riveted steel	9.14×10^{-4}
Rough riveted steel	9.14×10^{-3}

FIGURE 2.2
Moody diagram.

Alternatively, the explicit equation for the friction factor derived by Swamee and Jain (Equation 2.13) can be solved for the absolute roughness.

$$f = \frac{0.25}{\left[\log\left((\varepsilon/3.7D) + (5.74/\mathrm{Re}^{0.9})\right)\right]^2} \tag{2.13}$$

Head loss for turbulent flow

$$h_\mathrm{L} = \frac{\Delta P_\mathrm{L}}{\rho g} \tag{2.14}$$

The relative roughness of the pipe is ε/D, where ε is pipe roughness and D is the inner diameter of the pipe. The friction factor can be determined from the Moody diagram (Figure 2.2) or Equation 2.13. The useful power input is the amount needed to overcome the frictional losses in the pipe.

$$\dot{W}_\mathrm{pump} = Q\Delta P \tag{2.15}$$

Example 2.1: Pressure Drop in a Horizontal Pipe

Water is flowing in a 10-m horizontal smooth pipe at 4 m/s and 25°C. The density of water is 1000 kg/m^3 and the viscosity of water is 0.001 kg/m s. The pipe is Schedule 40, 1 in. nominal diameter (2.66 cm ID). Water inlet pressure is 2 atm. Calculate pressure drop in the pipe using hand calculations and compare the results with those obtained using Hysys, PRO/II, and Aspen software.

SOLUTION

HAND CALCULATIONS

Reynolds number is calculated to determine the flow regime:

$$\mathrm{Re} = \frac{\rho VD}{\mu} = \frac{(1000\ \mathrm{kg/m^3})(4\ \mathrm{m/s})(0.0266\ \mathrm{m})}{0.001\,\mathrm{kg/ms}} = 1.064 \times 10^5$$

Since Reynolds number is greater than 4000, the flow is turbulent. The relative roughness of the smooth pipe is

$$\varepsilon/D = \frac{0}{0.04\ \mathrm{m}} = 0$$

The friction factor, f, can be determined from the Moody chart (Figure 2.2) or Swamee and Jain alternative equation,

$$f = \frac{0.25}{\left[\log\left((0/3.7D) + (5.74/(1.064 \times 10^5)^{0.9})\right)\right]^2} = 0.0176$$

The calculated friction factor $f = 0.0176$. Then the pressure drop

$$\Delta P = P_1 - P_2 = \Delta P_L = f\frac{L}{D}\rho\frac{V^2}{2}$$

$$\Delta P = (0.0176)\frac{10\ \text{m}}{0.0266\ \text{m}}\frac{(1000\ \text{kg/m}^3)(4\ \text{m/s})^2}{2}\left(\frac{1\,\text{kN}}{1000\ \text{kg}\cdot\text{m/s}}\right)\left(\frac{1\,\text{kPa}}{1\,\text{kN/m}^2}\right)$$

$$= 52.93\,\text{kPa}$$

The head loss

$$h_L = \frac{\Delta P_L}{\rho g} = f\frac{L}{D}\frac{V^2}{2g} = 0.0176\frac{10\ \text{m}}{0.0266\ \text{m}}\frac{(4\ \text{m/s})^2}{2(9.81\,\text{m/s}^2)} = 5.13\,\text{m}$$

The volumetric flow rate

$$Q = VA = (4\ \text{m/s})\left(\frac{\pi(0.0266\ \text{m})^2}{4}\right) = 2.22 \times 10^{-3}\,\text{m}^3/\text{s}$$

The power input is needed to overcome the frictional losses in the pipe.

$$\dot{W}_{\text{pump}} = Q\Delta P = (2.22 \times 10^{-3}\,\text{m}^3/\text{s})(50.4\ \text{kPa})\left(\frac{1\,\text{kW}}{1\,\text{kPa}\cdot\text{m}^3/\text{s}}\right) = 0.12\,\text{kW}$$

Therefore, a useful power input of 0.12 kW is needed to overcome the frictional losses in the pipe.

HYSYS SIMULATION

In Hysys, the pipe segment in the object palette offers three calculation modes: pressure drop, flow rate, and pipe length. The appropriate mode will automatically be selected depending on the information supplied. The Hysys simulation of fluid flowing in a pipe is simulated as follows:

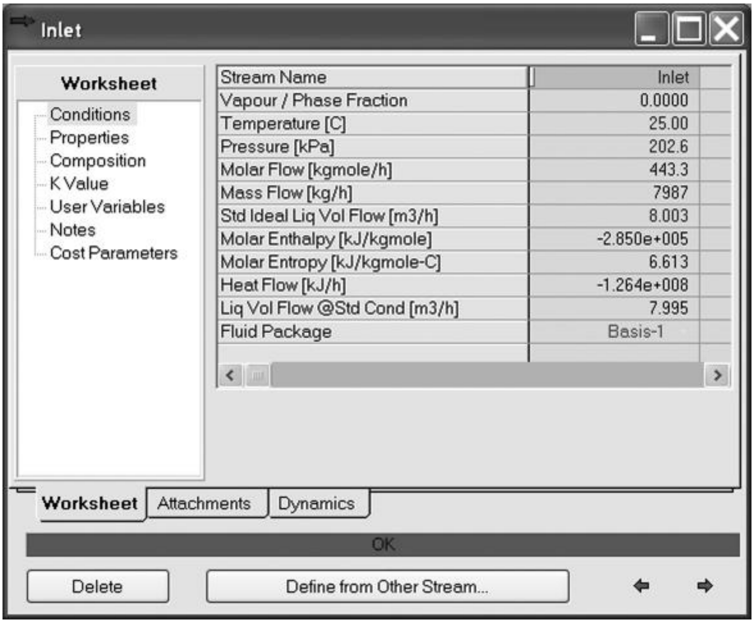
1. Start a new case in Hysys and use the SI units, from the *Tools* menu, *Preferences*, and then *Variables*. Choose water as the component flowing in the pipe, and ASME STEAM as Property packages and click *Enter the simulation Environment*.
2. Select a material stream by double clicking on the blue arrow from the top of the object palette and fill in the stream Name: Inlet.

3. Specify the volumetric feed rate, *Q*, based on the velocity of 4 m/s, and the inner pipe diameter of 0.0266 m,

$$Q = A_c \times V = \frac{\pi\left(0.0266\ \mathrm{m}\right)^2}{4} \times \frac{4\ \mathrm{m}}{\mathrm{s}}\left(\frac{3600\ \mathrm{s}}{1\ \mathrm{h}}\right) = \frac{8.03\ \mathrm{m}^3}{\mathrm{h}}$$

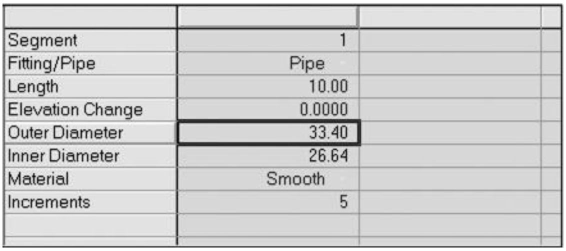
4. Enter values for feed pressure, temperature, and volumetric flow rate (Figure 2.3). In the composition menu, enter the mole fraction as 1 for water.
5. Add the pipe segment by double clicking on the pipe segment in the object palette. Click on the *Rating* tab and then on *Add Segment*. The pipe length is 10 m; specify the *Pipe Material* as "smooth" by choosing this value from the drop-down list (see Figure 2.4).
6. Click on *View Segment* and select Schedule 40. Then click on the nominal diameter entry and select 1 in. diameter. To choose one of the options, click on 25.4 mm (1 in.) and select *Specify* (Figure 2.5).

Double click on the product stream and enter 25°C for the temperature of the product stream (isothermal operation). To display the stream summary table below the PFD in the PFD area, click on the *Workbook* icon in the toolbar. Once the *Workbook* appears, from the workbook menu, click on the *Setup* command, and then click on *Add* in the workbook tabs group, and select the variable that needs to appear in the table. Right click on the PFD area below the PFD and click on *Add Workbook Table*; the result appears as given in Figure 2.6.



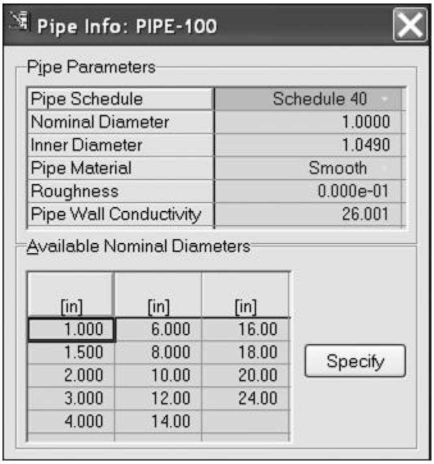
Stream Name	Inlet
Vapour / Phase Fraction	0.0000
Temperature [C]	25.00
Pressure [kPa]	202.6
Molar Flow [kgmole/h]	443.3
Mass Flow [kg/h]	7987
Std Ideal Liq Vol Flow [m3/h]	8.003
Molar Enthalpy [kJ/kgmole]	-2.850e+005
Molar Entropy [kJ/kgmole-C]	6.613
Heat Flow [kJ/h]	-1.264e+008
Liq Vol Flow @Std Cond [m3/h]	7.995
Fluid Package	Basis-1

FIGURE 2.3
Inlet stream conditions for Example 2.1.



Segment	1	
Fitting/Pipe	Pipe	
Length	10.00	
Elevation Change	0.0000	
Outer Diameter	33.40	
Inner Diameter	26.64	
Material	Smooth	
Increments	5	

FIGURE 2.4
Length and elevation profile of the pipe in Example 2.1.



Pipe Info: PIPE-100

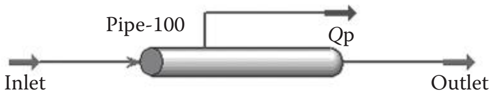
Pipe Parameters

Pipe Schedule	Schedule 40
Nominal Diameter	1.0000
Inner Diameter	1.0490
Pipe Material	Smooth
Roughness	0.000e-01
Pipe Wall Conductivity	26.001

Available Nominal Diameters

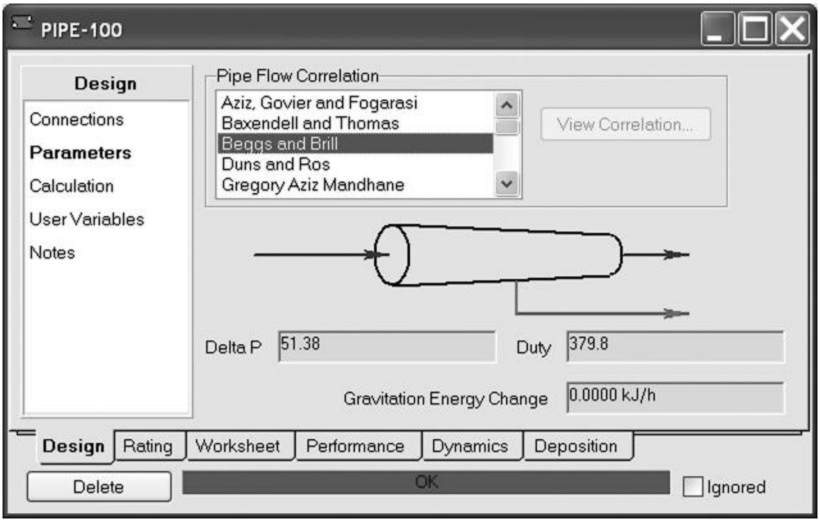
[in]	[in]	[in]
1.000	6.000	16.00
1.500	8.000	18.00
2.000	10.00	20.00
3.000	12.00	24.00
4.000	14.00	

FIGURE 2.5
Selection of pipe nominal diameter.



Streams			
		Inlet	Outlet
Temperature	C	25.00	25.00
Pressure	kPa	202.6	151.3
Mass flow	kg/h	7987	7987
Comp mass frac (H_2O)		1.0000	1.0000

FIGURE 2.6
Pipe process flow sheet.



Pipe Flow Correlation

- Aziz, Govier and Fogarasi
- Baxendell and Thomas
- Beggs and Brill
- Duns and Ros
- Gregory Aziz Mandhane

Delta P 51.38

Duty 379.8

Gravitation Energy Change 0.0000 kJ/h

FIGURE 2.7
Pipe Delta *P* calculated.

While on the Design page, click on the parameters; the Hysys calculated pressure drop is 51.69 kPa (see Figure 2.7).

PRO/II SIMULATION

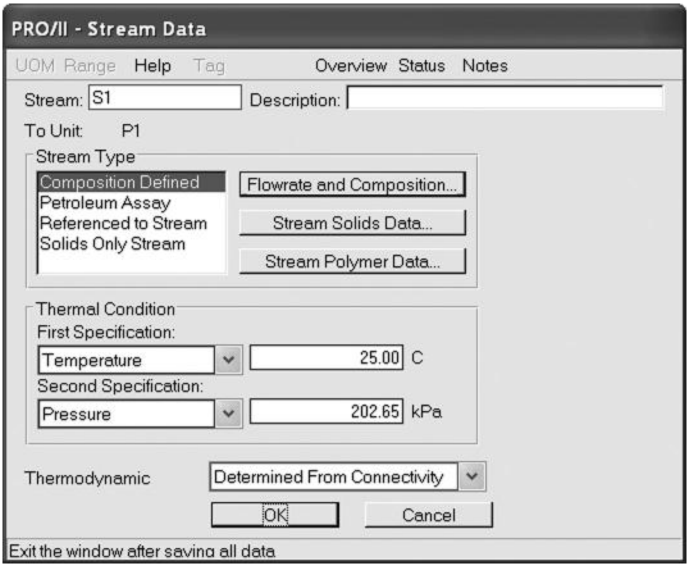
Open a new case in PRO/II, click on the component selection icon (the benzene ring in the toolbar), select water, and then select the stream fluid package. Click on the pipe segment in the object palette and then click anywhere in the PFD area to place the pipe. Click on *Stream* in the object palette then generate the inlet stream (S1) and the exit stream (S2). Double click on stream S1 and specify inlet temperature and pressure feed stream (Figure 2.8).

Click on *Flowrate and Composition* and specify inlet flow rate and stream composition; then double click on the *Pipe* icon in the PFD and specify nominal pipe diameter, pipe length, elevation change, and *K* factor when available. For a smooth pipe, the relative roughness is zero. See Figure 2.9. Click on *Run* or the small arrow in the toolbar. After the run is successfully converged, generate the results report. The converged process flow sheet is shown in Figure 2.10.

Select *Generate Report* under *Output* in the PRO/II toolbar menu to display the results. The calculated total pressure drop is 52.1 kPa as shown in Figure 2.11.

ASPEN SIMULATION

Start the Aspen program, select *Aspen Plus User Interface*, and when the *Connect to Engine* window appears, use the default Server Type *Local PC*. Select *Pipe* under the *Pressure Changes* tab from the *Equipment Model Library* and then click on the flow sheet window where you would like the piece of equipment to appear. In order to add material streams to the simulation, select the material stream from the *Stream Library*. When the material stream option is selected, a number of arrows will appear on each of the unit operations. Red arrows indicate a required stream and blue arrows indicate an optional stream.



PRO/II - Stream Data

Stream: S1

Description:

To Unit: P1

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Thermal Condition

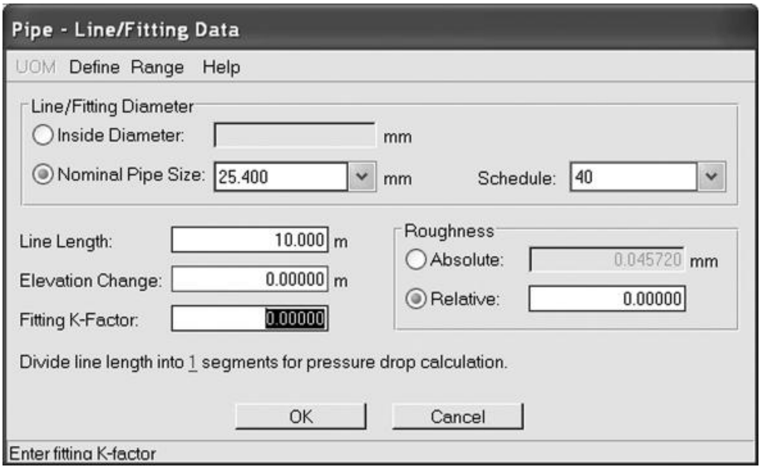
First Specification: Temperature 25.00 C

Second Specification: Pressure 202.65 kPa

Thermodynamic: Determined From Connectivity

Exit the window after saving all data

FIGURE 2.8
Inlet stream conditions.



Pipe - Line/Fitting Data

Line/Fitting Diameter

○ Inside Diameter: mm

● Nominal Pipe Size: 25.400 mm

Schedule: 40

Line Length: 10.000 m

Elevation Change: 0.00000 m

Fitting K-Factor: 0.00000

Roughness

○ Absolute: 0.045720 mm

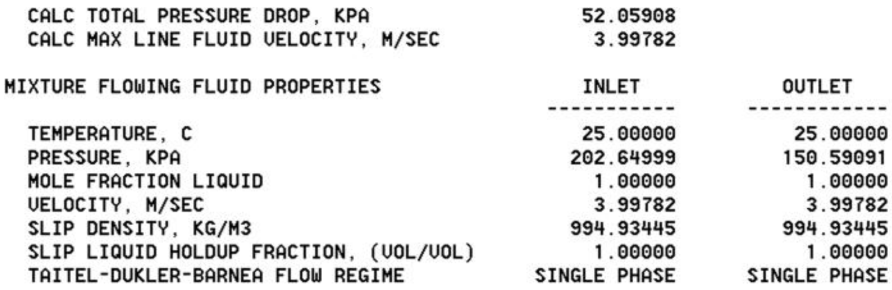
● Relative: 0.00000

Divide line length into 1 segments for pressure drop calculation.

Enter fitting K-factor

FIGURE 2.9
Pipe segment input menu completed.

FIGURE 2.10
Process flow sheet of Example 2.1.



```
  CALC TOTAL PRESSURE DROP, KPA                 52.05908
  CALC MAX LINE FLUID VELOCITY, M/SEC            3.99782

MIXTURE FLOWING FLUID PROPERTIES                 INLET          OUTLET
                                              -----------    ------------
  TEMPERATURE, C                                25.00000        25.00000
  PRESSURE, KPA                                202.64999       150.59091
  MOLE FRACTION LIQUID                           1.00000         1.00000
  VELOCITY, M/SEC                                3.99782         3.99782
  SLIP DENSITY, KG/M3                          994.93445       994.93445
  SLIP LIQUID HOLDUP FRACTION, (VOL/VOL)         1.00000         1.00000
  TAITEL-DUKLER-BARNEA FLOW REGIME            SINGLE PHASE    SINGLE PHASE
```

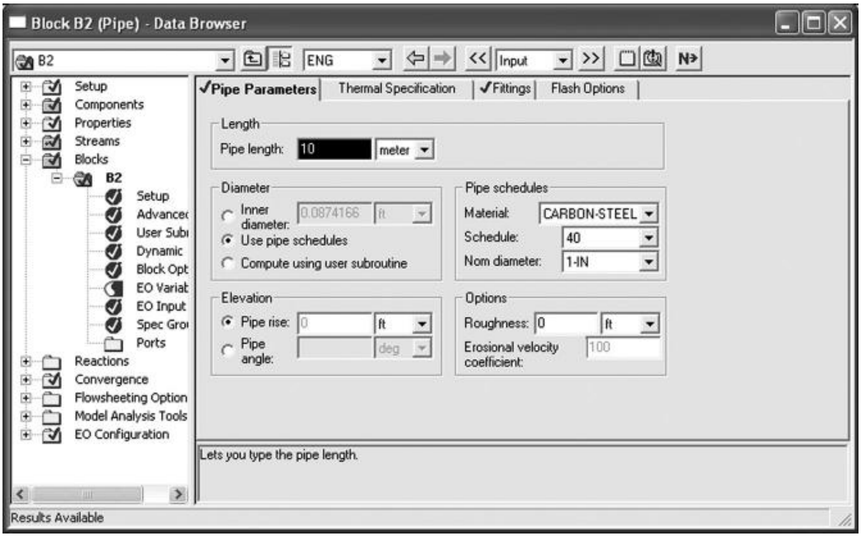
FIGURE 2.11
Pressure drop and stream properties of Example 2.1.

Streams were added by clicking on the process flow sheet where one would like the stream to begin and clicking again where you would like the stream to end. In a fashion similar to that of the equipment, each click will add a new stream to the process flow sheet until you click on *Select Mode* (the arrow at the left button corner). For this example, add one stream into the pipe, and one product stream leaves the pipe. At this point, the process flow sheet should be complete and it should somewhat resemble the one shown in Figure 2.12.

Under the *Components* tab, select *water*. The user input under the *Property* tab is probably the most critical input required to run a successful simulation. This key input is the *Base Method* found under the *Specifications* option. The *Base Method* is the thermodynamic basis for all the simulation calculations. Since the fluid is water, select steam fluid package. Aspen has a tool in the toolbar that will automatically take the user through the required data input in a stepwise fashion. The button that does this is the blue *N* with the arrow next to it in the toolbar, an alternative method is to double click on the material stream and specify the feed stream conditions, and then double click on the pipe segment and specify pipe conditions as shown in Figure 2.13.

After the feed stream is specified and the pipe segment is defined, the simulation status changes to *Required Input is Complete*. There are few ways to run the simulation; the user could select either *Next* in the toolbar that will say whether the required inputs are completed and ask whether you would like to run the simulation. The user can also run the simulation by selecting *Run* in the toolbar. After the simulation is run and converged, the *Results Summary* Tab on the *Data Browser Window* has a blue check mark. Clicking on that tab will open the *Run Status*. If simulation has converged, it should state, *Calculations were completed normally*. Adding stream tables to the process flow sheet is a simple process, but we will first go over some options for formatting and modifying the stream tables.

FIGURE 2.12
Process flow sheet of Example 2.1.



Pipe length: 10 meter

○ Inner diameter: 0.0874166 ft
● Use pipe schedules
○ Compute using user subroutine

Material: CARBON-STEEL
Schedule: 40
Nom diameter: 1-IN

● Pipe rise: 0 ft
○ Pipe angle: deg

Roughness: 0 ft
Erosional velocity coefficient: 100

Lets you type the pipe length.

Results Available

FIGURE 2.13
Pipe length and the pipe schedule.

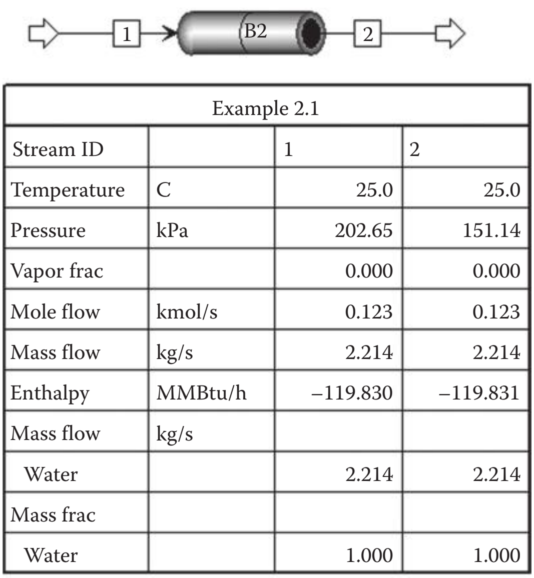
On the current screen you will see two of the options for varying the stream table: Display and Format. Under the *Display* drop-down menu there are two options, *All streams* or *Streams*. The streams option allows the user to choose the streams they would like to present, one by one. Under the Format drop-down menu there are a number of types of stream tables. Each of the options presents the data in a slightly different fashion, depending on the intended application. The CHEM_E option gives the results. To add a stream table to process the flow sheet, click on *Stream Table* and a stream table will be added to your process flow sheet. The process flow sheet and stream results are shown in Figure 2.14.

CONCLUSIONS

The comparison between pressure drop values calculated by hand calculation (50.4 kPa), Hysys (51.69 kPa), PRO/II (52.1 kPa), and Aspen (51.51 kPa) reveals that there is a slight deviation between hand calculations and software simulations. The discrepancy in the hand-calculated value is due to the assumption made by taking the inlet conditions in calculating Reynolds number, while the average of inlet and exit streams should be considered to have better results.

Example 2.2: Pressure Drop of Natural Gas in Horizontal Pipe

Natural gas contains 85 mol% methane and 15 mol% carbon dioxide (density, $\rho = 2.879\ \text{kg/m}^3$ and the viscosity, $\mu = 1.2 \times 10^{-5}\ \text{kg/m s}$) is pumped through a horizontal Schedule 40, 6-in.-diameter cast-iron pipe at a mass flow rate of 363 kg/h. If the pressure at the pipe inlet is 3.45 bars and 25°C, the pipe length is 20 km downstream, assume incompressible flow. Calculate the pressure drop across the pipe. Is the assumption of incompressible flow reasonable?



Example 2.1			
Stream ID		1	2
Temperature	C	25.0	25.0
Pressure	kPa	202.65	151.14
Vapor frac		0.000	0.000
Mole flow	kmol/s	0.123	0.123
Mass flow	kg/s	2.214	2.214
Enthalpy	MMBtu/h	−119.830	−119.831
Mass flow	kg/s		
Water		2.214	2.214
Mass frac			
Water		1.000	1.000

FIGURE 2.14
Process flow sheet and stream table conditions.

SOLUTION

HAND CALCULATIONS

The energy equation for the pipe flow is

$$gz_1 + \frac{p_1}{\rho} + \frac{V_1^2}{2} = gz_2 + \frac{p_2}{\rho} + \frac{V_2^2}{2} + f\frac{L}{D}\frac{V_2^2}{2} + \Sigma F + W_s$$

Since the pipe is horizontal $z_1 = z_2$, and the flow is assumed to be incompressible (this assumption is not accepted with gases) with a constant diameter $V_1 = V_2$, the pressure drop in this case can be calculated by using the following equation:

$$\frac{p_1 - p_2}{\rho} = f\frac{L}{D}\frac{V_2}{2}$$

The nominal pipe diameter is 6 in. Schedule 40; consequently, the inner pipe diameter is 0.154 m and the velocity is

$$V = \frac{\dot{m}}{\rho A} = \frac{\dot{m}}{\rho\left(\pi D_1^2/4\right)} = \frac{\dfrac{363\,\text{kg}}{\text{h}}\left(\dfrac{\text{h}}{3600\,\text{s}}\right)}{2.879\dfrac{\text{kg}}{\text{m}^3}\pi\left(0.154\,\text{m}\right)^2/4} = \frac{1.98\,\text{m}}{\text{s}}$$

Reynolds number,

$$\text{Re} = \frac{\rho VD}{\mu} = \frac{(2.879\ \text{kg/m}^3)(1.98\ \text{m/s})(0.154\ \text{m})}{1.2 \times 10^{-5}\ \text{kg/ms}} = 7.14 \times 10^4$$

Since Reynolds number is greater than 4000, the flow is turbulent and the roughness factor for the cast-iron pipe is $\varepsilon = 0.00026$ m (Table 2.1). The relative roughness of a cast-iron pipe is $(\varepsilon/D) = (0.00026\ \text{m})/(0.15\ \text{m}) = 0.0017$. From the relative roughness and $\text{Re} = 7.14 \times 10^4$, we can find the friction factor $f = 0.024$ (Figure 2.2). Using the calculated friction factor, the pressure drop

$$P_1 - P_2 = \rho\left(f\frac{L}{D}\frac{V_2}{2}\right) = \left(2.879\ \text{kg/m}^3\right)\left((0.024)\frac{20{,}000\ \text{m}}{0.154\ \text{m}}\frac{(1.98\ \text{m/s})^2}{2}\right) = 17{,}590\ \text{kg/ms}^2$$

$$P_1 - P_2 = 17{,}590\ \text{kg/ms}^2\left(\frac{N}{1\,\text{kg m/s}^2}\right)\left(\frac{1\,\text{kPa}}{1000\ \text{N/m}^2}\right) = 17.59\ \text{kPa}$$

If the initial pressure is 3.45 bars, the downstream pressure (P_2) is

$$P1 - P2 = 17.59\ \text{kPa} \Rightarrow P2 = P1 - 17.59\ \text{kPa} = 345 - 17.59\ \text{kPa} = 327\ \text{kPa}$$

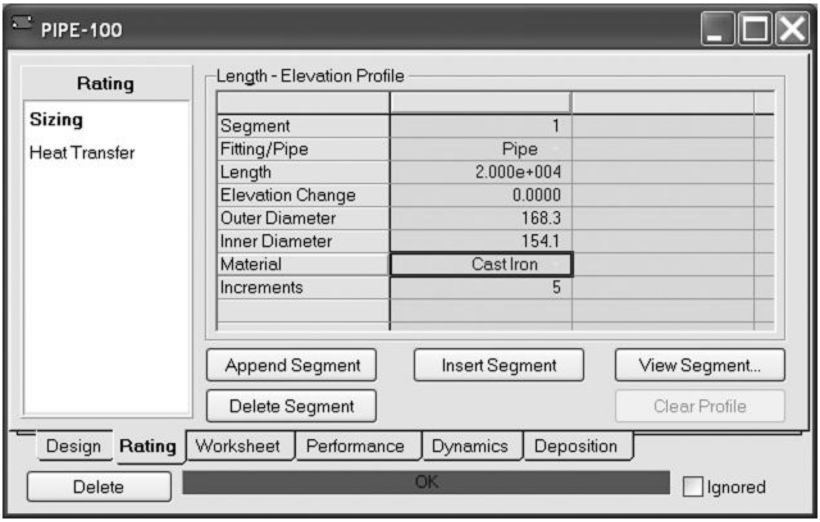
HYSYS SIMULATION

Open a new case in Hysys; select methane and carbon dioxide as components and Peng–Robinson as fluid package, respectively. Specify the feed stream conditions and compositions. Specify the temperature of the exit stream as that for inlet stream. Click on the pipe segment and then on *Append Segment* which is in rating page; then specify pipe length as 20 km. The inlet and the exit of the pipe are at the same level, elevation should be changed to be zero, click on *View Segment*, and specify the pipe schedule and pipe material (Figure 2.15).

TABLE 2.1

Roughness Factors Used by Hysys

Pipe Material Type	Absolute Roughness (ε), m
Smooth	0.0
Drawn tube	1.52×10^{-6}
Mild steel	4.57×10^{-5}
Asphalted iron	1.22×10^{-4}
Galvanized iron	1.52×10^{-4}
Cast iron	2.59×10^{-4}
Smooth riveted steel	9.14×10^{-4}
Rough riveted steel	9.14×10^{-3}



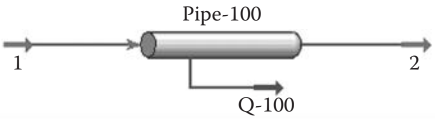
Segment	1
Fitting/Pipe	Pipe
Length	2.000e+004
Elevation Change	0.0000
Outer Diameter	168.3
Inner Diameter	154.1
Material	Cast Iron
Increments	5

FIGURE 2.15
Appended pipe segment.

To display the result to as shown in Figure 2.16, click on the *Workbook* icon in the toolbar. The *Workbook* appears. From the workbook menu click on *Setup*. Once the setup view appears, click on *Add* in the workbook tabs group and select the variable desired to be displayed in the table. Right click on the PFD area below the PFD and click on *Add Workbook Table*.

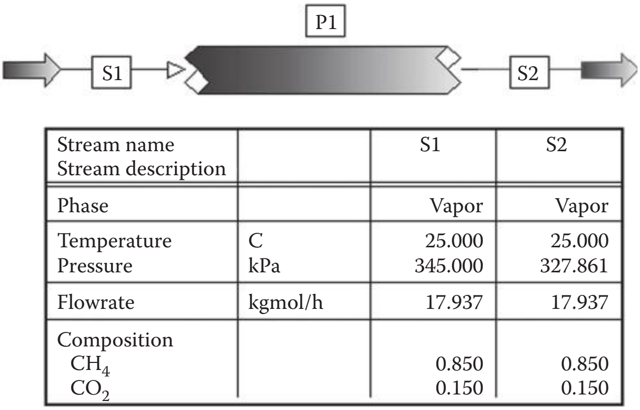
SIMULATION WITH PRO/II

Repeating the same procedure used to construct the process flow sheet of Example 2.1 with PRO/II, the pressure drop is 17.14 kPa as shown in Figure 2.17.



Streams			
		1	2
Temperature	C	25.00	25.00
Pressure	kPa	345.0	327.7
Mass flow	kg/h	363.0	363.0
Comp molar flow (Methane)	kgmol/h	15.2461	15.2461
Comp molar flow (CO_2)	kgmol/h	2.6905	2.6905

FIGURE 2.16
Pressure drop through the pipeline is 17 kPa.



Stream name Stream description		S1	S2
Phase		Vapor	Vapor
Temperature	C	25.000	25.000
Pressure	kPa	345.000	327.861
Flowrate	kgmol/h	17.937	17.937
Composition			
CH_4		0.850	0.850
CO_2		0.150	0.150

FIGURE 2.17
Pressure drop across the pipe of Example 2.2.

ASPEN SIMULATIONS

Following the same procedure used in constructing the process flow sheet of Example 2.1 with Aspen, remember that the pipe has no fittings. The simulation results are shown in Figure 2.18.

CONCLUSION

Hand-calculated pressure drop value is 17.59 kPa, and according to Hysys, PRO/II, and Aspen it was found to be 17 kPa, 17.14 kPa, and 17.16 kPa, respectively. Simulation software results were very close to each other; on the contrary, hand calculation is greater than all the other results, and this is attributed to the incompressibility assumption made during hand calculation. It is clear from the solution of this example that the density of gases is a function of both temperature and pressure.

Example 2.3: Calculate Pipe Inlet Flow (Given D and ΔP)

Water at 2 atm and 25°C is flowing in a horizontal 10 m mild steel pipe; the pressure drop in the pipe is equal to 118 kPa. The pipe is Schedule 40 and has 1 in. nominal diameter (1.049 in. or 0.0266 m ID). Calculate the water inlet water velocity and liquid volumetric flow rate.

SOLUTION

HAND CALCULATIONS

In this example, the diameter and pressure drop between the inlet and the exit pipe are provided, and the inlet velocity and/or flow rate are to be determined. Since there is no fitting in the pipe, the pressure drop is a function of pipe skin friction only as the following:

$$\Delta P = f\frac{L}{D}\rho\frac{V^2}{2}$$

Example 2.2			
Stream ID		1	2
Temperature	C	25.0	25.0
Pressure	kPa	345.00	327.00
Vapor frac		1.000	1.000
Mole flow	kmol/s	0.005	0.005
Mass flow	kg/s	0.101	0.101
Enthalpy	MMBtu/h	–2.082	–2.081
Mass flow	kg/s		
Methane		0.068	0.068
CO_2		0.033	0.033
Mass frac			
Methane		0.674	0.674
CO_2		0.326	0.326

FIGURE 2.18
Stream table of Example 2.2 using Aspen.

Substituting values into the above equation,

$$118 \times 10^3\,\text{Pa} = f\frac{10\,\text{m}}{0.0266\,\text{m}}(1000\,\text{kg/m}^3)\frac{V^2}{2}$$

The friction factor can be found from the Moody diagram or calculated:

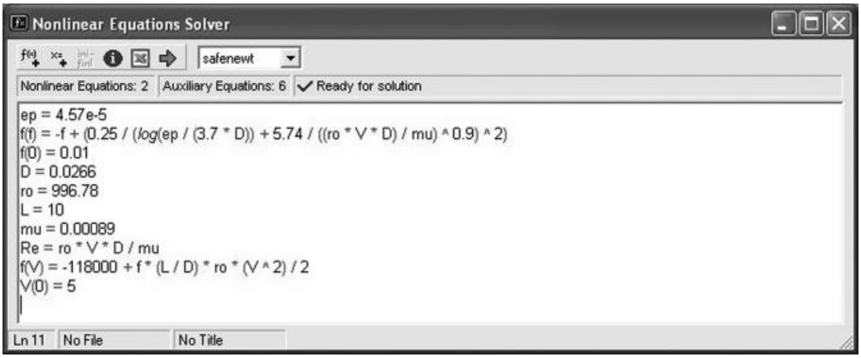
$$f = \frac{0.25}{\left[\log\left((\varepsilon/3.7D) + (5.74/\text{Re}^{0.9})\right)\right]^2}$$

Friction factor is a function of Reynolds number,

$$f = \frac{0.25}{\left[\log\left(\frac{4.57 \times 10^{-5}\,\text{m}}{3.7 \times 0.0266\,\text{m}} + \frac{5.74}{\text{Re}^{0.9}}\right)\right]^2}$$

The Reynolds number

$$\text{Re} = \frac{\rho VD}{\mu} = \frac{1000\,\text{kg/m}^3\,(V)0.0266\,\text{m}}{0.001\,\text{kg/ms}}$$

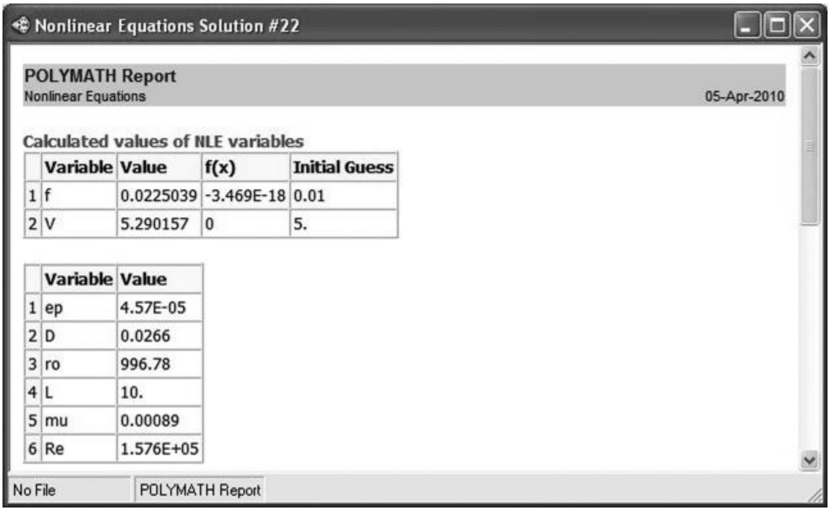


```
ep = 4.57e-5
f(f) = -f + (0.25 / (log(ep / (3.7 * D)) + 5.74 / ((ro * V * D) / mu) ^ 0.9) ^ 2)
f(0) = 0.01
D = 0.0266
ro = 996.78
L = 10
mu = 0.00089
Re = ro * V * D / mu
f(V) = -118000 + f * (L / D) * ro * (V ^ 2) / 2
V(0) = 5
```

FIGURE 2.19
Polymath code of Example 2.3.

Reynolds number is a function of velocity. And that is why a trial-and-error solution is needed here to calculate the pressure drop.

Assume velocity *V*, and calculate Reynolds number. From Reynolds number, calculate the friction factor from the Moody diagram shown in Figure 2.2, otherwise it can be obtained from the above-mentioned equations. Calculate the pressure drop and then compare the calculated result with the given value of pressure drop which is 118 kPa in the question of the example. Repeat until the desired pressure drop is reached. Polymath software can be used instead (Figure 2.19). The calculated velocity is 5.29 m/s as shown in Figure 2.20.



POLYMATH Report
Nonlinear Equations
05-Apr-2010

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	f	0.0225039	-3.469E-18	0.01
2	V	5.290157	0	5.

	Variable	Value
1	ep	4.57E-05
2	D	0.0266
3	ro	996.78
4	L	10.
5	mu	0.00089
6	Re	1.576E+05

FIGURE 2.20
Polymath results for velocity calculation.

Hysys Simulation

Select a new case in Hysys. For components, select water; and for fluid package, select ASME steam. Enter the simulation environment. Select the pipe segment from the object palette. Specify the feed stream conditions, stream composition, and product stream temperature.

Click on the *Rating* tab. While on the rating page, click on *Append Segment* and enter the pipe specification as shown in Figure 2.21.

While on the pipe *Design* page, click on *Parameters*, and enter the pressure drop *Delta P* as 118 kPa. "The pressure drop is greater than 10%" is only a warning and can be ignored (Figure 2.22).

To view the velocity; click on the *Performance* tab, then click on *View Profile* (Figure 2.23).

The Hysys calculated velocity is 5.13 m/s (Figure 2.24).

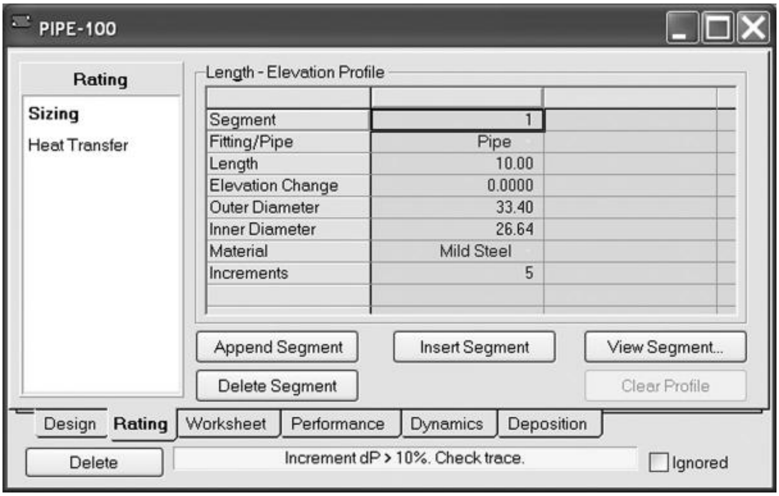
The volumetric flow rate = velocity × pipe cross section

$$Q = VA = (6.336\ \text{m/s})\left(\frac{\pi(0.0266\ \text{m})^2}{4}\right) = 3.52 \times 10^{-3}\ \text{m}^3/\text{s}$$

Simulation with PRO/II

The option of having the pressure drop and calculating velocity in Hysys is not available in PRO/II; instead, a case study or assuming flow rate and calculating pressure drop are needed. The process flow sheet of the pipe using PRO/II is demonstrated in Figure 2.25.

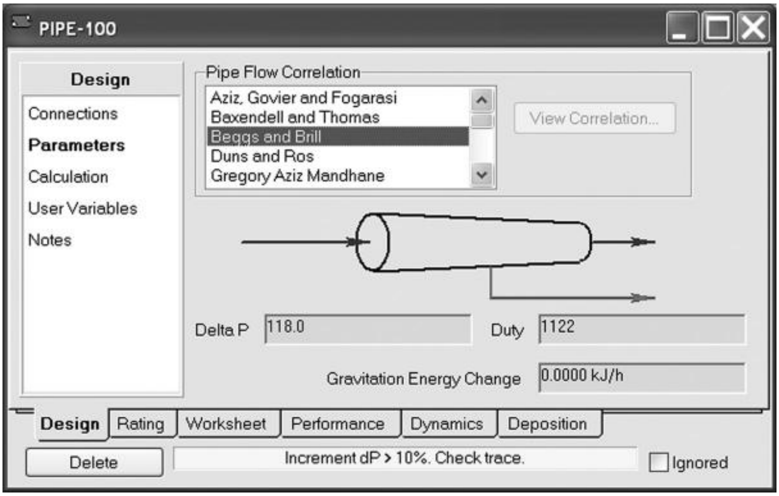
Click the *Pipe* icon in the PFD and specify the pipe length as 10 m, zero elevation, and zero fittings. Mild steel absolute roughness is 4.57×10^{-5}m entered in the PRO/II pipe-line/fittings menu as shown in Figure 2.26.



Segment	1
Fitting/Pipe	Pipe
Length	10.00
Elevation Change	0.0000
Outer Diameter	33.40
Inner Diameter	26.64
Material	Mild Steel
Increments	5

Increment dP > 10%. Check trace.

FIGURE 2.21
Pipe length–elevation profile.



Delta P 118.0

Duty 1122

Gravitation Energy Change 0.0000 kJ/h

Increment dP > 10%. Check trace.

FIGURE 2.22
Pipe parameters window.

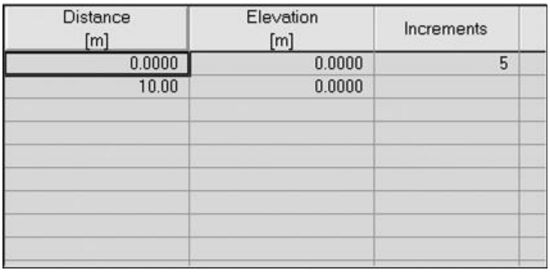
The trial-and-error procedure is used to estimate the required pressure drop of 118 kPa. Assume the inlet liquid volumetric flow rate, run the simulator, and then check the pressure drop. Keep repeating the process until a pressure drop of 118 kPa is achieved. The generated report is shown in Figure 2.27.

ASPEN SIMULATION

With Aspen, also a trial-and-error procedure is required and in the same way as that used with PRO/II. Following the same procedure using Aspen shown in Example 2.1, the process flow sheet and stream table simulation results are depicted in Figure 2.28. Volumetric flow rate is 0.00287 m^3/s (velocity = 5.17 m/s).

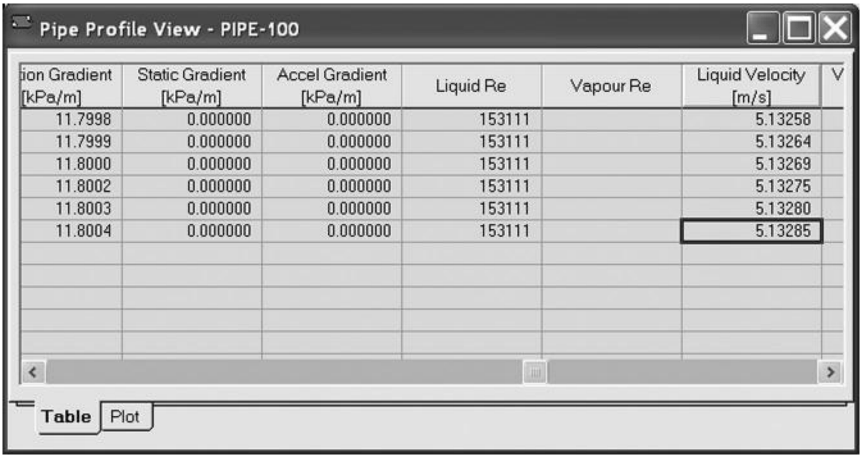
CONCLUSIONS

The velocity obtained by hand calculation (5.29 m/s) is slightly larger than that obtained by Hysys (5.13 m/s) and closer to those obtained by PRO/II (5.21 m/s) and Aspen (5.17 m/s).



Distance [m]	Elevation [m]	Increments
0.0000	0.0000	5
10.00	0.0000	

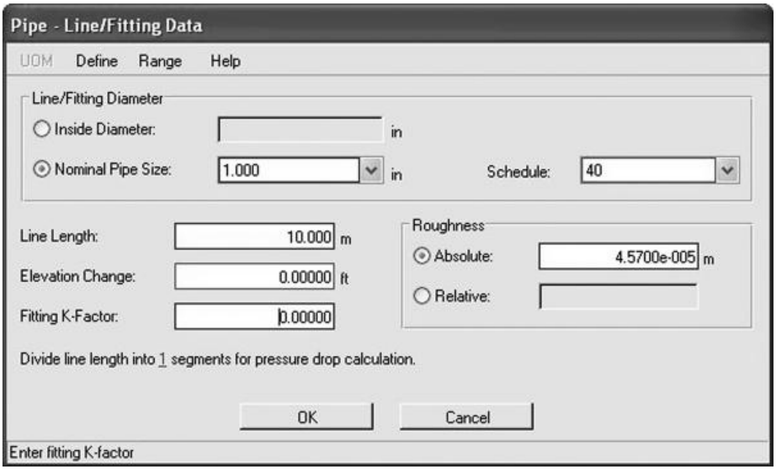
FIGURE 2.23
Pipe performance profiles.



ion Gradient [kPa/m]	Static Gradient [kPa/m]	Accel Gradient [kPa/m]	Liquid Re	Vapour Re	Liquid Velocity [m/s]	V
11.7998	0.000000	0.000000	153111		5.13258	
11.7999	0.000000	0.000000	153111		5.13264	
11.8000	0.000000	0.000000	153111		5.13269	
11.8002	0.000000	0.000000	153111		5.13275	
11.8003	0.000000	0.000000	153111		5.13280	
11.8004	0.000000	0.000000	153111		5.13285	

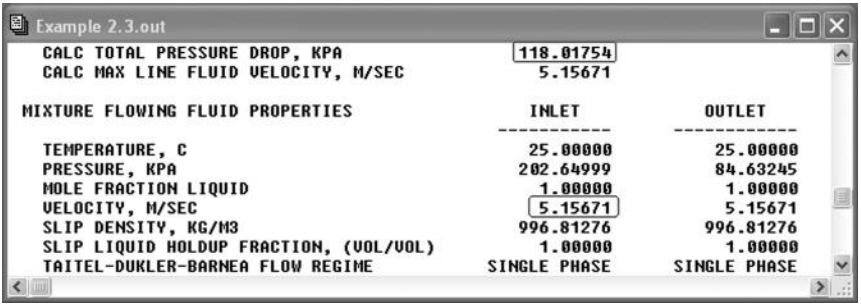
FIGURE 2.24
Liquid velocities inside the pipe.

FIGURE 2.25
Process flow sheet of Example 2.3.



Line/Fitting Diameter
○ Inside Diameter: in
● Nominal Pipe Size: 1.000 in Schedule: 40
Line Length: 10.000 m
Elevation Change: 0.00000 ft
Fitting K-Factor: 0.00000
Roughness
● Absolute: 4.5700e-005 m
○ Relative:
Divide line length into 1 segments for pressure drop calculation.
Enter fitting K-factor

FIGURE 2.26
Pipe fitting menu in PRO/II.



```
   CALC TOTAL PRESSURE DROP, KPA                        118.01754
   CALC MAX LINE FLUID VELOCITY, M/SEC                    5.15671

 MIXTURE FLOWING FLUID PROPERTIES                       INLET            OUTLET
                                                     -----------      ------------
   TEMPERATURE, C                                      25.00000          25.00000
   PRESSURE, KPA                                      202.64999          84.63245
   MOLE FRACTION LIQUID                                 1.00000           1.00000
   VELOCITY, M/SEC                                      5.15671           5.15671
   SLIP DENSITY, KG/M3                                996.81276         996.81276
   SLIP LIQUID HOLDUP FRACTION, (VOL/VOL)               1.00000           1.00000
   TAITEL-DUKLER-BARNEA FLOW REGIME                 SINGLE PHASE      SINGLE PHASE
```

FIGURE 2.27
Inlet fluid velocities that lead to a pressure drop of 118 kPa.

Example 2.4: Effect of Liquid Flow Rate on Pressure Drop

Water is flowing in a pipeline at 20°C. The pipeline which is 6 in. nominal diameter, Schedule 40 commercial steel pipe (length, $L = 1500$ m), pipe inlet pressure, $P_1 = 20$ atm, exit pressure, $P_2 = 2$ atm, and $z_1 = 0$ ft and $z_2 = 100$ m. Plot inlet volumetric flow rate versus pressure drop across the pipe.

SOLUTION

Hand Calculations

Assume an inlet liquid volumetric flow rate of 0.01 m^3/s, find the fluid velocity and then Reynolds number using calculated velocity. Use the Moody diagram to

Example 2.3			
Stream ID		1	2
Temperature	C	25.0	25.0
Pressure	kPa	202.65	84.95
Vapor frac		0.000	0.000
Mole flow	kmol/s	0.159	0.159
Mass flow	kg/s	2.862	2.862
Volume flow	cum/s	0.003	0.003
Enthalpy	MMBtu/h	−154.916	−154.917
Mass flow	kg/s		
Water		2.862	2.862
Mass frac			
Water		1.000	1.000

FIGURE 2.28
Aspen results of Example 2.3.

calculate the friction factor and then calculate the pressure drop. Repeat for flow rates 0.02, 0.04, and 0.06 m^3/s, and plot the calculated pressure drop versus the inlet liquid flow rate using excel.

HYSYS SIMULATION

Open a new case in Hysys, select water as the pure component, ASME steam for the fluid package, and then enter the simulation environment. Select the pipe segment from the object palette, double click on the pipe and fill in the connection page. Click on the *Worksheet* tab; set the feed and product stream temperatures to 20°C (isothermal condition) and the feed pressure to 20 atm. Click on the *Rating* tab; then click on *Append segment* and specify the parameters of the pipe as shown in Figure 2.29.

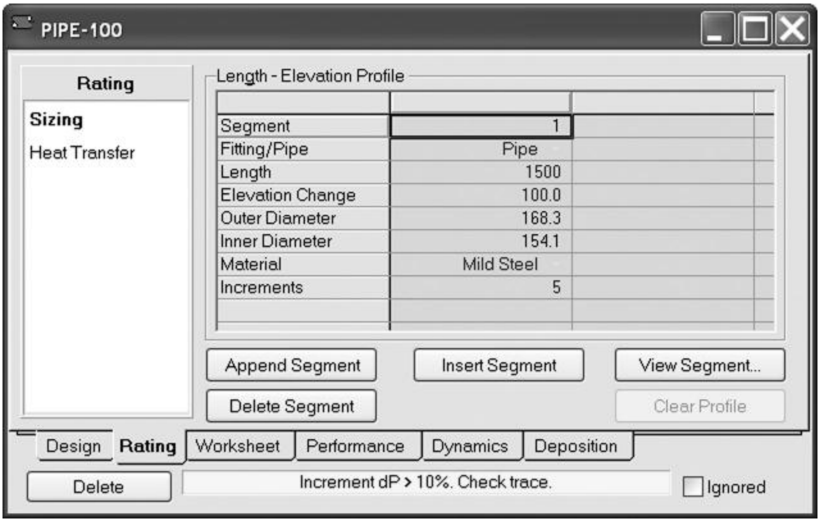
The outer and inner diameters of the pipe were specified by double clicking on the *View Segment*, select pipe Schedule 40, 6 in. nominal diameter and the pipe material as mild steel (Figure 2.30).

The problem requests the plot of the flow rate versus the pressure drop with 18 atm as the maximum bound. A useful tool in Hysys is the *DataBook*. From the *Tools* menu, select *DataBook*. Click on *Insert* and add the following variables: Feed and Actual Liquid flow. Thereafter, click on *OK* as shown in Figure 2.31.

Under the *Object* column, select PIPE 100 and for *Variable*, select Pressure drop as shown in Figure 2.32 and then click *OK* to close.

The data book variables are shown in Figure 2.33.

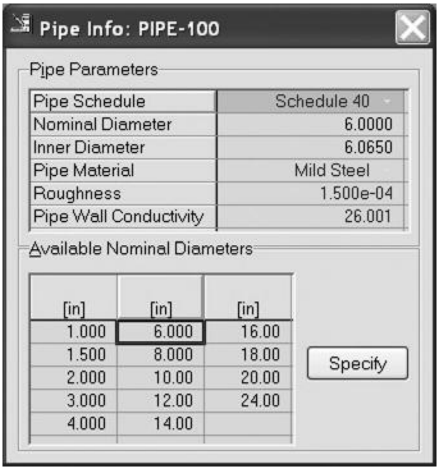
Click on the *Case Studies* tab at the bottom of Figure 2.33; choose the pressure drop as the independent variable and actual liquid flow as the dependent variable (Figure 2.34).



Segment	1
Fitting/Pipe	Pipe
Length	1500
Elevation Change	100.0
Outer Diameter	168.3
Inner Diameter	154.1
Material	Mild Steel
Increments	5

Increment dP > 10%. Check trace.

FIGURE 2.29
Pipe segment specifications.



Pipe Info: PIPE-100

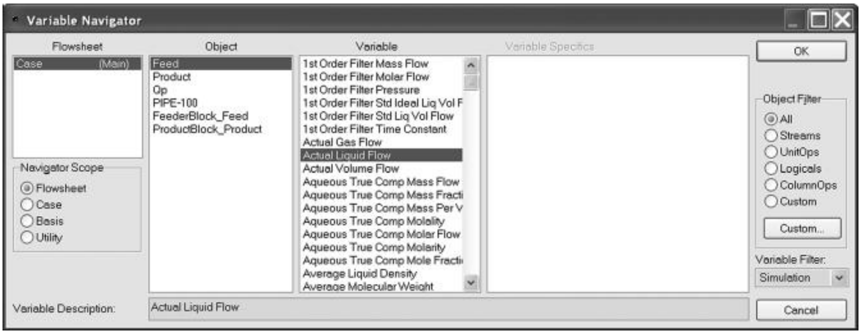
Pipe Parameters

Pipe Schedule	Schedule 40
Nominal Diameter	6.0000
Inner Diameter	6.0650
Pipe Material	Mild Steel
Roughness	1.500e-04
Pipe Wall Conductivity	26.001

Available Nominal Diameters

[in]	[in]	[in]
1.000	6.000	16.00
1.500	8.000	18.00
2.000	10.00	20.00
3.000	12.00	24.00
4.000	14.00	

FIGURE 2.30
Pipe schedule and material selection page.



Variable Navigator

Flowsheet: Case (Main)

Object: Feed

Variable: Actual Liquid Flow

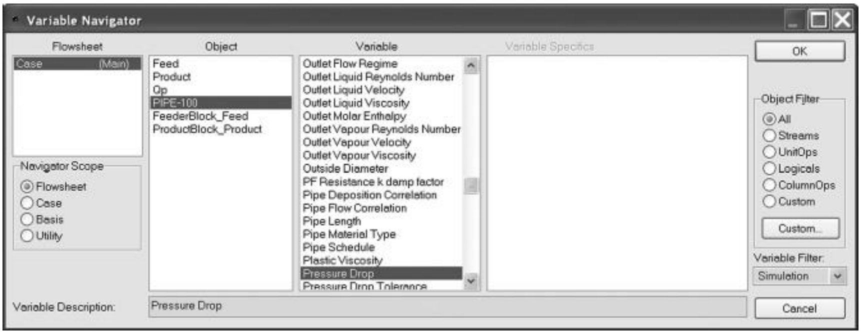
Navigator Scope: Flowsheet

Object Filter: All

Variable Filter: Simulation

Variable Description: Actual Liquid Flow

FIGURE 2.31
Feed stream actual liquid flow.



Variable Navigator

Flowsheet: Case (Main)

Object: PIPE-100

Variable: Pressure Drop

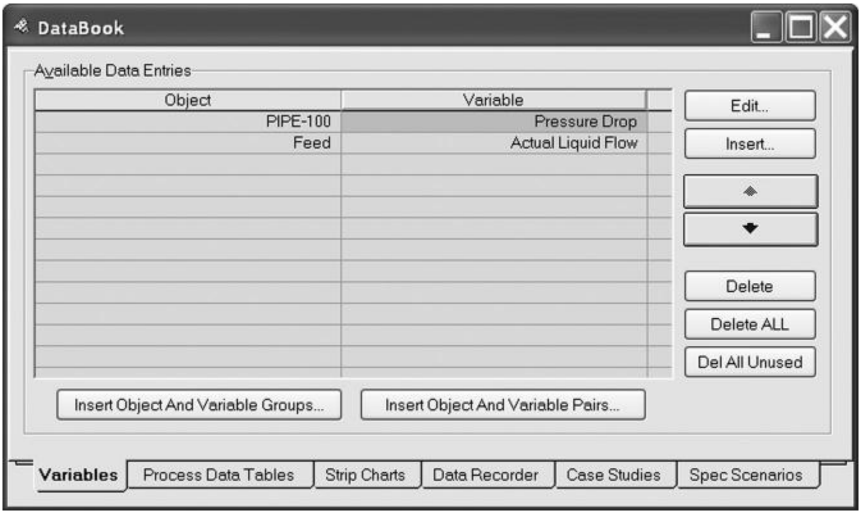
Navigator Scope: Flowsheet

Object Filter: All

Variable Filter: Simulation

Variable Description: Pressure Drop

FIGURE 2.32
Selection of pipe pressure drop variable.

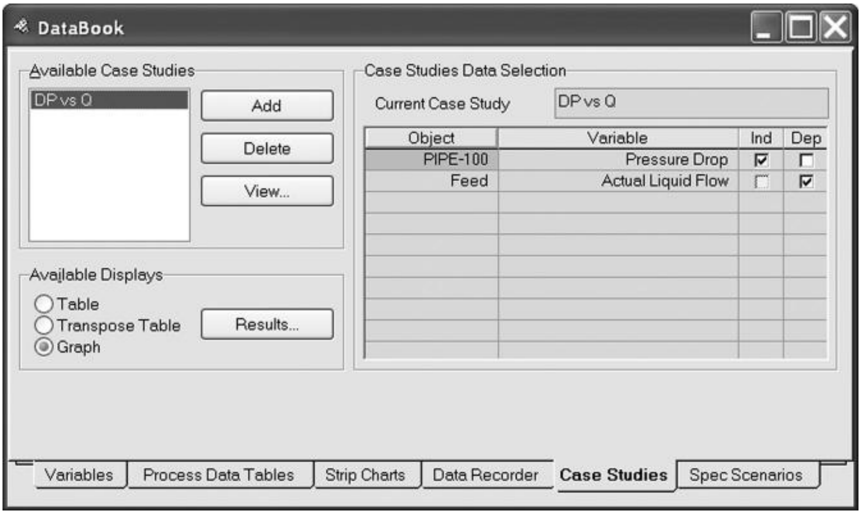


Object	Variable
PIPE-100	Pressure Drop
Feed	Actual Liquid Flow

FIGURE 2.33
Variables used in the sensitivity study of pressure drop versus feed flow rate.

Rename the current case study to DP versus *Q*. Click on *View* and specify the low bound as 10 atm and the high bound as 18 atm, and the *Step Size* as 0.5 (Figure 2.35).

Click on *Start*. When the calculations are complete, click on *Results*. Then click on *View* to see the generated graph (Figure 2.36).



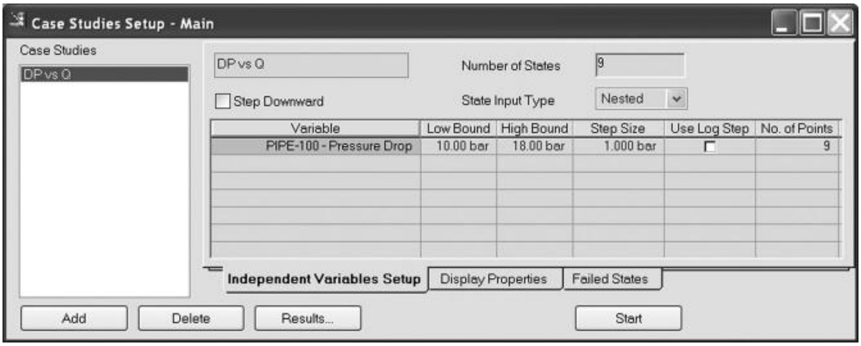
DP vs Q

○ Table
○ Transpose Table
● Graph

Current Case Study: DP vs Q

Object	Variable	Ind	Dep
PIPE-100	Pressure Drop	☑	☐
Feed	Actual Liquid Flow	☐	☑

FIGURE 2.34
Available case studies window.



Case Studies: DP vs Q

DP vs Q

Number of States: 9

☐ Step Downward

State Input Type: Nested

Variable	Low Bound	High Bound	Step Size	Use Log Step	No. of Points
PIPE-100 - Pressure Drop	10.00 bar	18.00 bar	1.000 bar	☐	9

FIGURE 2.35
Low- and high-bound page.

PRO/II SIMULATION

In order to plot pressure drop versus liquid flow rate using the PRO/II software package carry out the following steps: click on the *Case Study* icon in the toolbar and rename PAR1 or leave as default, in this case PAR1 was renamed to FLOW. Clicking on the red word *Parameter*, a menu will pop up, since the inlet stream flow rate is set as the manipulated variable, select *Stream* from the pull-down menu under *Stream/Unit*. Under *Stream Name* select S1 and then click on the *Parameter* below the *Stream/Unit* cell and select *Flow rate*. Specify cycles from 1 through 6. Set the offset of the base case value to 0.002 and the step size to 0.001. After the parameter is set, the *Result* in the second row is to be specified. Click on result and rename it as pressure drop DP. Under *Stream/Unit* select *Pipe* and for the name select the name of the pipe (PI1). Click on the red word *Parameter* just

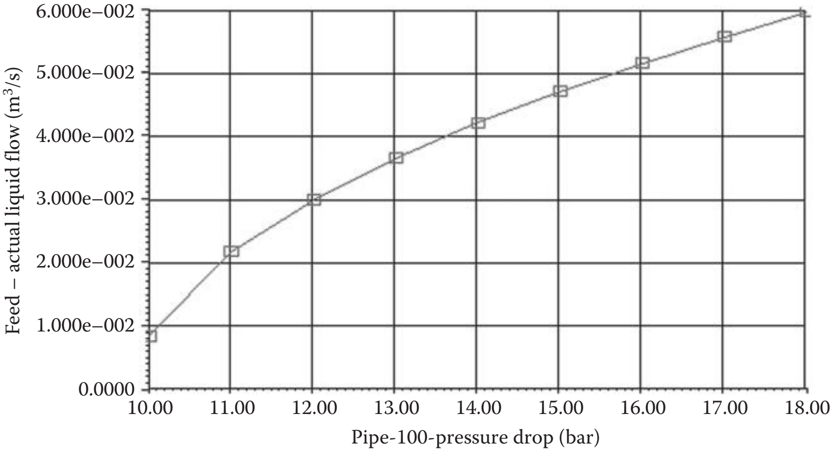
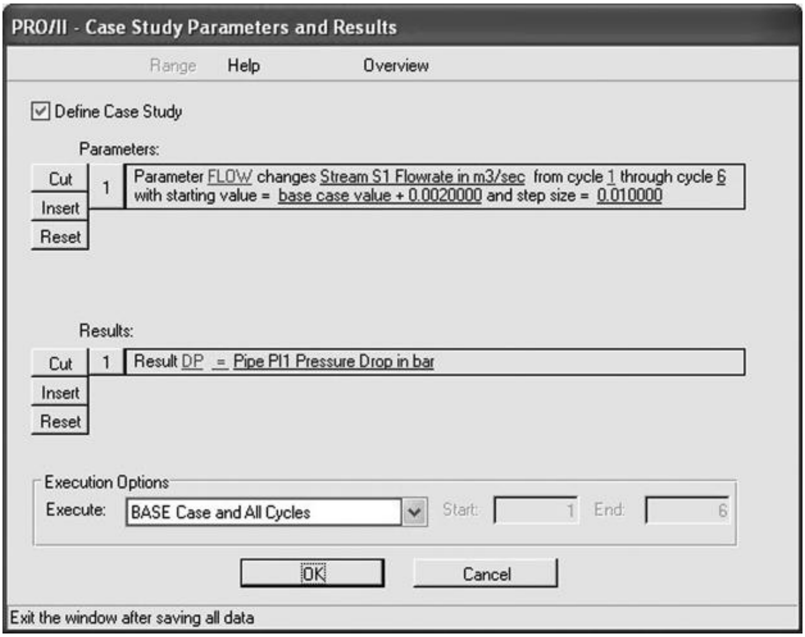


FIGURE 2.36
Effect of pressure drop on actual liquid flow rate.



PRO/II - Case Study Parameters and Results

☑ Define Case Study

Parameters:

1 Parameter FLOW changes Stream S1 Flowrate in m3/sec from cycle 1 through cycle 6 with starting value = base case value + 0.0020000 and step size = 0.010000

Results:

1 Result DP = Pipe PI1 Pressure Drop in bar

Execution Options

Execute: BASE Case and All Cycles Start: 1 End: 6

Exit the window after saving all data

FIGURE 2.37
Case study parameters with PRO/II.

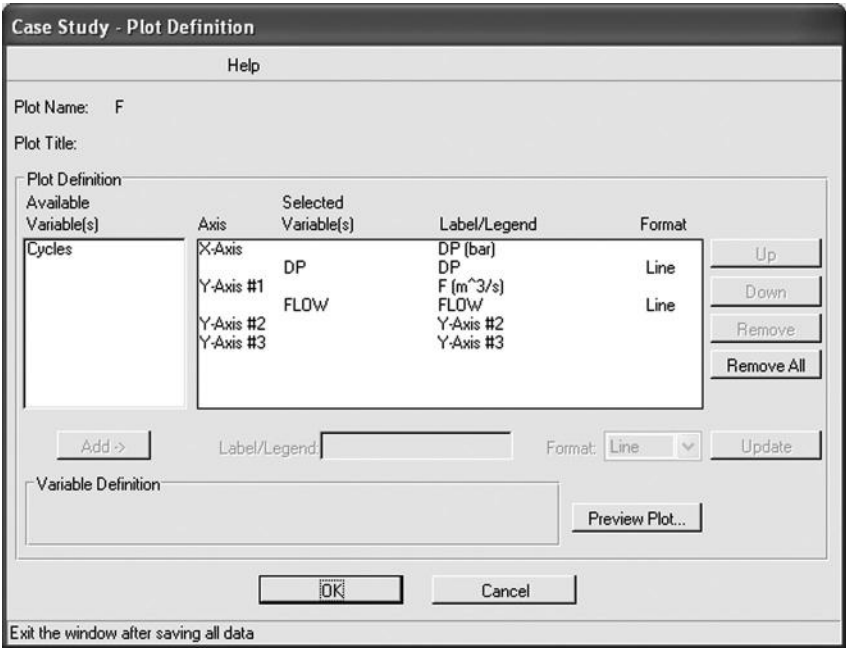
below the *Stream/Unit* cell and select the parameter as the *Pressure drop* and the units in *bar*. The final case study and the *Parameter* menu should appear as that in Figure 2.37. Click on *OK* to close the case study window. Click on *Run*, and then select case study under *Output* in the toolbar, and then select plots. Enter plot name and title and then click on *Data*. Select the DP as the *x*-axis and Flow as the *y*-axis; the final windows should appear like that in Figure 2.38. From the *Options* menu select *Plot Setup*, then select "Excel 97 and above." When generating a plot, PRO/II will open Excel and give a plot on one worksheet and the source data on another. The case study tabular output can also be exported to Excel. In the case study table setup window, click on *View Table*, and you will get a view of the table; click on *Copy to Clipboard*. You can now paste into Excel and use any Excel plot option as per your choice.

Figure 2.39 shows the effect of flow rate on pressure drop generated using the PRO/II case study option. Figure 2.39 reveals that as the liquid volumetric flow rate increases, pressure drop across the pipe increases.

ASPEN SIMULATION

Open a blank case in Aspen following the same procedure used by Aspen to construct process flow sheet of the pipe as that done in Example 2.1; the pipe has no fittings. The simulation result is shown in Figure 2.40.

To plot the pressure drop versus the flow rate using Aspen; from *Data* in the toolbar select *Model Analysis Tool*, and then *Sensitivity*. Click on *New*, the default name is *S-1*. Click *New* again, name the first variable for pressure drop



Plot Name: F

Plot Title:

Available Variable(s): Cycles

Axis	Selected Variable(s)	Label/Legend	Format
X-Axis		DP (bar)	
	DP	DP	Line
Y-Axis #1		F (m^3/s)	
	FLOW	FLOW	Line
Y-Axis #2		Y-Axis #2	
Y-Axis #3		Y-Axis #3	

Exit the window after saving all data

FIGURE 2.38
Case study plot definition.

as DP, edit the variable as shown in Figure 2.41, and repeat the same for the liquid volume flow rate FR as shown in Figure 2.42. Click on **N** to run the Sensitivity analysis. To plot the figure, click on *Result* and select *x* and *y* data as shown in Figure 2.43. The plot of pressure drop versus the flow rate is shown in Figure 2.44.

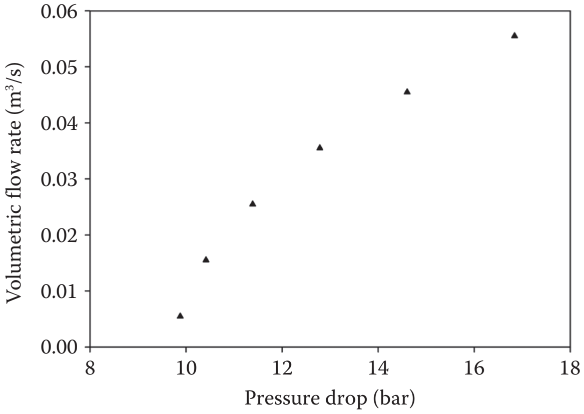
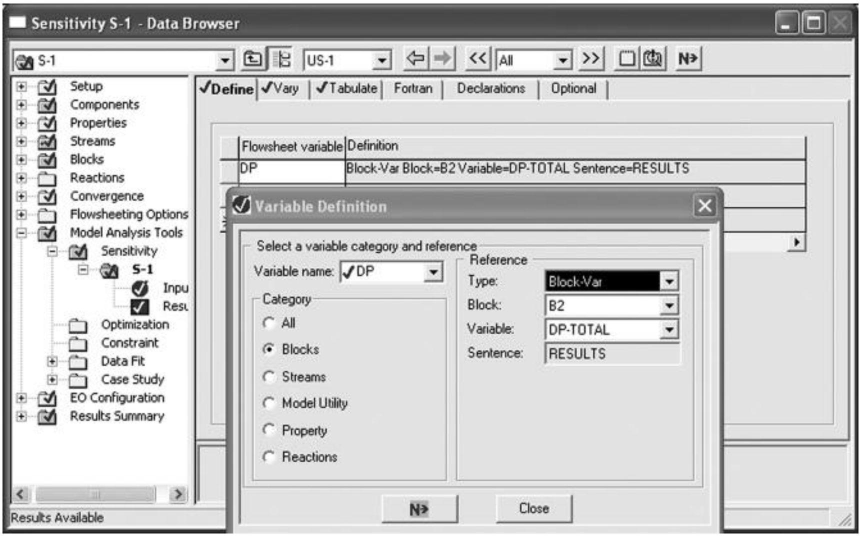


FIGURE 2.39
Liquid volumetric flow rates versus pressure drop.

Example 2.4			
Stream ID		1	2
Temperature	C	25.0	25.0
Pressure	kPa	2026.500	1020.550
Vapor frac		0.000	0.000
Mole flow	kmol/s	0.554	0.554
Mass flow	kg/s	9.979	9.979
Volume flow	cum/s	0.010	0.010
Enthalpy	MMkcal/h	–136.121	–136.129
Mass flow	kg/s		
Water		9.979	9.979
Mass frac			
Water		1.000	1.000

FIGURE 2.40
Process flow sheet and stream table for Example 2.4.



Flowsheet variable	Definition
DP	Block-Var Block=B2 Variable=DP-TOTAL Sentence=RESULTS

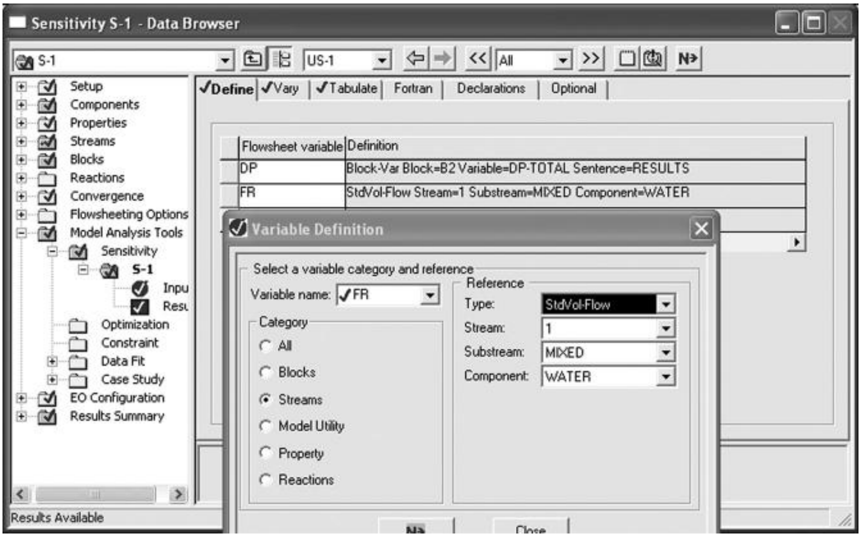
Select a variable category and reference

Variable name: ✓DP

Category
○ All
● Blocks
○ Streams
○ Model Utility
○ Property
○ Reactions

Reference
Type: Block-Var
Block: B2
Variable: DP-TOTAL
Sentence: RESULTS

FIGURE 2.41
Specify pressure drop as a variable.



Flowsheet variable	Definition
DP	Block-Var Block=B2 Variable=DP-TOTAL Sentence=RESULTS
FR	StdVol-Flow Stream=1 Substream=MIXED Component=WATER

Variable name: FR

Category: ○ All ○ Blocks ● Streams ○ Model Utility ○ Property ○ Reactions

Type: StdVol-Flow

Stream: 1

Substream: MIXED

Component: WATER

FIGURE 2.42
Setting liquid flow rate as variable.

Example 2.5: Pipeline with Fitting and Pump

Water at 20°C is being pumped from the feed tank at 5 atm pressure to an elevated storage tank 15 m high at the rate of 18 m^3/h. All pipes are 4-in. Schedule 40 commercial steel pipes. The pump has an efficiency of 65%. The PFD is shown in Figure 2.45. Calculate the power needed for the pump to overcome the pressure loss in the pipeline.

DATA

Density of water $\rho = 998\ kg/m^3$, viscosity $\mu = 1.0 \times 10^{-3}$ kg/ms, pipe diameter for 4-in. Schedule 40 is ID = 0.1023 m, and pipe cross-sectional area $A = 8.2 \times 10^{-3}\ m^2$.

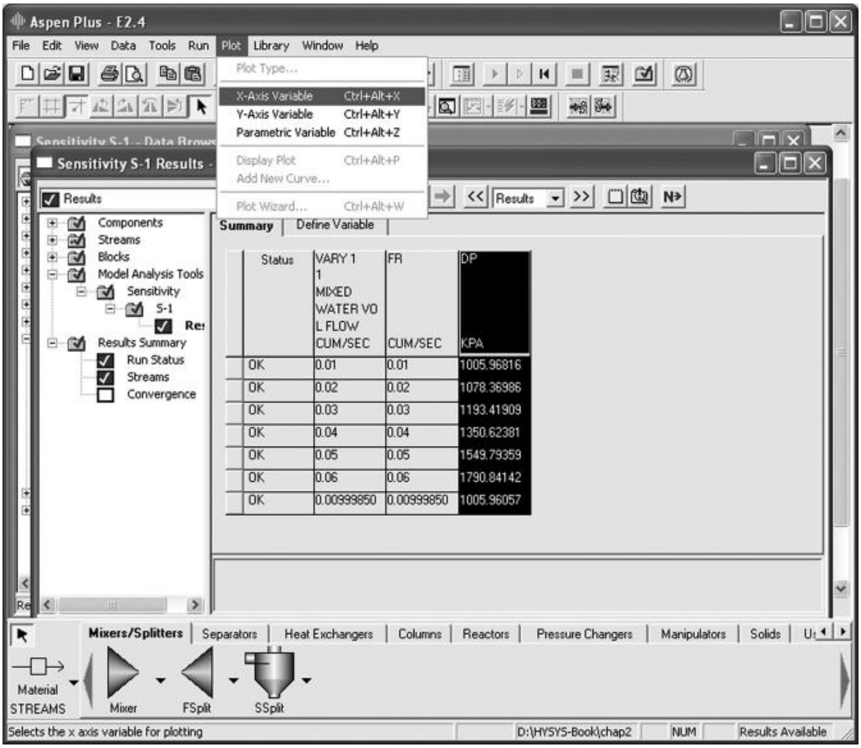
SOLUTION

HAND CALCULATIONS

In the previous example there were no pumps installed in the pipelines; however, in many practical situations the driving force is usually provided by a pump.

Energy equation,

$$\frac{P_1}{\rho} + gz_1 + \frac{V_1^2}{2} = \frac{P_2}{\rho} + gz_2 + \frac{V_2^2}{2} + W_s + \Sigma F$$



Status	VARY 1 1 MIXED WATER VOL FLOW CUM/SEC	FR CUM/SEC	DP KPA
OK	0.01	0.01	1005.96816
OK	0.02	0.02	1078.36986
OK	0.03	0.03	1193.41909
OK	0.04	0.04	1350.62381
OK	0.05	0.05	1549.79359
OK	0.06	0.06	1790.84142
OK	0.00999850	0.00999850	1005.96057

FIGURE 2.43
Selection of pressure drop as the *x*-axis for the sensitivity analysis.

Reynolds number,

$$\mathrm{Re} = \frac{\rho V D}{\mu} = \frac{(998\ \mathrm{kg/m^3})\left(\dfrac{5\times 10^{-3}\ \mathrm{m^3/s}}{8.22\times 10^{-3}\ \mathrm{m^2}}\right)}{1\times 10^{-3}\ \mathrm{kg/ms}} = 6.18\times 10^{4}$$

Since Reynolds number is greater than 4000 and the flow is turbulent, from the Moody chart

$$\frac{\varepsilon}{D} = \frac{4.6\times 10^{-5}}{0.1023} = 0.00045, \quad \text{hence } f = 0.02$$

The friction losses

$$\Sigma F = f\frac{L}{D}\frac{V^2}{2} + \frac{V^2}{2}\left(K_\mathrm{c} + 2K_\mathrm{e} + K_\mathrm{ex}\right)$$

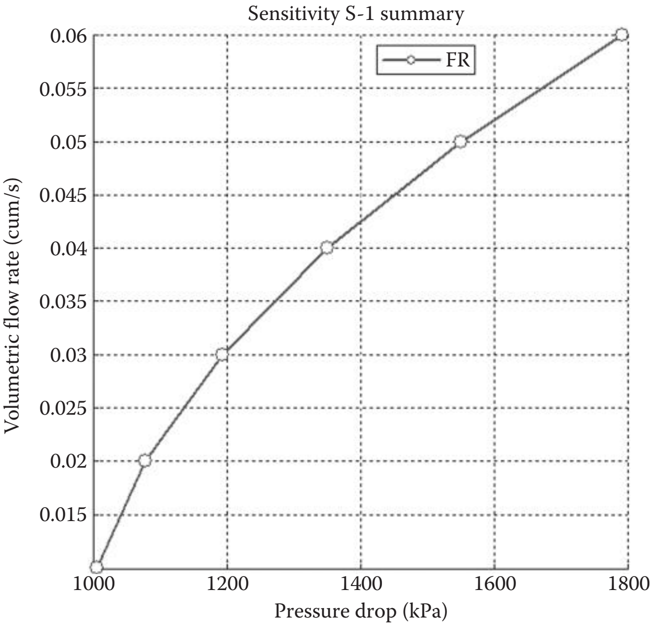


FIGURE 2.44
Pressure drop versus inlet liquid feed rate.

Contraction loss at the exit feed tank, $A_2/A_1 = 0$, since $A_1 \gg A_2 = 0$

$$K_c = 0.55\left(1 - \frac{A_2}{A_1}\right) = 0.55(1 - 0) = 0.55$$

Expansion loss at the inlet of the storage tank, $A_1/A_2 = 0$, since $A_2 \gg A_1 = 0$

$$K_{ex} = \left(1 - \frac{A_1}{A_2}\right)^2 = (1 - 0) = 1.0$$

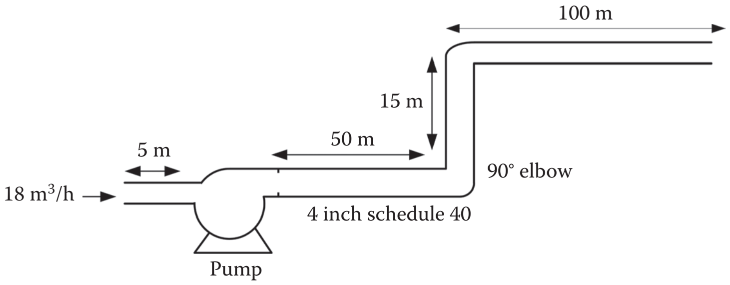


FIGURE 2.45
Process flow diagram for Example 2.5.

Summation of friction losses

$$\Sigma F = 0.02 \frac{170\,\text{m}}{0.1023\,\text{m}} \frac{(0.608\,\text{m/s})^2}{2} + \frac{(0.608\,\text{m/s})^2}{2}(0.55 + 2(0.75) + 1) = 6.84\,\text{m}^2/\text{s}^2$$

Energy equations:

$$0 = \frac{P_2 - P_1}{\rho} + g(z_2 - z_1) + \frac{V_2^2 - V_1^2}{2} + W_s + \Sigma F$$

$$0 = 0 + 9.806\,\text{m/s}^2(15 - 0) + 0 + W_s + 6.84\,\text{m}^2/\text{s}^2$$

Shaft work,

$$W_s = -154\,\text{m}^2/\text{s}^2$$

Pump kW power, mW_p

$$W_s = -\eta W_p$$

$$-154 = -0.65 W_p$$

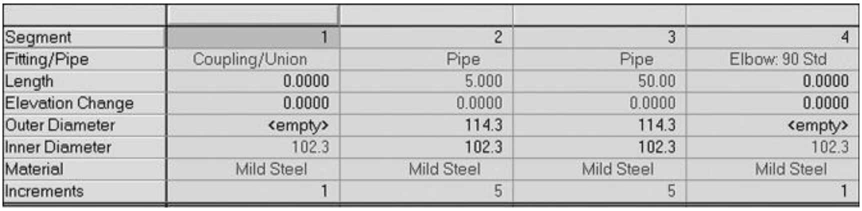
$$W_p = 234\,\text{m}^2/\text{s}^2$$

$$\text{Brake kW} = mW_p = (5 \times 10^{-3}\,\text{m}^3/\text{s})(998\,\text{kg/m}^3)\left(234\,\text{m}^2/\text{s}^2\right)\left(\frac{1\,\text{kJ}}{1000\,\text{kg}\,\text{m}^2/\text{s}^2}\right) = 1.17\,\text{kW}$$

$$\text{Pump hp} = 1.17\,\text{kW}\frac{1\,\text{hp}}{0.7457\,\text{kW}} = 1.57\,\text{hp}$$

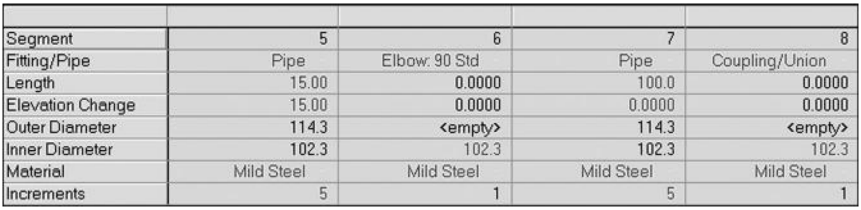
HYSYS SIMULATION

Open a new case in Hysys, select water for component, ASME Steam as fluid package, and then enter simulation environment. Build pipe flow sheet. Double click on feed stream and specify feed stream conditions. Double click on the pipe segment on the object palette, switch to the *Rating* page, and click on the *Append Segment*, and then add pipes and fitting as shown in Figures 2.46 and 2.47.



Segment	1	2	3	4
Fitting/Pipe	Coupling/Union	Pipe	Pipe	Elbow: 90 Std
Length	0.0000	5.000	50.00	0.0000
Elevation Change	0.0000	0.0000	0.0000	0.0000
Outer Diameter	<empty>	114.3	114.3	<empty>
Inner Diameter	102.3	102.3	102.3	102.3
Material	Mild Steel	Mild Steel	Mild Steel	Mild Steel
Increments	1	5	5	1

FIGURE 2.46
Pipe segment specifications for the section from the pipe inlet to the elbow.



Segment	5	6	7	8
Fitting/Pipe	Pipe	Elbow: 90 Std	Pipe	Coupling/Union
Length	15.00	0.0000	100.0	0.0000
Elevation Change	15.00	0.0000	0.0000	0.0000
Outer Diameter	114.3	<empty>	114.3	<empty>
Inner Diameter	102.3	102.3	102.3	102.3
Material	Mild Steel	Mild Steel	Mild Steel	Mild Steel
Increments	5	1	5	1

FIGURE 2.47
Pipe segment specifications for the section from elbow to exit of the pipe.

Click on the *Design* tab, and then *Parameters*, to find the pressure drop across the pipe (Figure 2.48). The pump horsepower (hp) required is shown in Figure 2.49.

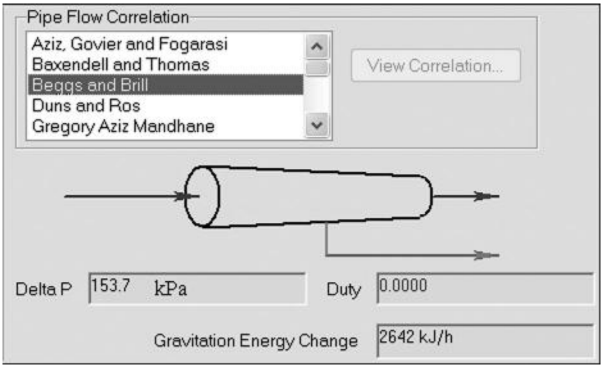
The PFD with set logical operator is shown in Figure 2.50.

SIMULATION WITH PRO/II

Build the process flow sheet shown in Figure 2.51 using PRO/II. Double click on stream S1 to enter inlet stream conditions (temperature, pressure, total flow rate, and molar composition). Double click on the pipe segment and specify the pipe nominal size, length, roughness, elevation, and fitting *K* factor (Figure 2.52). Double click on the pump and enter the outlet pressure which is equal to the feed pressure (stream S1) so as to maintain zero pressure drops in the system as shown in Figure 2.53. Run the system and generate the output report as shown in Figure 2.54.

ASPEN SIMULATION

Follow the same procedure shown in the previous example for constructing the process flow sheet using Aspen. Specify feed stream conditions. Double click on pipe segment and set the pipe rise to 15 m. The pump exit pressure should be defined as the pipe inlet pressure (506.3 kPa) to overcome the pressure drop in the pipeline. The Aspen process flow sheet and stream table are shown in Figure 2.55. The pump brake hp is shown in Figure 2.56.

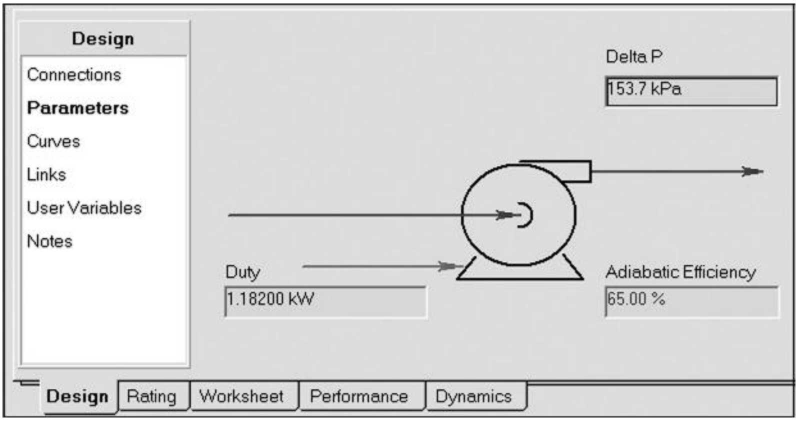


Delta P 153.7 kPa

Duty 0.0000

Gravitation Energy Change 2642 kJ/h

FIGURE 2.48
Pressure drop across the pipe.

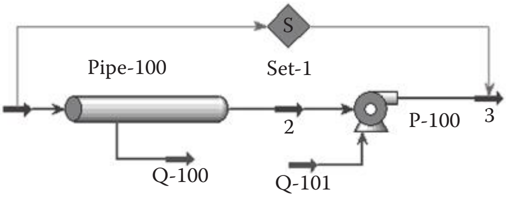


Delta P: 153.7 kPa

Duty: 1.18200 kW

Adiabatic Efficiency: 65.00 %

FIGURE 2.49
Pump hp required.



Streams				
		1	2	3
Temperature	C	20.00	20.00	20.02
Pressure	kPa	506.6	352.9	506.6
Mass flow	kg/h	1.796e + 004	1.796e + 004	1.796e + 004
Comp mass frac (H_2O)		1.0000	1.0000	1.0000

FIGURE 2.50
Process flow sheet of Example 2.5 generated with Hysys.

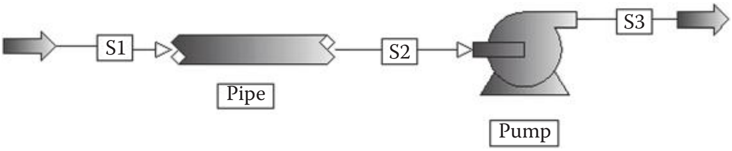
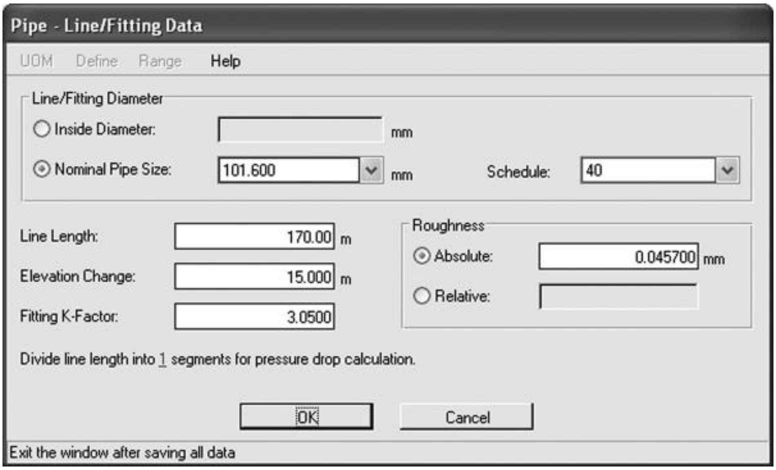


FIGURE 2.51
PFD of Example 2.5 constructed with PRO/II.



Line/Fitting Diameter

○ Inside Diameter: mm

● Nominal Pipe Size: 101.600 mm Schedule: 40

Line Length: 170.00 m

Elevation Change: 15.000 m

Fitting K-Factor: 3.0500

Roughness

● Absolute: 0.045700 mm

○ Relative:

Divide line length into 1 segments for pressure drop calculation.

Exit the window after saving all data

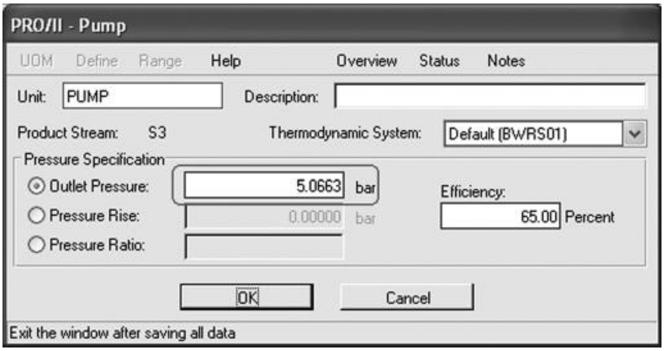
FIGURE 2.52
Pipe line/fitting data of Example 2.5.

Conclusions

Pump brake power was calculated using three methods; with hand calculation the brake power is 1.57 hp, Hysys value is 1.58 hp, PRO/II result is 1.1859 kW (1.589 hp), and Aspen Plus result is 1.585 hp. Al results were almost the same.

Example 2.6: Pressure Drop through Pipeline and Fitting

Water at 25°C (density 1000 kg/m^3) and 2.5 atm pressure is being transferred with a 2 hp pump that is 75% efficient at a rate of 15 m^3/h. All the piping is 4 in. Schedule 40 mild steel pipe except for the last section, which is a 2-in. Schedule 40 steel pipe. There are three 4-in. nominal diameter standard 90° elbows and



Unit: PUMP Description:

Product Stream: S3 Thermodynamic System: Default (BWRS01)

Pressure Specification

● Outlet Pressure: 5.0663 bar

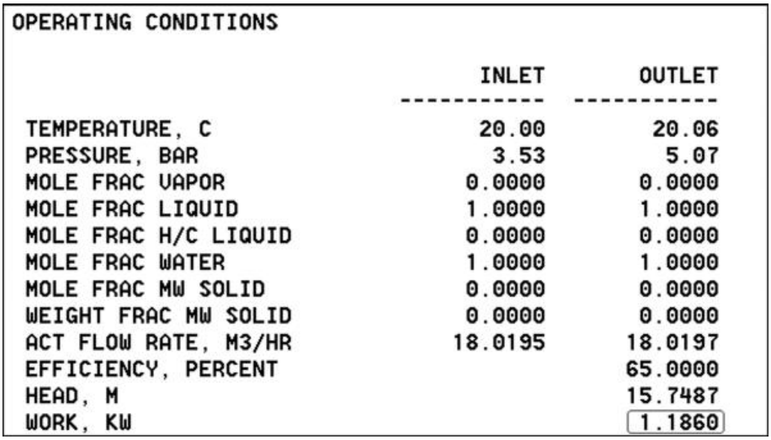
○ Pressure Rise: 0.00000 bar

○ Pressure Ratio:

Efficiency: 65.00 Percent

Exit the window after saving all data

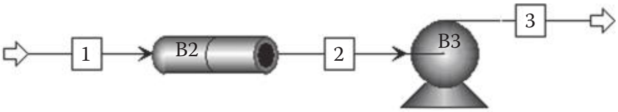
FIGURE 2.53
Pump exit pressure and percent efficiency specified.



```
OPERATING CONDITIONS

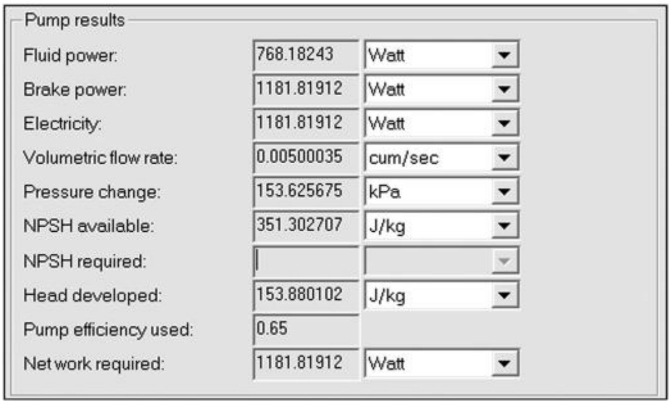
                                    INLET        OUTLET
                                 -----------  -----------
 TEMPERATURE, C                        20.00        20.06
 PRESSURE, BAR                          3.53         5.07
 MOLE FRAC VAPOR                      0.0000       0.0000
 MOLE FRAC LIQUID                     1.0000       1.0000
 MOLE FRAC H/C LIQUID                 0.0000       0.0000
 MOLE FRAC WATER                      1.0000       1.0000
 MOLE FRAC MW SOLID                   0.0000       0.0000
 WEIGHT FRAC MW SOLID                 0.0000       0.0000
 ACT FLOW RATE, M3/HR                18.0195      18.0197
 EFFICIENCY, PERCENT                              65.0000
 HEAD, M                                          15.7487
 WORK, KW                                          1.1860
```

FIGURE 2.54
Pump calculated horsepower generated with PRO/II for Example 2.5.



Example 2.5			
Stream ID		1	2
Temperature	C	20.0	20.0
Pressure	kPa	506.63	353.00
Vapor frac		0.000	0.000
Mole flow	kmol/s	0.277	0.277
Mass flow	kg/s	4.992	4.992
Volume flow	cum/s	0.005	0.005
Enthalpy	MMBtu/h	–270.594	–270.597
Mass flow	kg/s		
Water		4.992	4.992
Mass frac			
Water		1.000	1.000

FIGURE 2.55
Process flow sheet and stream table of Example 2.5.



Pump results

Fluid power:	768.18243	Watt
Brake power:	1181.81912	Watt
Electricity:	1181.81912	Watt
Volumetric flow rate:	0.00500035	cum/sec
Pressure change:	153.625675	kPa
NPSH available:	351.302707	J/kg
NPSH required:		
Head developed:	153.880102	J/kg
Pump efficiency used:	0.65	
Net work required:	1181.81912	Watt

FIGURE 2.56
Pump brake power of Example 2.5.

one reducer to connect the 2 in. pipe (Figure 2.57). Calculate the pressure drop across the system.

SOLUTION

HAND CALCULATION

The average density of water is 1000 kg/m^3 and the average viscosity of water is 0.001 kg/(m s). The pipe line consists of two piping diameters:

a. ID = 102.3 mm, OD = 114.3 mm (4 in. Schedule 40).
b. ID = 52.50 mm, OD = 60.33 mm (2 in. Schedule 40).

For the mild steel pipe, the roughness, ε, is 4.57×10^{-5} m

$$V_1 = \frac{Q}{A_1} = \frac{Q}{\pi D_1^2/4} = \frac{(15\ \text{m}^3/\text{h})(\text{h}/3600\ \text{s})}{\pi(0.1023\ \text{m})^2/4} = 0.507\ \text{m/s}$$

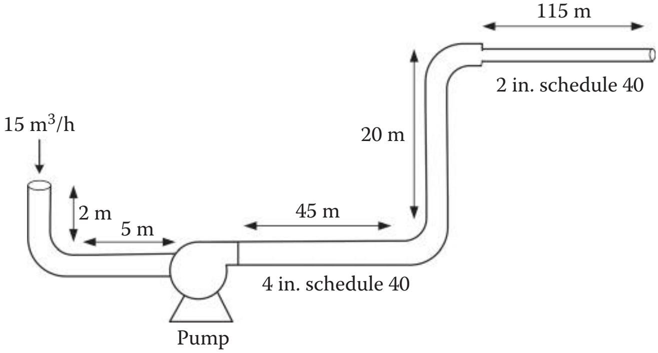


FIGURE 2.57
PFD for Example 2.6.

Reynolds number for the 4 in. Schedule 40 pipe,

$$\mathrm{Re}_1 = \frac{\rho V_1 D_1}{\mu} = \frac{(1000\ \mathrm{kg/m^3})(0.507\ \mathrm{m/s})(0.1023\ \mathrm{m})}{0.001\,\mathrm{kg/m.s}} = 5.2 \times 10^4$$

The relative roughness for the 4 in. Schedule 40 pipe,

$$\frac{\varepsilon}{D_1} = \frac{4.57 \times 10^{-5}\,\mathrm{m}}{0.1023\,\mathrm{m}} = 4.47 \times 10^{-4}$$

Using the Moody chart (Figure 2.2),

$$\mathrm{f}_1 = 0.022$$

The average velocity for the 2 in. Schedule 40 pipe is

$$V_2 = \frac{Q}{A_2} = \frac{Q}{\pi D_2{}^2/4} = \frac{(15\ \mathrm{m^3/h})(\mathrm{h}/3600\ \mathrm{s})}{\pi(0.0.0525\ \mathrm{m})^2/4} = 1.93\ \mathrm{m/s}$$

Reynolds number for the 2 in. Schedule 40 pipe is

$$\mathrm{Re}_2 = \frac{\rho V_2 D_2}{\mu} = \frac{(1000\ \mathrm{kg/m^3})(1.93\ \mathrm{m/s})(0.0525\ \mathrm{m})}{0.001\,\mathrm{kg/m\cdot s}} = 1.0 \times 10^4$$

Relative roughness of the in. Schedule 40 pipe is

$$\frac{\varepsilon}{D_2} = \frac{4.57 \times 10^{-5}\,\mathrm{m}}{0.0525\,\mathrm{m}} = 8.7 \times 10^{-4}$$

Using the Moody chart (Figure 2.2)

$$\mathrm{f}_2 = 0.028$$

Friction loss in the line before the pump, ΣF_1: There is 1 elbow 90° in this segment

Friction loss

$$\Sigma F_1 = f_1 \frac{L_1}{D_1}\frac{V_1^2}{2} + K_\mathrm{e}\frac{V_1^2}{2}$$

Substituting values,

$$\Sigma F_1 = (0.022)\frac{(7\,\mathrm{m})}{0.1023\mathrm{m}}\frac{(0.507\,\mathrm{m/s})^2}{2} + (0.75)\frac{(0.507\,\mathrm{m/s})^2}{2} = 0.19\ \mathrm{m^2/s^2} + 0.096\ \mathrm{m^2/s^2}$$

$$= 0.29\ \mathrm{m^2/s^2}$$

Pressure drop for the line before the pump is

$$\Delta P_1 = \rho\left[g(z_2 - z_1) + \frac{V_2^2 - V_1^2}{2} + \Sigma F_1\right]$$

$$= \left(1000\text{ kg/m}^3\right)\left[\left(9.806\text{ m/s}^2\right)(0\text{ m} - 2\text{ m}) + \frac{(0.507\text{ m/s})^2 - (0.507\text{ m/s})^2}{2} + 0.29\text{ m/s}^2\right]$$

$$= 1000\text{ kg/m}^3(-19.61 + 0 + 0.29)\text{ m}^2/\text{s}^2 = -19320\text{ kg/m s}^2$$

$$= -19320\text{ kg/m s}^2\left(\frac{N}{\text{kg m/s}^2}\right)\left(\frac{1\text{Pa}}{1N/\text{m}^2}\right)\left(\frac{1\text{kPa}}{1000\text{Pa}}\right) = -19.30\text{ kPa}$$

Friction loss in the line after the pump, ΣF_2: In this line segment there are two different pipes (4 in. and 2 in. diameter); consequently, two velocities. There are also two 90° elbows and one sudden contraction joining the two pipes.

$$\Sigma F_2 = 4f_2\frac{L_3}{D_2}\frac{V_2^2}{2} + 2K_e\frac{V_1^2}{2} + K_c\frac{V_2^2}{2}$$

Contraction loss

$$K_c = 0.55\left(1 - \frac{A_2}{A_1}\right) = 0.55\left(1 - \frac{\pi D_2^2/4}{\pi D_1^2/4}\right) = 0.55\left(1 - \frac{D_2^2}{D_1^2}\right)$$

$$= 0.55\left(1 - \frac{(0.0525\text{ m})^2}{(0.1023\text{ m})^2}\right) = 0.405$$

$$\Sigma F_2 = (0.022)\frac{(65\text{ m})}{0.1023\text{ m}}\frac{(0.507\text{ m/s})_1^2}{2} + (0.028)\frac{(115\text{ m})}{0.0525}\frac{(1.93\text{ m/s})^2}{2}$$

$$+2(0.75)\frac{(0.507\text{ m/s})^2}{2} + (0.405)\frac{(1.93\text{ m/s})^2}{2}$$

Solving for ΣF_2:

$$\Sigma F_2 = (1.6 + 114.2 + 0.19 + 0.754)\text{ m}^2/\text{s}^2 = 116\text{ m}^2/\text{s}^2$$

Pressure drop in the line after the pump

$$\Delta P_2 = \rho\left[g(z_2 - z_1) + \frac{V_2^2 - V_1^2}{2} + \Sigma F\right]$$

Substituting required values

$$\Delta P_2 = \left(1000\ \text{kg/m}^3\right)\left[\left(9.806\ \text{m/s}^2\right)(20\ \text{m} - 2\ \text{m}) + \frac{(1.93\ \text{m/s})^2 - (0.507\ \text{m/s})^2}{2} + 116\ \text{m}^2/\text{s}^2\right]$$

$$= 1000\ \text{kg/m}^3\left(176.51 + 1.73 + 116\ \text{m}^2/\text{s}^2\right) = 294{,}000\ \text{kg/ms}^2$$

The pressure drop in the second pipe segment in kPa is

$$\Delta P_2 = 2.94 \times 10^5\ \text{kg/ms}^2\left(\frac{N}{\text{kgm/s}}\right)\left(\frac{1\,\text{Pa}}{1N/\text{m}^2}\right)\left(\frac{1\,\text{kPa}}{1000\ \text{Pa}}\right) = 294\ \text{kPa}$$

The mass flow rate in kg/s

$$m = \rho Q = \left(1000\ \text{kg/m}^3\right)\left(15\ \text{m/h}\right)\left(\frac{1\,\text{h}}{3600\ \text{s}}\right) = 4.17\ \text{kg/s}$$

The shaft work

$$W_s = \frac{-\eta W_p}{\dot{m}} = -0.75(2\ \text{hp})\left(\frac{0.7457\ \text{kW}}{1\,\text{hp}}\right)\left(\frac{1\,\text{kJ/s}}{1\,\text{kW}}\right)\left(\frac{1000\ \text{Nm}}{1\,\text{kJ}}\right)\left(\frac{1\,\text{kg m/s}^2}{1\,\text{N}}\right)\Big/ 4.17\ \text{kg/s}$$

$$= \frac{-\eta W_p}{\dot{m}} = -268.4\ \text{m}^2/\text{s}^2$$

Pump pressure rise, $\Delta\ P_p$

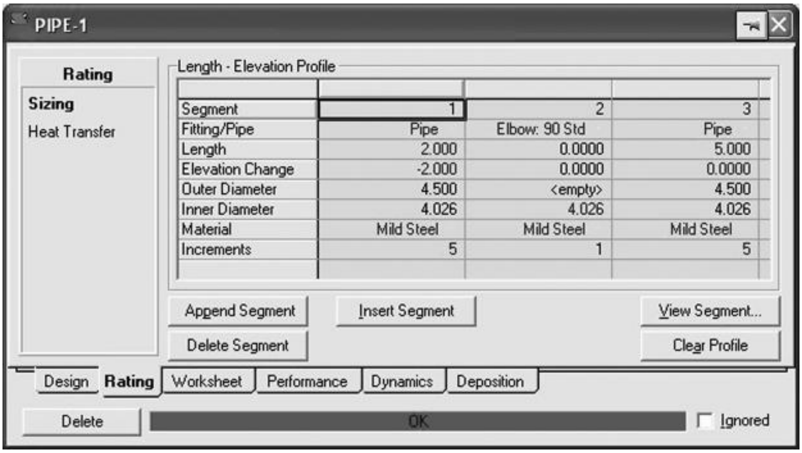
$$\Delta P_p = \rho W_s = \left(\frac{1000\ \text{kg}}{\text{m}^3}\right)\left(\frac{268.4\ \text{m}^2}{\text{s}^2}\right)\left(\frac{1\,\text{kPa}}{1000\ \cancel{N}/\text{m}^2}\right)\left(\frac{1\,\cancel{N}}{1\,\text{kg m/s}^2}\right) = 268.4\ \text{kPa}$$

The negative sign is just because the calculated pressure drop was inlet minus exit. However, across the pump, pressure always increased.

HYSYS SIMULATION

Open a new case in Hysys. Add water as the pure component, and select ASME steam for the fluid package. Construct the pipe process flow sheet and specify the feed stream conditions. Double click on *Pipe Segment* on the process flow sheet, click on the *Rating* tab, and then click on *Append Segment* to add the pipe specification (length, nominal size, elevation, and fittings) as shown in Figures 2.58 and 2.59.

While on the design page, click on *Parameters* to enter the pressure drop in the line before the pump (pressure drop = –19.3 kPa). The negative sign indicates the pressure rise due to the negative elevation of first pipe segment.



Segment	1	2	3
Fitting/Pipe	Pipe	Elbow: 90 Std	Pipe
Length	2.000	0.0000	5.000
Elevation Change	-2.000	0.0000	0.0000
Outer Diameter	4.500	<empty>	4.500
Inner Diameter	4.026	4.026	4.026
Material	Mild Steel	Mild Steel	Mild Steel
Increments	5	1	5

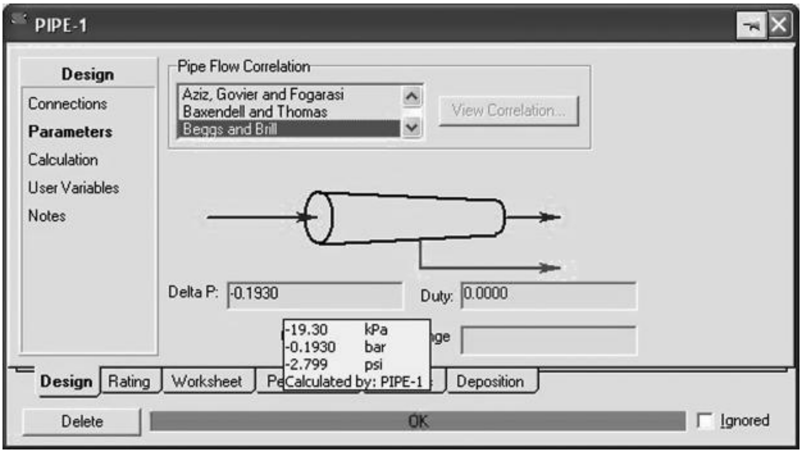
FIGURE 2.58
The first pipe segment conditions.

Add a new pipe segment to specify the line after the pump, while on the rating page, click on *Append Segment* and enter the data shown in Figure 2.60.

Double click on the pump segment in the flow sheet area and while the *Design* page is open, click on *Parameters*, and specify the pressure drop as shown in Figure 2.61.

While in the design page click on *Parameter* and type 2.0 hp in the Duty cell.

The pressure rise across the pump is 268.2 kPa as shown in Figure 2.62. The final flow sheet should appear as that shown in Figure 2.63.

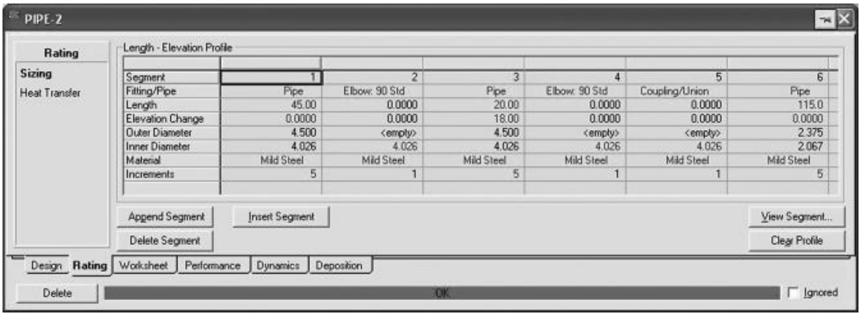


Delta P: -0.1930

Duty: 0.0000

-19.30 kPa
-0.1930 bar
-2.799 psi
Calculated by: PIPE-1

FIGURE 2.59
Pressure drop across the first pipe segment.



Segment	1	2	3	4	5	6
Fitting/Pipe	Pipe	Elbow: 90 Std	Pipe	Elbow: 90 Std	Coupling/Union	Pipe
Length	45.00	0.0000	20.00	0.0000	0.0000	115.0
Elevation Change	0.0000	0.0000	18.00	0.0000	0.0000	0.0000
Outer Diameter	4.500	<empty>	4.500	<empty>	<empty>	2.375
Inner Diameter	4.026	4.026	4.026	4.026	4.026	2.067
Material	Mild Steel	Mild Steel	Mild Steel	Mild Steel	Mild Steel	Mild Steel
Increments	5	1	5	1	1	5

FIGURE 2.60
Pipe specifications for line after the pump.

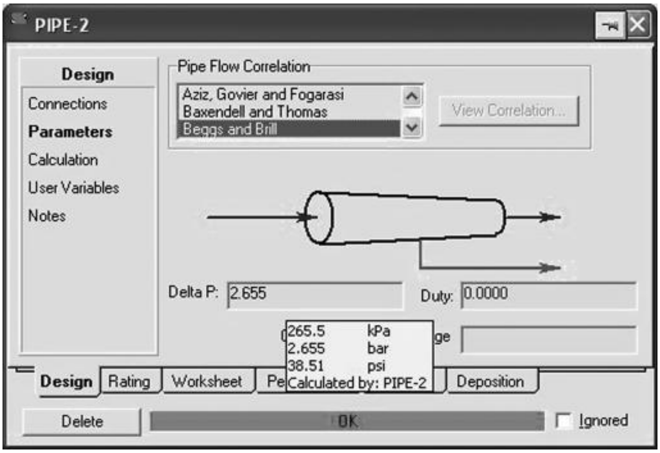
Simulation with PRO/II

In PRO/II; there should be one pipe segment for each change in diameter, length, height, and fitting *K* factors as shown in Figure 2.64.

The stream conditions are shown in Figure 2.65.

Aspen Simulation

Using Aspen, a procedure similar to that used in PRO/II is applied as shown in Figure 2.66. In the first pipe segment, specify the *Pipe length* as 2 m, the *Pipe rise* as –2 m. In the second pipe segment, the length is 5 m, elevation is zero, and fitting is one 90° elbow. For the pump, set the power required to 2 hp. The length of the third pipe is 45 m and that of the fourth pipe is 20 m. The pipe rise is also 20 m and the number of *90° elbows* is 2. For the fifth pipe, the length is 115 m, elevation is zero, and pipe nominal size is 2 in. Schedule 40. Click on the *Thermal Specification* tab and select *Adiabatic*. The Aspen process flow sheet and the stream table is shown in Figure 2.66.

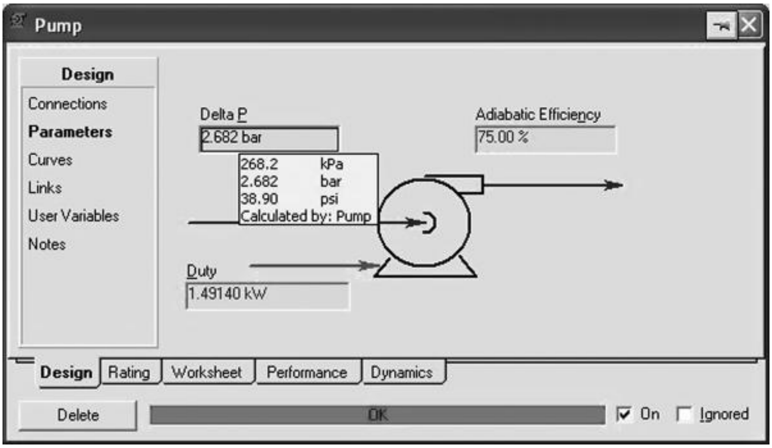


Delta P: 2.655

Duty: 0.0000

265.5 kPa
2.655 bar
38.51 psi
Calculated by: PIPE-2

FIGURE 2.61
Pressure drop the pipe segment.



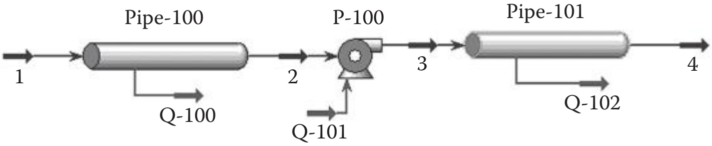
Delta P: 2.682 bar

268.2 kPa
2.682 bar
38.90 psi
Calculated by: Pump

Adiabatic Efficiency: 75.00 %

Duty: 1.49140 kW

FIGURE 2.62
Duty of the pump is 2 hp (1.49140 kW) at 75% adiabatic efficiency.



Streams					
		1	2	3	4
Temperature	C	25.00	25.00	25.01	25.03
Pressure	kPa	253.3	272.7	541.0	237.3
Mass flow	kg/h	18000.00	18000.00	18000.00	18000.00
Comp mass frac (H_2O)		1.0000	1.0000	1.0000	1.0000

FIGURE 2.63
Process flow sheet of Example 2.6 with Hysys.

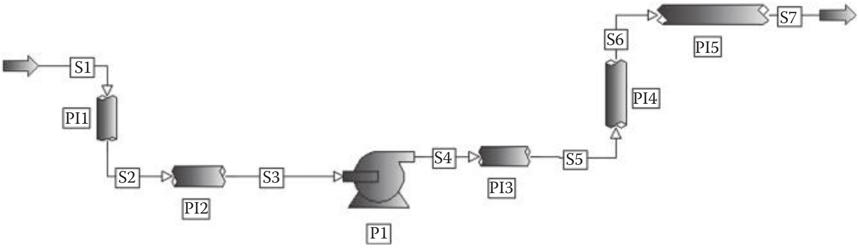


FIGURE 2.64
Process flow sheet of Example 2.6 with provision.

Stream name stream description		S1	S2	S3	S4	S5	S6	S7
Phase		Water	Water	Water	Water	Water	Water	Water
Temperature	F	77.000	77.001	77.001	77.048	77.050	77.044	77.078
Pressure	psia	36.740	39.554	39.534	78.434	77.846	49.371	36.628
Flowrate	lb-mol/h	1833.819	1833.819	1833.819	1833.819	1833.819	1833.819	1833.819
Composition Water		1.000	1.000	1.000	1.000	1.000	1.000	1.000

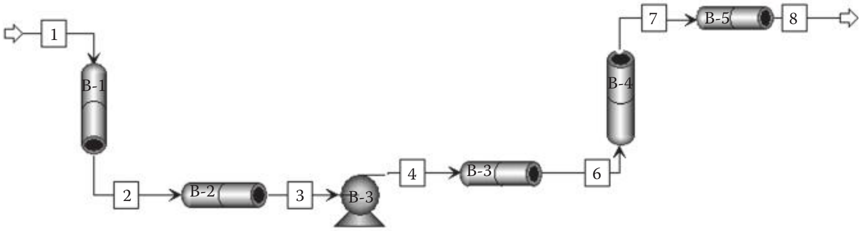
FIGURE 2.65
Stream specifications with PRO/II.

CONCLUSIONS

The pressure rise across the pump using hand calculation is 268.4 kPa, Hysys is 268.2 kPa, PRO/II is 268.1 kPa, and Aspen Plus is 268.46 kPa and all values were in good agreement.

2.2 Fluid Flow in Pumps

Pumps are used to move liquids in a closed conduit or pipe. The pump increases the pressure of the liquid.



Example 2.6								
Stream ID		1	2	3	4	6	7	8
Temperature	C	25.0	25.0	25.0	25.0	25.0	25.0	25.0
Pressure	kPa	253.31	272.64	272.46	540.92	539.61	343.40	255.95
Vapor frac		0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mole flow	kmol/s	0.231	0.231	0.231	0.231	0.231	0.231	0.231
Mass flow	kg/s	4.155	4.155	4.155	4.155	4.155	4.155	4.155
Volume flow	cum/s	0.004	0.004	0.004	0.004	0.004	0.004	0.004
Enthalpy	MMBtu/h	−224.912	−224.911	−224.911	−224.906	−224.906	−224.909	−224.909
Mass flow	kg/s							
Water		4.155	4.155	4.155	4.155	4.155	4.155	4.155
Mass frac								
Water		1.000	1.000	1.000	1.000	1.000	1.000	1.000

FIGURE 2.66
Process flow sheet and stream table of Example 2.6 with Aspen.

2.2.1 Power and Work Required

Using mechanical energy balance equation around the pump system, the actual or theoretical mechanical energy W_S (kJ/kg) added to fluid by the pump can be calculated. If η is the fractional efficiency and W_p the shaft work delivered to the pump,

$$W_p = -\frac{W_s}{\eta} \tag{2.16}$$

$$W_s = -\frac{P_b - P_a}{\rho} \tag{2.17}$$

$$\text{Brake power kW} = mW_p = -\frac{mW_s}{\eta} \tag{2.18}$$

The mechanical energy W_S in kJ/kg added to the fluid is often expressed as the developed head H of the pump in meters of fluid being pumped, where

$$-W_s = Hg \tag{2.19}$$

the head is

$$H = \frac{\Delta P_L}{\rho g} = \frac{32\mu LV}{\rho g D^2} \tag{2.20}$$

2.3 Fluid Flow in Compressors

In compressors and blowers, pressure changes are large and also the compressible flow occurs. In compression of gases the density changes and so the mechanical energy balance equation must be written in differential form and then integrated to obtain the work of compression.

$$dW = \frac{dp}{\rho} \tag{2.21}$$

Integration between the suction pressure P_1 and discharge pressure P_2 gives the work of compression.

$$W = \int_{P_1}^{P_2} \frac{dp}{\rho} \tag{2.22}$$

For adiabatic compression, the fluid follows an isentropic path and

$$\frac{P_1}{P} = \left(\frac{\rho_1}{\rho}\right)^{\gamma} \tag{2.23}$$

where the ratio of heat capacities, $\gamma = C_p/C_v$,

$$-W_s = \frac{\gamma}{\gamma - 1}\frac{RT_1}{M}\left[\left(\frac{P_2}{P_1}\right)^{(\gamma-1)/\gamma} - 1\right] \tag{2.24}$$

The adiabatic temperatures are related by

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{(\gamma-1)/\gamma} \tag{2.25}$$

The brake power

$$\text{Brake kW} = \frac{-W_s\,\text{m}}{\eta} \tag{2.26}$$

Example 2.7: Flow through Pump

Pure water is fed at a rate of 100 lb/h into a pump at 250°F, 44.7 psia. The exit pressure is 1200 psig. Use the pump module in HYSYS, PRO/II, and Aspen programs to model the pumping process. The pump adiabatic efficiency is 10%. Find the energy required.

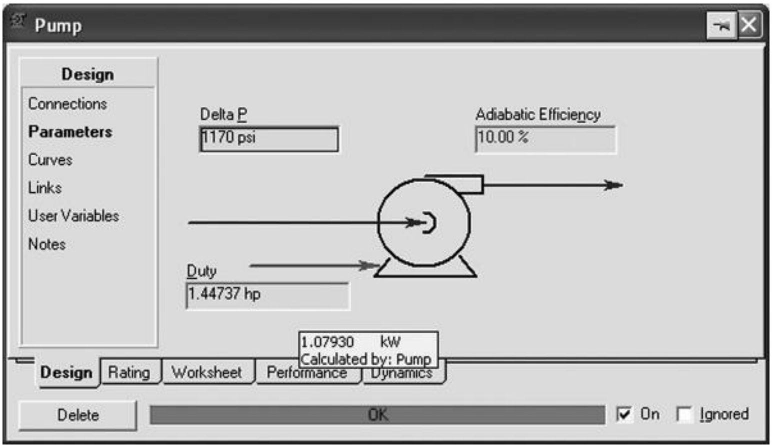
SOLUTION

HAND CALCULATION

$$-W_s = \frac{(P_1 - P_2)}{\rho} = \frac{((1200 + 14.7) - 44.7)}{58.9\ \text{lb/ft}^3}\text{lb}_\text{f}/\text{in}^2\ 144\,\text{in}^2/\text{ft}^2 = 2860.44\ \text{lb}_\text{f}\ \text{ft/lb}$$

The density of water at 250°F is 58.9 $\text{lb}_\text{f}/\text{ft}^3$, the horsepower for 10% efficiency pump:

$$W_p = \frac{-W_s \times \dot{m}}{\eta} = \frac{1}{0.1}(2860.44\ \text{lb}_\text{f}\text{ft/lb})(100\ \text{lb/h})\left(\frac{1\,\text{h}}{3600\ \text{s}}\right)\left(\frac{1\,\text{hp}}{550\,\text{lb}_\text{f}.\text{ft/s}}\right) = 1.445\ \text{hp}$$



Delta P: 1170 psi

Adiabatic Efficiency: 10.00 %

Duty: 1.44737 hp

1.07930 kW
Calculated by: Pump

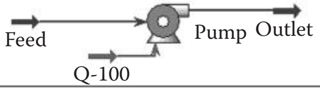
FIGURE 2.67
Specifying of pump adiabatic efficiency.

Simulation with Hysys

Open a new case in Hysys and then perform process flow sheet of the pump with inlet, exit, and the red color energy stream connected to the pump. Specify the feed stream conditions and exit stream pressure to 1200 psig. Click on the *Design* tab, and then click on *Parameters*. In the *Adiabatic Efficiency* box on the parameter page, enter 10. Click on the *Worksheet* tab to view the results as in Figure 2.67.

Click the *Workbook* icon in the toolbar. The *Workbook* appears. From the workbook menu click on *Setup*. Once the setup view appears, click on *Add* in the Workbook Tabs group and select the variable that should appear in the table. Right click on the PFD area below the PFD and click on *Add Workbook Table*. The stream conditions for the pump are shown in Figure 2.68.

The new outlet temperature of the water is 283.9°F for the 10% efficient pump. Hand calculations and Hysys results are not different from each other.



Streams			
		Feed	Outlet
Temperature	C	121.1	140.0
Pressure	kPa	308.2	8375
Mass flow	kg/h	45.36	45.36
Comp mass frac (H_2O)		1.0000	1.0000

FIGURE 2.68
Converged stream conditions.

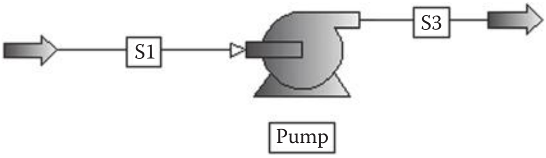


FIGURE 2.69
PFD of Example 2.7.

Simulation with PRO/II

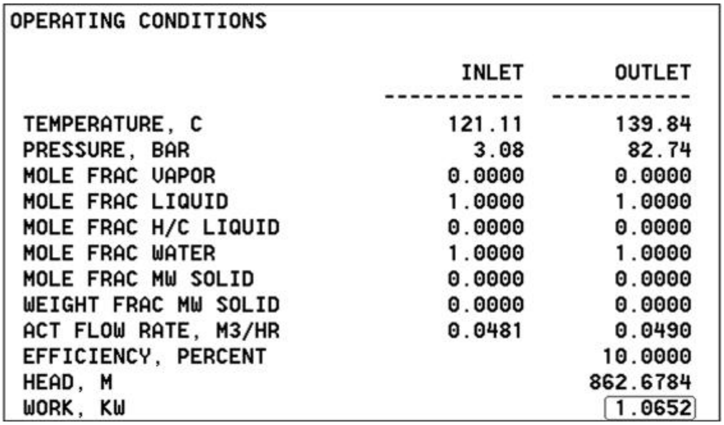
Using PRO/II, add water as the pure component. For fluid package select PRSV or PR. Perform the pump process flow sheet. Specify the feed stream conditions. The pump exit pressure is 1200 psig (Figure 2.69). Run the system and generate the output report; it should appear as in Figure 2.70.

Aspen Simulation

Aspen is used to construct the pump process flow sheet shown in Figure 2.71. Add pure water as the only component. Click on *Physical Property* in the toolbar, and select *Stream-TA* as the base method. Double click on the feed stream and specify inlet stream conditions (temperature, pressure, total flow rate, and composition). Double click on the pump icon and set the *Discharge Pressure* to 1200 psig and the pump efficiency to 0.1. Note that in the status bar, the message "*Required Input Completed*" means that the system is ready to be run. Click *Run* after the message run is successfully completed, click on results, and then click on block results. The process flow sheet and the stream table are shown in Figure 2.71. The brake power of the pump is shown in Figure 2.72.

Conclusions

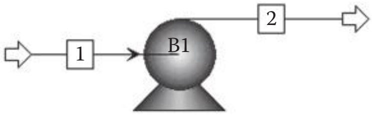
This example shows that pumping liquid can increase its temperature and pressure. In this case, the pump was only 10% efficient and it caused 15°F in the



```
OPERATING CONDITIONS

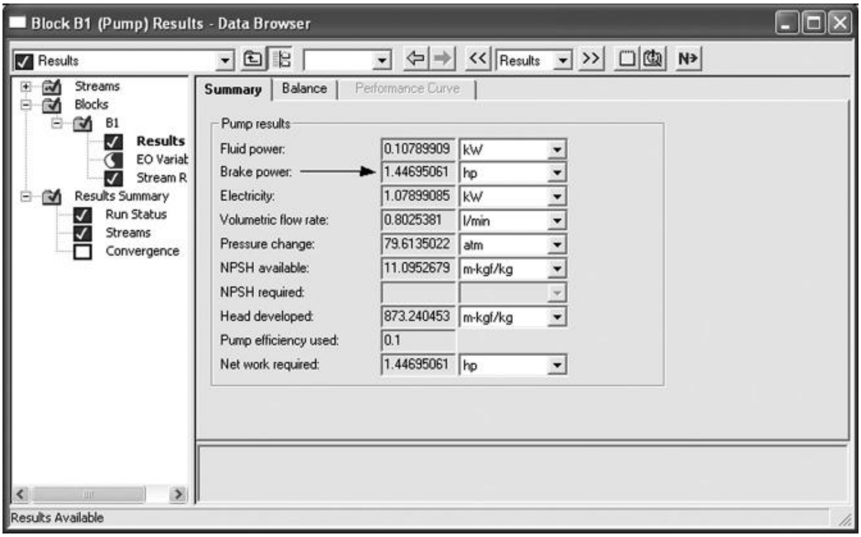
                                   INLET        OUTLET
                                -----------  -----------
 TEMPERATURE, C                     121.11       139.84
 PRESSURE, BAR                        3.08        82.74
 MOLE FRAC VAPOR                    0.0000       0.0000
 MOLE FRAC LIQUID                   1.0000       1.0000
 MOLE FRAC H/C LIQUID               0.0000       0.0000
 MOLE FRAC WATER                    1.0000       1.0000
 MOLE FRAC MW SOLID                 0.0000       0.0000
 WEIGHT FRAC MW SOLID               0.0000       0.0000
 ACT FLOW RATE, M3/HR               0.0481       0.0490
 EFFICIENCY, PERCENT                            10.0000
 HEAD, M                                       862.6784
 WORK, KW                                        1.0652
```

FIGURE 2.70
Pump required work for Example 2.7.



Example 2.7			
Stream ID		1	2
Temperature	K	394.3	413.1
Pressure	atm	3.04	82.66
Vapor frac		0.000	0.000
Mole flow	kmol/h	2.518	2.518
Mass flow	kg/h	45.359	45.359
Volume flow	L/min	0.803	0.813
Enthalpy	MMBtu/h	–0.665	–0.661
Mole flow	kmol/h		
Water		2.518	2.518

FIGURE 2.71
Process flow sheet and stream table of Example 2.7.



Pump results

Fluid power: 0.10789909 kW

Brake power: 1.44695061 hp

Electricity: 1.07899085 kW

Volumetric flow rate: 0.8025381 l/min

Pressure change: 79.6135022 atm

NPSH available: 11.0952679 m-kgf/kg

NPSH required:

Head developed: 873.240453 m-kgf/kg

Pump efficiency used: 0.1

Net work required: 1.44695061 hp

FIGURE 2.72
The pump results generated by Aspen.

temperature of the water. The less efficient a pump is, the greater is the increase in the temperature of the fluid being pumped. This is attributed to the reason that in a low-efficiency pump, more energy is needed to pump the liquid to get the same outlet pressure of a more efficient pump. So, extra energy gets transferred to the fluid. The brake power calculated by hand calculation, Hysys, PRO/II, and Aspen is 1.45, 1.45, 1.43, and 1.45 hp, respectively. Results were close to each other.

Example 2.8: Compression of Natural Gas

A compressor is used to compress 100 kg/h of natural gas consisting of 80 mol% methane, 10% ethane, 5% carbon dioxide, and the remaining nitrogen from 3 bars and 30°C to 10 bars. Find the compressor duty (brake kW) for 75% and 10% efficiency.

SOLUTION

HAND CALCULATION

The compressor shaft work,

$$-W_s = \frac{\gamma}{\gamma - 1}\frac{RT_1}{M}\left[\left(\frac{P_2}{P_1}\right)^{(\gamma-1)/\gamma} - 1\right]$$

Natural gas average molecular weight (M)

$$M = 0.8(16) + 0.1(30) + 0.05(44) + 0.05(28) = 19.4 \text{ kg/kgmol}$$

Assuming that gas is incompressible,

$$-W_s = \left(\frac{1.31}{1.31-1}\right)\frac{8.3143(\text{kJ/kgmolK})(30 + 273.15)\text{K}}{19.4 \text{ kg/kgmol}}\left[\left(\frac{10}{3}\right)^{(1.31-1)/1.31} - 1\right]$$

The shaft work in kJ/kg

$$-W_s = 181 \text{ kJ/kg}$$

The compressor brake kW,

$$\text{Brake kW} = \frac{-W_s m}{\eta}$$

The brake power for a compressor, 75% adiabatic efficiency,

$$\text{Brake kW} = \frac{(181 \text{ kJ/kg})\left(100 \text{ kg/h}\dfrac{\text{h}}{3600 \text{ s}}\right)}{0.75} = 6.69 \text{ kW}$$

For 10% adiabatic efficiency,

$$\text{Brake kW} = \frac{(181\,\text{kJ/kg})\left(100\,\text{kg/h}\,\dfrac{\text{h}}{3600\,\text{s}}\right)}{0.10} = 50.175\,\text{kW}$$

SIMULATION WITH HYSYS

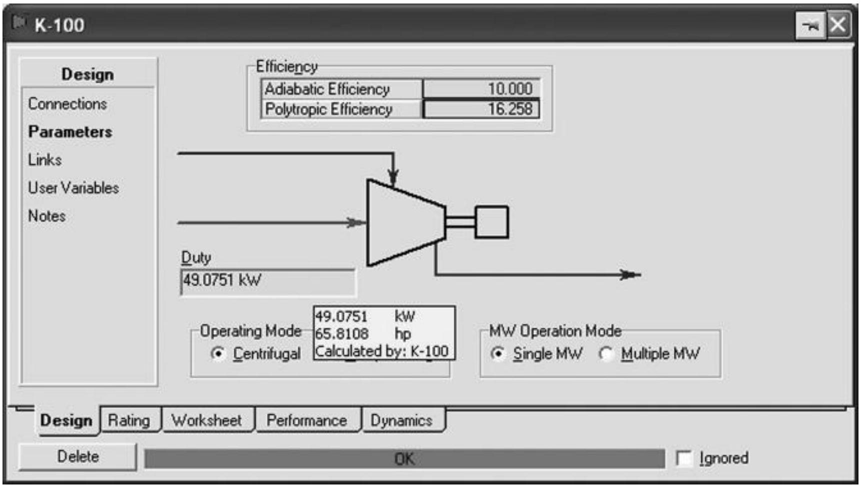
The pump simulation is done by opening a new Hysys case and selecting the components methane, ethane, CO_2, and N_2. PRSV is selected as the property estimation method. The basis of calculation is assumed as 100 kg/h of natural gas stream. Select a compressor from the object palette and specify the stream conditions and keep the Hysys default compressor efficiency and then determine the outlet temperature and compressor duty. Neglect the heat loss or gain from the environment. Enter the Pressure for the outlet stream which is 10 bars. Click on the *Design* tab, and then click on *Parameters* and see the Hysys default adiabatic efficiency and calculated Polytropic efficiency. In the *Adiabatic Efficiency* box on the parameter page, enter 10 (Figure 2.73). Click on the *Worksheet* tab to view the results.

Double click on the pump PFD and click on the Worksheet tab. The stream conditions for the pump are shown in Figures 2.74 and 2.75 for 75% and 10% adiabatic efficiency, respectively.

The new outlet temperature is of 652.4°C for the 10% adiabatic efficient and 144.4°C for an adiabatic efficiency of 75%.

SIMULATION WITH PRO/II

Following the same procedure as done previously with PRO/II, construct the process flow sheet shown in Figure 2.76, enter the inlet temperature, pressure, total



Efficiency

Adiabatic Efficiency	10.000
Polytropic Efficiency	16.258

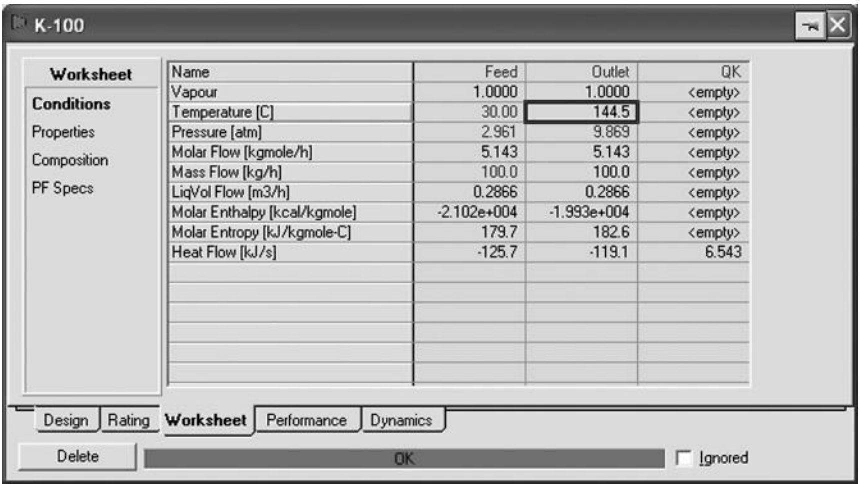
Duty: 49.0751 kW

49.0751 kW
65.8108 hp
Calculated by: K-100

Operating Mode: ● Centrifugal

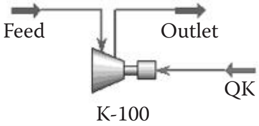
MW Operation Mode: ● Single MW ○ Multiple MW

FIGURE 2.73
Specifying of compressor adiabatic efficiency.



Name	Feed	Outlet	QK
Vapour	1.0000	1.0000	<empty>
Temperature [C]	30.00	144.5	<empty>
Pressure [atm]	2.961	9.869	<empty>
Molar Flow [kgmole/h]	5.143	5.143	<empty>
Mass Flow [kg/h]	100.0	100.0	<empty>
LiqVol Flow [m3/h]	0.2866	0.2866	<empty>
Molar Enthalpy [kcal/kgmole]	-2.102e+004	-1.993e+004	<empty>
Molar Entropy [kJ/kgmole-C]	179.7	182.6	<empty>
Heat Flow [kJ/s]	-125.7	-119.1	6.543

FIGURE 2.74
Conditions of the simulated compressor (75% adiabatic efficiency).



Streams			
		Feed	Outlet
Temperature	C	30.00	652.4
Pressure	kPa	300.0	1000
Mass flow	kg/h	100.0	100.0

FIGURE 2.75
Conditions of the simulated compressor (10% adiabatic efficiency).

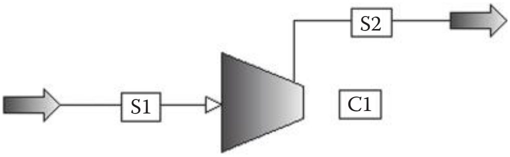


FIGURE 2.76
Compressor process flow sheet.

inlet flow rate, and molar compositions. For 10% efficiency, the results are shown in Figure 2.77.

ASPEN PLUS SIMULATION

Open the Aspen user interface and then click on the *Pressure Changes* tab on the model library and select compressor. Click anywhere in the process flow sheet area. Click on *Material Streams* in the model library and connect inlet and exit stream lines. Click on the arrow on the left of the model library to cancel the insert mode. Click on *Component* on the toolbar, and select methane, ethane, CO_2, and N_2.

Click on *Physical Property* in the toolbar, and select *Peng–Robinson* as the base method. Double click on the feed stream and specify inlet stream conditions (temperature, pressure, total flow rate, and composition). Double click on the *Compressor* icon and set the *Discharge pressure* to 10 bars and the compressor efficiency to 0.10 for the 10% efficiency. Note that in the status bar, the message *Required Input Completed* is displayed, which means that the system is ready to run. Click on run or F5; after the run *is successfully completed* click on results and then click on the block icon in the results menu. The process flow sheet and the stream table are shown in Figure 2.78. The brake power of the 10% efficiency pump is shown in Figure 2.79.

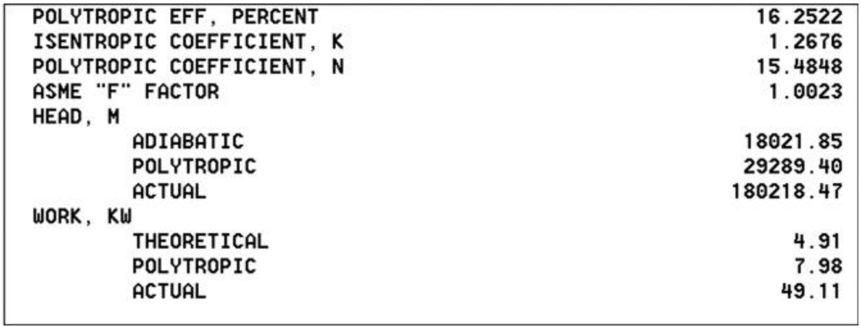
CONCLUSIONS

Results of the actual work of the pump with 10% efficiency with hand calculations are 50 kW; on the contrary, results obtained by Hysys, PRO/II, and Aspen were in good agreement and around 49 kW. The discrepancy in hand calculations is due to the ideal gas assumption.

PROBLEMS

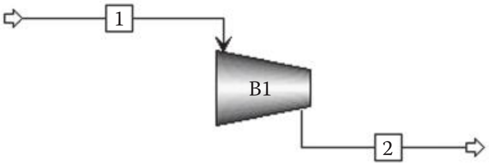
2.1 Pressure Drop through a Smooth Pipe

Water is flowing in a 15 m horizontal smooth pipe at 8 m^3/h and 35°C. The density of water is 998 kg/m^3 and the viscosity of water is 0.8 cP. The pipe is Schedule 40, 1 in. nominal diameter (2.66 cm ID). Water inlet pressure is 2 atm. Calculate the pressure drop.



```
POLYTROPIC EFF, PERCENT                                    16.2522
ISENTROPIC COEFFICIENT, K                                   1.2676
POLYTROPIC COEFFICIENT, N                                  15.4848
ASME "F" FACTOR                                             1.0023
HEAD, M
        ADIABATIC                                         18021.85
        POLYTROPIC                                        29289.40
        ACTUAL                                           180218.47
WORK, KW
        THEORETICAL                                           4.91
        POLYTROPIC                                            7.98
        ACTUAL                                               49.11
```

FIGURE 2.77
Pressure drop for the compressor with 10% efficiency.



Example 2.8			
Stream ID		1	2
Temperature	C	30.0	652.6
Pressure	Bar	3.000	10.000
Vapor frac		1.000	1.000
Mole flow	kmol/h	5.143	5.143
Mass flow	kg/h	100.000	100.000
Volume flow	cum/h	42.889	39.680
Enthalpy	MMkcal/h	–0.108	–0.065
Mole flow	kmol/h		
Methane		4.115	4.115
Ethane		0.514	0.514
CO_2		0.257	0.257
N_2		0.257	0.257

FIGURE 2.78
Process flow sheet and stream table of Example 2.8.

2.2 Pressure Drop in a Horizontal Pipe

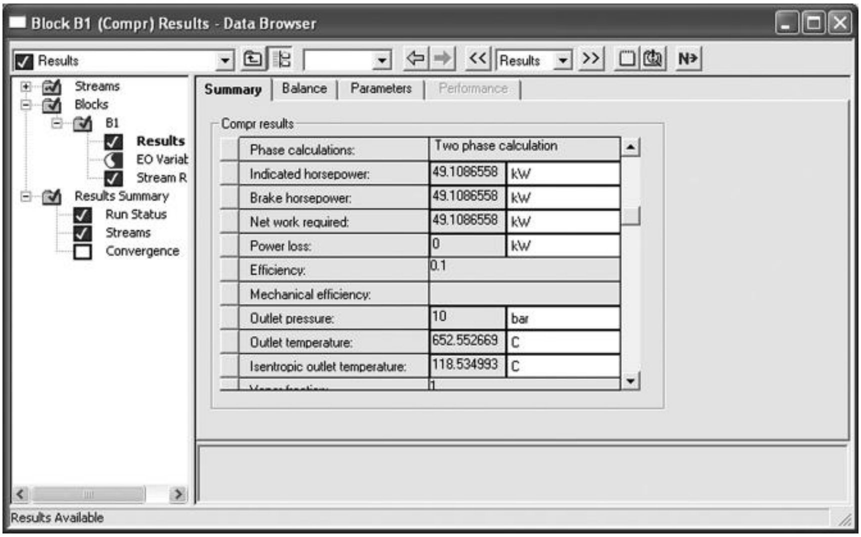
Calculate the pressure drop of water through a 50-m long smooth horizontal pipe. The inlet pressure is 100 kPa, the average fluid velocity is 1 m/s. The pipe diameter is 10 cm and the pipe relative roughness is zero. Fluid density is 1 kg/L and viscosity is 1 cP.

2.3 Pressure Drop in a Pipe with Elevation

Calculate the pressure drop of water through a pipe 50 m long (relative roughness is 0.01 m/m). The inlet pressure is 100 kPa; the average fluid velocity is 1 m/s. The pipe diameter is 10 cm. Fluid density is 1 kg/L and viscosity is 1 cP. The water is discharged at an elevation 2 m higher than water entrance.

2.4 Pumping of Natural Gas in a Pipeline

Natural gas contains 85 mol% methane and 15 mol% ethane is pumped through a horizontal Schedule 40, 6-in-diameter cast-iron pipe at a mass



Compr results

Phase calculations:	Two phase calculation	
Indicated horsepower:	49.1086558	kW
Brake horsepower:	49.1086558	kW
Net work required:	49.1086558	kW
Power loss:	0	kW
Efficiency:	0.1	
Mechanical efficiency:		
Outlet pressure:	10	bar
Outlet temperature:	652.552669	C
Isentropic outlet temperature:	118.534993	C

FIGURE 2.79
Compressor bakes power of Example 2.8.

flow rate of 363 kg/h. If the pressure at the pipe inlet is 3.5 bars and 25°C and the pipe length is 20 km downstream, assume incompressible flow. Calculate the pressure drop across the pipe using Hysys, Aspen Plus, and PRO/II.

2.5 Compression of Gas Mixture

The mass flow rate of a gas stream 100 kg/h of feed contains 60 wt% methane and 40% ethane at 20 bars and 35°C is being compressed to 30 bars (use PR fluid package). Determine the temperature of the exit stream in °C.

2.6 Compression of Nitrogen

Find the compressor horsepower required to compress 100 kmol/h of nitrogen from 1 atm and 25°C to 5 atm.

2.7 Pumping of Pure Water

Pure water is fed at a rate of 100 lb/h into a pump at 250°F, 44.7 psia. The exit pressure is 1200 psig. Plot the pump adiabatic efficiency versus the energy required.

2.8 Pumping of Water to Top of Building

Calculate the size of the pump required to pump 100 kmol/min of pure water at 1 atm and 25°C to the top of a building 12 m high.

References

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3

Material and Energy Balance

At the end of this chapter you should be able to

1. Provide meaningful experience in solving mass balances for physical and chemical processes.
2. Perform energy balance on reactive and nonreactive processes.
3. Verify hand calculation results with Hysys, PRO/II, Aspen, and SuperPro Designer.

3.1 Introduction

Material balances are based on the fundamental law of conservation of mass. In particular, chemical engineers are concerned with doing mass balances around chemical processes. Chemical engineers do a mass balance to account for what happens to each of the chemicals that is used in a chemical process. By accounting for material entering and leaving a system, mass flows can be identified which might have been unknown, or difficult to measure without this technique. Heat transfer is the transition of thermal energy from a hotter mass to a cooler mass. When an object is at a different temperature from its surroundings or another object, transfer of thermal energy (also known as heat flow or heat exchange) occurs in such a way that the heat is transferred until the object and the surroundings reach thermal equilibrium.

3.2 Material Balance without Reaction

To apply a material balance, one needs to define the system and the quantities of interest.

System is a region of space defined by a real or imaginary closed envelope (envelope = system boundary); it can be a single process unit, collection of process units, or an entire process.

The general material balance equation is

$$\begin{Bmatrix}\text{Accumulation within the}\\ \text{system (buildup)}\end{Bmatrix} = \{\text{Input through system boundary}\} \\ -\{\text{Output through system boundary}\} \\ +\{\text{Generation within the system}\} \\ -\{\text{Consumption within the system}\}$$

At steady state, accumulation = 0.
If there is no reaction, generation and consumptions = 0.
The general material balance is reduced to

Input through system boundary = Output through system boundary.

Example 3.1: Mixing Process

Two streams each containing ethanol and water is to be mixed together at 5 atm pressure and 25°C

Stream 1: 20 kmol/h ethanol (ethyl alcohol)
80 kmol/h water
Stream 2: 40 kmol/h ethanol (ethyl alcohol)
60 kmol/h water

Find the compositions and molar flow rates of product stream.

SOLUTION

HAND CALCULATIONS

The process is just physical mixing and no reaction is involved. The PFD is shown in Figure 3.1.

Basis: 100 kmol/h of stream 1
Total mass balance:
S1 + S2 = S3
100 + 100 = S3, S3 = 200 kmol/h

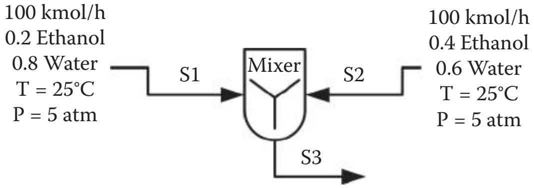


FIGURE 3.1
Mixing PFD.

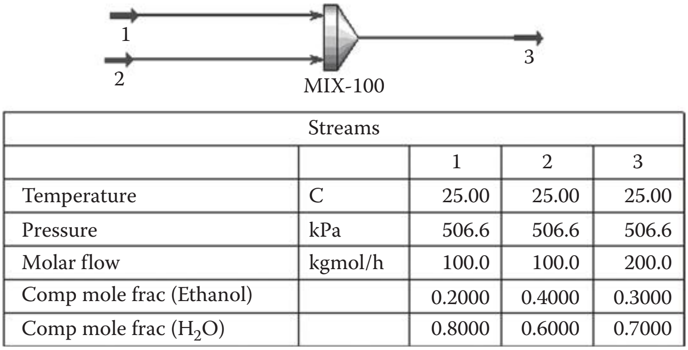
Component balance (ethanol):
0.2 (100) + 0.4(100) = x(200); hence, $x = 0.3$ (mole fraction of ethyl alcohol)
The exit stream consists of 0.3 mole fraction ethanol and the rest is water.

HYSYS/UNISIM SIMULATION

Select a new case in Hysys. For *Components*, select ethanol and water; for *Fluid Package*, select Non-Random Two Liquid (activity coefficient model), NRTL, and then enter the simulation environment. From the object palette, select *Mixer* and place it in the PFD area. Create two inlet streams and connect one exit stream. Click on stream 1 and enter 25°C for temperature, 5 atm for pressure, and 100 kmol/h for molar flow rate. In the composition page enter the value 0.2 for ethanol and 0.8 for water. Click on stream S2 and enter 25°C for temperature and 5 atm for pressure to ensure that both the ethanol and water are in the liquid phase, and 100 kmol/h for molar flow rate. In the composition page, enter 0.4 for ethanol and 0.6 mole fraction for water. To display the result below the process flow sheet, right click on each stream and select the show table, double click on each table and click on *Add Variable*, select the component mole fraction and click on *Add Variable* for both ethanol and water. Remove units and label for stream 2 and remove labels for stream 3. Results should appear like that shown in Figure 3.2.

PRO/II SIMULATION

The PRO/II process simulation program performs rigorous mass and energy balances for a range of chemical processes. The following procedure is used to build the mixing process with PRO/II: Open a new case in PRO/II; click *File* and then *New*. This will bring the user to the basic simulation environment. It is called the PFD screen. Then click the *Component Selection* button in the top toolbar. This button appears like a benzene ring. Next, click on *Thermodynamic Data*. Once entered, click on *Liquid Activity* and then on *NRTL*. Then click *Add* and then *OK* to return back to the PFD screen. Now it is ready to insert units and streams. The unit that we want to put in the simulation is the mixer. Scroll down the toolbar



Streams				
		1	2	3
Temperature	C	25.00	25.00	25.00
Pressure	kPa	506.6	506.6	506.6
Molar flow	kgmol/h	100.0	100.0	200.0
Comp mole frac (Ethanol)		0.2000	0.4000	0.3000
Comp mole frac (H_2O)		0.8000	0.6000	0.7000

FIGURE 3.2
Mixing process flow sheet and the stream summary generated by Hysys.

until you see an icon that looks like a mixer. Next, click on *Streams*. First create a feed stream, S1, entering into one side of the mixer. Next, create stream S2 from the other side of the mixer. The next stream, S3, should be moved from the bottom side of the mixer to wherever you would like to, as this will be the product stream.

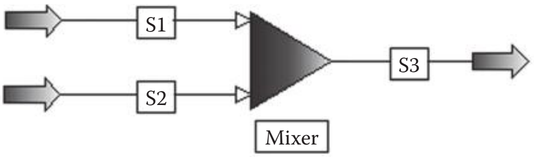
The next task at hand is entering the known data into the simulation. We will begin with the feed stream data. Double click on S1 and the *Stream Data* screen will appear. Click on *Flowrate and Composition*, then *Individual Component Flowrates*, and then enter in all the given feed flow rates. Once this is done, click *OK* and the *Stream Data* screen should reappear with *Flowrate and Composition* now outlined in blue. The two streams each containing ethanol and water is mixed together at 5 atm pressure and 25°C.

Stream S1: 20 kmol/h ethanol (ethyl alcohol)
80 kmol/h water
Stream S2: 40 kmol/h ethanol (ethyl alcohol)
60 kmol/h water

Now it is time to run the simulation. Click on *Run* on the toolbar, and the simulation should turn blue. If it does not, one can double click on the controller and then increase the number of iterations until it converges. Otherwise, one should retrace steps to find the error and fix it. The next thing to do is to view the results. For this, click on *Output* and then *Stream Property Table*. Double click on the generated table and then select *Material Balance List* under the property list to be used. Click on *Add All* to add available streams. Sample results are shown in Figure 3.3.

ASPEN PLUS SIMULATION

Select the mixer from the *Mixer/Splitter* submenu and place it in the PFD area. Create the inlet streams, by first clicking on *Material Streams* at the bottom-left



Stream name Stream description		S1	S2	S3
Phase		Liquid	Liquid	Liquid
Temperature pressure	C kg/cm^2	25.000 5.166	25.000 5.166	25.000 5.166
Flowrate	kgmol/h	100.000	100.000	200.000
Composition Ethanol Water		 0.200 0.800	 0.400 0.600	 0.300 0.700

FIGURE 3.3
Mixer process flow sheet and the stream summary generated by PRO/II.

corner of the window and move the cursor over the mixer. Red and blue arrows appear around the mixer. A red arrow signifies that a stream is required for the flow simulation, whereas a blue arrow signifies that it is optional. Click on *Next* to begin entering data. While in the *Property Method*, select the NRTL option from the list. Enter the data for the inlet stream labeled 1, enter 25°C for temperature and 5 atm for pressure. In the box labeled water, enter the value 80 and enter 20 in the box labeled EtOH. Note that the units of the values you just entered are displayed in the box labeled *Composition*s. These units can be changed by first clicking on the arrow by the box and selecting the appropriate units from the options. Click next. Enter 25°C for temperature and 5 atm for pressure to ensure that both the ethanol and water are in the liquid phase. Enter the flow rate values for both water and ethanol as instructed above. Enter 60 and 40 kmol/h for water and ethanol, respectively.

Stream summary results can be displayed on the process flow sheet by clicking on *Report Options* under the *Setup* folder. Then click on the Stream folder tab. For detailed data, make sure that both the boxes beside Mole and Mass contain a checkmark. Also, make sure that both the boxes are checked under Fraction basis. Click on *Next*. For summary results, just check the box below mole fraction basis (Figure 3.4).

Click on *Check Results* to view the results. Click on *Stream Table* to display the stream summary as shown in Figure 3.5.

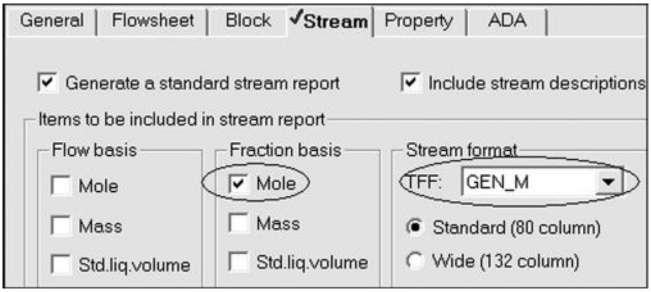
SuperPro Designer

Opening a new case in SuperPro and selecting all components involved the mixing process: Tasks >> Enter Pure Components

Ethyl alcohol is selected. Water, oxygen, and nitrogen exist as default components. Select a mixing process:

Unit Procedures >> Mixing >> Bulk flow >> 2 streams

Connecting two inlet streams and one exit stream; double click on the inlet streams and enter temperature, pressure, and molar flow rate of each stream. To run the system, click on *Solve ME Balance* (the calculator icon) or press F9. Click on *Toggle Stream Summary Table* in the toolbar. Right click on the empty area in the PFD and click on update data. Select all streams. Results should appear like that shown in Figure 3.6.



☑ Generate a standard stream report
☑ Include stream descriptions

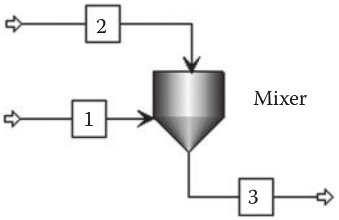
Items to be included in stream report

Flow basis
☐ Mole
☐ Mass
☐ Std.liq.volume

Fraction basis
☑ Mole
☐ Mass
☐ Std.liq.volume

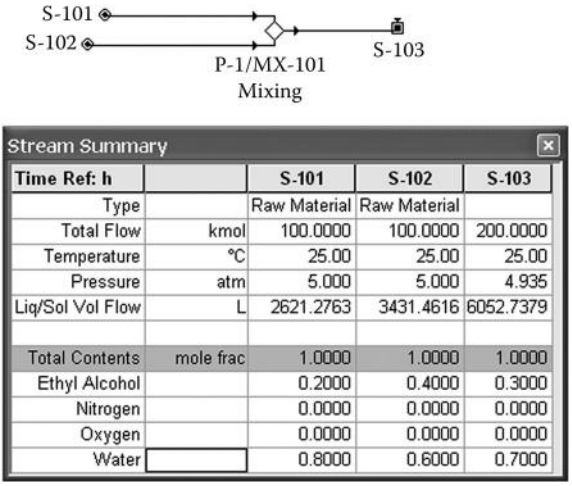
Stream format
TFF: GEN_M
● Standard (80 column)
○ Wide (132 column)

FIGURE 3.4
Stream report options in Aspen Plus.



Example 3.1				
Stream ID		1	2	3
Temperature	K	298.1	298.1	298.4
Pressure	atm	5.000	5.000	5.000
Vapor Frac		0.000	0.000	0.000
Mole flow	kmol/h	100.000	100.000	200.000
Mass flow	kg/h	2362.603	2923.678	5286.282
Volume flow	L/min	43.623	57.295	100.890
Enthalpy	MMkcal/h	–6.791	–6.751	–13.543
Mole frac				
Ethanol		0.200	0.400	0.300
Water		0.800	0.600	0.700

FIGURE 3.5
Streams summary generated by Aspen.



Time Ref: h		S-101	S-102	S-103
Type		Raw Material	Raw Material	
Total Flow	kmol	100.0000	100.0000	200.0000
Temperature	°C	25.00	25.00	25.00
Pressure	atm	5.000	5.000	4.935
Liq/Sol Vol Flow	L	2621.2763	3431.4616	6052.7379
Total Contents	mole frac	1.0000	1.0000	1.0000
Ethyl Alcohol		0.2000	0.4000	0.3000
Nitrogen		0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000
Water		0.8000	0.6000	0.7000

FIGURE 3.6
Process flow sheet and streams summary generated by SuperPro.

3.3 Material Balance on Reactive Processes

The extent of reaction ξ (or $\dot{\xi}$) is the amount of moles (or molar flow rate) that gets converted in a given reaction. The extent of reaction is a quantity that characterizes the reaction and simplifies our calculations. For a continuous process at steady state,

$$\dot{n}_i = \dot{n}_i^o + v_i\dot{\xi}$$

where, $\dot{n}_i^o$ and $\dot{n}_i$ are the molar flow rates of species i in the feed and outlet streams, respectively. For a batch process,

$$n_i = n_i^o + v_i\xi$$

where n_i^o and n_i are the initial and final molar amounts of species i, respectively. The extent of reaction ξ (or $\dot{\xi}$) has the same units as n (or $\dot{n}$). Generally, the syntheses of chemical products do not involve a single reaction but rather multiple reactions. The goal is to maximize the production of the desirable product and minimize the production of unwanted by-products. For example, ethylene is produced by dehydrogenation of ethane [1]:

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

$$C_2H_6 + H_2 \rightarrow 2CH_4$$

$$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$$

This leads to the following definitions:

$$\text{Yield} = \frac{\text{Moles of desired product formed}}{\begin{array}{c}\text{Moles formed if there were no side reactions and}\\ \text{limiting reactant reacts completely}\end{array}}$$

$$\text{Selectivity} = \frac{\text{Moles of desired product formed}}{\text{Moles of undesired product formed}}$$

The concept of extent of reaction can also be applied to multiple reactions, with each reaction having its own extent. If a set of reactions takes place in a batch or continuous, steady-state reactor, we can write

$$n_i = n_i^o + \sum_j v_{ij}\xi_j$$

where v_{ij} is the stoichiometric coefficient of substance i in reaction j; ξ_j is the extent of reaction for reaction j.

For a single reaction, the above equation reduces to the equation reported in a previous section.

Example 3.2: Conversion Reactor, Single Reaction

Ammonia is burned to produce nitric oxide. The fractional conversion of the limiting reactant is 0.5. The inlet molar flow rates of NH_3 and O_2 are 5 kmol/h each. The operating temperature and pressure are 25°C and 1 atm. Calculate the exit components' molar flow rates. Assume that the reactor is operating adiabatically.

SOLUTION

HAND CALCULATION

The process flow sheet is shown in Figure 3.7.

The reaction stoichiometric coefficients:

$$v_{NH_3} = -4, \quad v_{O_2} = -5, \quad v_{NO} = 4, \quad v_{H_2O} = 6$$

The extent of reaction method (ξ) can be used to find the molar flow rates of the product stream. The material balance can be written using the extent of reaction method as follows:

$$n_i = n_i^o + v_i\xi$$

$$NH_3\text{: } n_{NH_3} = n_{NH_3}^o - 4\xi$$

$$O_2\text{: } n_{O_2} = n_{O2}^o - 5\xi$$

$$NO\text{: } n_{NO} = n_{NO}^o + 4\xi$$

$$H_2O\text{: } n_{H_2O} = n_{H_2O}^o + 6\xi$$

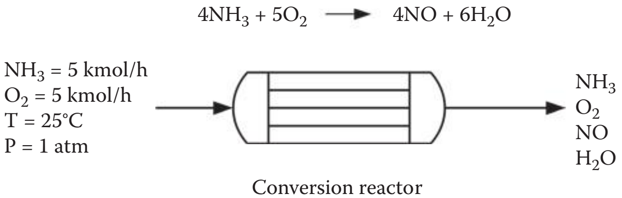


FIGURE 3.7
Process flow sheet of Example 3.2.

Total number of moles at the outlet of the reactor:

$$n = n^{o} + (-4 - 5 + 4 + 6)\xi = n^{o} + \xi$$

$$n = n^{o} + \xi$$

Inlet molar feed rates:

$$n^{o}_{NH_3} = 5\,\text{kmol/h}, \quad n^{o}_{O_2} = 5\,\text{kmol/h}, \quad n^{o}_{NO} = 0, \quad n^{o}_{H_2O} = 0$$

Since the limiting reactant is oxygen, the fractional conversion of oxygen:

$$x = \frac{n^{o}_{O_2} - n_{O_2}}{n^{o}_{O_2}}$$

$$0.5 = \frac{5 - n_{O_2}}{5}, \quad n_{O_2} = 2.5\,\text{kmol/h}$$

Substituting in the oxygen material balance equation,

$$2.5 = 5 - 5\xi, \quad \Rightarrow \xi = 0.5$$

Solving the set of the material balance equations gives the following results:

$$\xi = 0.5, \quad n_{NH_3} = 3\,\text{kmol/h}, \quad n_{O_2} = 2.5\,\text{kmol/h},$$

$$n_{NO} = 2\,\text{kmol/h}, \quad n_{H_2O} = 3\,\text{kmol/h}$$

HYSYS SOLUTION

Five types of reactors are built in Hysys (conversion, equilibrium, Gibbs, plug flow reactor (PFR), and continuous stirred tank reactor (CSTR). Conversion, equilibrium, and Gibbs reactors do not need reaction rates. On the contrary, CSTR and PFR reactors require reaction rate constants and order of reaction. There are also five different types of reaction rates that may be simulated in Hysys (conversion, equilibrium, simple rate, kinetic, and catalytic). Gibbs reactors are based on minimizing the Gibbs free energy of all components involved in the reactions. Hysys reaction rates are given in units of moles per volume of gas phase per time.

$$r_{HYSYS}[=]\frac{\text{mol}}{\text{m}^3_{\text{gas}} \cdot \text{s}}$$

For catalytic reactions, reaction rates are given in moles per mass of catalyst per time. For example, the following reaction rate is in units of mole per kilogram catalyst.

$$r[=]\frac{\text{mol}}{\text{kg}_{\text{cat}} \cdot \text{s}}$$

To convert to unit of moles per volume of gas, the following equation is used:

$$r_{\mathrm{HYSYS}} = r\rho_c \frac{(1-\phi)}{\phi}$$

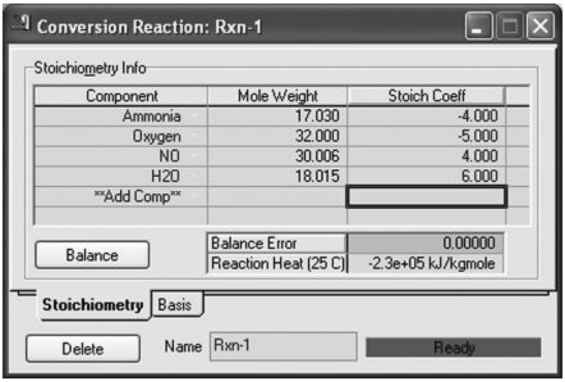
where ϕ is the reactor void fraction and ρ_c is the catalyst density. For this example, a conversion reactor will be sufficient to perform the material balance. Select a new case in Hysys, and add all components involved the reaction and also components produced (ammonia, oxygen, NO, and H_2O). Select Peng–Robinson as the fluid package. From the object palette, click on *General Reactors*, and then select *Conversion Reactor* and then click anywhere in the PFD area. Double click on the reactor and attach feed and product streams. Double click on the feed stream; enter feed conditions (1 atm, 25°C, and total molar flow rate 10 kmol/h). In the compositions page, set 0.5 mole fraction for ammonia and oxygen. From *Flowsheet* in the toolbar menu, select *Reaction Package* and then select *Conversion Reaction*; fill in the *Stoichiometry* page as in Figure 3.8 and the *Basis* page as in Figure 3.9.

The percent conversion is constant and is not a function of temperature; so C0 = 50 and the C1 and C2 are set to zero. The process flow sheet and stream conditions are shown in Figure 3.10. The results are the same as those obtained by hand calculation.

PRO/II Simulation

The PRO/II process simulation program performs rigorous mass and energy balances for a range of chemical processes. The conversion reactor in PRO/II is used as follows.

Open a new case in PRO/II and select the conversion reactor from the object palette; then, connect inlet and exit streams. Click on the *Component* tab (benzene ring in the toolbar) and select the components, NH_3, O_2, NO, and H_2O. From the thermodynamic data, select the most commonly used fluid package, the Peng–Robinson EOS. Double click on the inlet stream (S1) and the *Stream Data* screen should appear. Click on *Flowrate and Composition*, then *Individual*



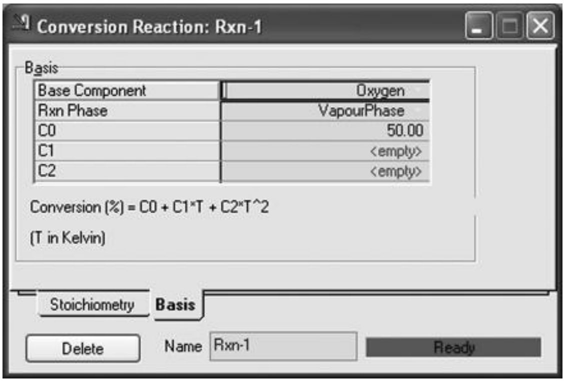
Component	Mole Weight	Stoich Coeff
Ammonia	17.030	-4.000
Oxygen	32.000	-5.000
NO	30.006	4.000
H2O	18.015	6.000
Add Comp		

Balance Error: 0.00000

Reaction Heat (25 C): -2.3e+05 kJ/kgmole

Name: Rxn-1

FIGURE 3.8
Stoichiometry of the reaction.



Conversion Reaction: Rxn-1

Basis

Base Component	Oxygen
Rxn Phase	VapourPhase
C0	50.00
C1	<empty>
C2	<empty>

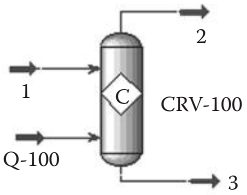
Conversion (%) = C0 + C1*T + C2*T^2

(T in Kelvin)

FIGURE 3.9
Reaction in the vapor phase; 50% conversion; O_2 is the base component.

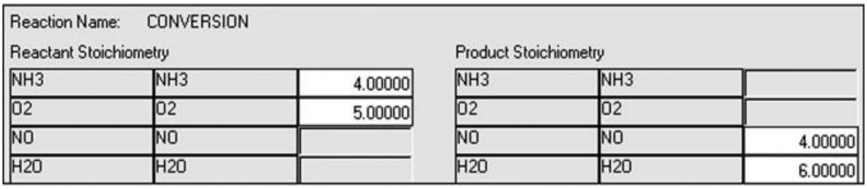
Component Flowrates, and then enter in all component flowrates; 5 kmol/h for NH_3 and 5 kmol/h for O_2. For thermal condition, set the pressure to 1 atm and temperature to 25°C. From *Input* in the toolbar menu, select *Reaction Data*, enter the reaction name and description and then click on *Reaction = Product*. Enter the reactant and the product as shown in Figure 3.11. Double click on the reactor R1 and from the pull-down menu of *Reaction Set Name*, select the conversion or the name being selected by the user. Save the file and click on *Run*.

Generate the results from the *Output* menu, and select *Generate Text Report*. The results are shown in Figure 3.12.



Streams				
		1	2	3
Temperature	C	25.00	1103	1103
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	10.00	10.50	0.0000
Comp molar flow (Ammonia)	kgmol/h	5.00	3.00	0.00
Comp molar flow (Oxygen)	kgmol/h	5.00	2.50	0.00
Comp molar flow (NO)	kgmol/h	0.00	2.00	0.00
Comp molar flow (H_2O)	kgmol/h	0.00	3.00	0.00

FIGURE 3.10
Process flow sheet and exit molar flow rates.



Reaction Name: CONVERSION

Reactant Stoichiometry

NH3	NH3	4.00000
O2	O2	5.00000
NO	NO	
H2O	H2O	

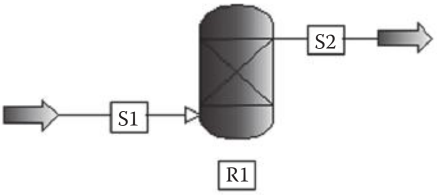
Product Stoichiometry

NH3	NH3	
O2	O2	
NO	NO	4.00000
H2O	H2O	6.00000

FIGURE 3.11
Reaction component and stoichiometry.

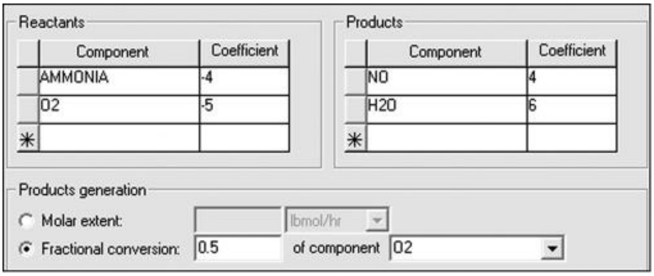
ASPEN SIMULATION

Aspen is capable of modeling chemical reactions. It can handle single and multiple reactions. Material balance can be done in the stoichiometric reactor, *Rstoic* from *Reactors* in the model library. Click on *Material Streams*, and connect the inlet and product streams. Click on *Components* and choose the components involved. Peng–Robinson EOS is selected as the thermodynamic fluid package. Double click on the conversion reaction block. Click on the *Specification* tab; enter pressure as 1 atm and temperature as 25°C. Then click on the *Reactions* tab, click on *New* and enter the components involved in the reaction, stoichiometric coefficient, and fractional conversion as shown in Figure 3.13. Close the stoichiometric windows and then double click on the inlet stream, specify temperature, pressure, flow rate, and composition. Click *Run* and then generate the stream table as shown in Figure 3.14.



Stream name Stream description Phase		S1 Vapor	S2 Mixed
Temperature	K	298.1500	298.1500
Pressure	kPa	101.3250	101.3250
Enthalpy	M∗kJ/h	0.1251	0.0810
Molecular weight		24.5147	23.3473
Mole fraction vapor		1.0000	0.7371
Mole fraction Liquid		0.0000	0.2629
Rate	kgmol/h	10.000	10.500
Fluid rates	kgmol/h		
NH_3		5.0000	3.0000
O_2		5.0000	2.5000
NO		0.0000	2.0000
H_2O		0.0000	3.0000

FIGURE 3.12
Process flow sheet and molar flow rates of streams of Example 3.2.



Reactants

Component	Coefficient
AMMONIA	-4
O2	-5

Products

Component	Coefficient
NO	4
H2O	6

Products generation

○ Molar extent: lbmol/hr

● Fractional conversion: 0.5 of component O2

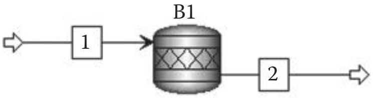
FIGURE 3.13
Reaction stoichiometry and fractional conversion.

SuperPro Designer Simulation

With SuperPro it is possible to simulate the conversion reaction in a continuous stoichiometric CSTR or PFR reactors (Figure 5.11). The well-mixed reactor expects some solid/liquid material in the feed stream. A small amount of water must be added. The PFR does not have such a requirement (Figure 3.15).

Start by registering the components. Under *Tasks* menu select *Edit Pure Components* (Figure 3.16).

Select the unit procedure, a continuous CSTR with a stoichiometric reaction (Figure 3.17).



Example 3.2			
Stream ID		1	2
Temperature	K	298.1	298.1
Pressure	atm	1.00	1.00
Vapor frac		1.000	0.678
Mole flow	kmol/h	10.000	10.500
Mass flow	kg/h	245.147	245.147
Volume flow	L/min	4061.555	2893.744
Enthalpy	MMBtu/h	–0.218	–0.787
Mole flow	kmol/h		
Ammonia		5.000	3.000
O_2		5.000	2.500
NO			2.000
H_2O			3.000

FIGURE 3.14
Process flowsheet and stream table properties.

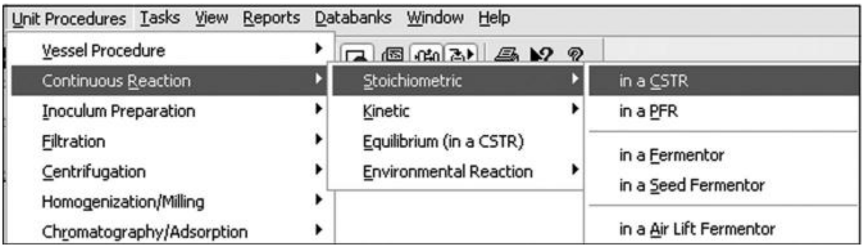
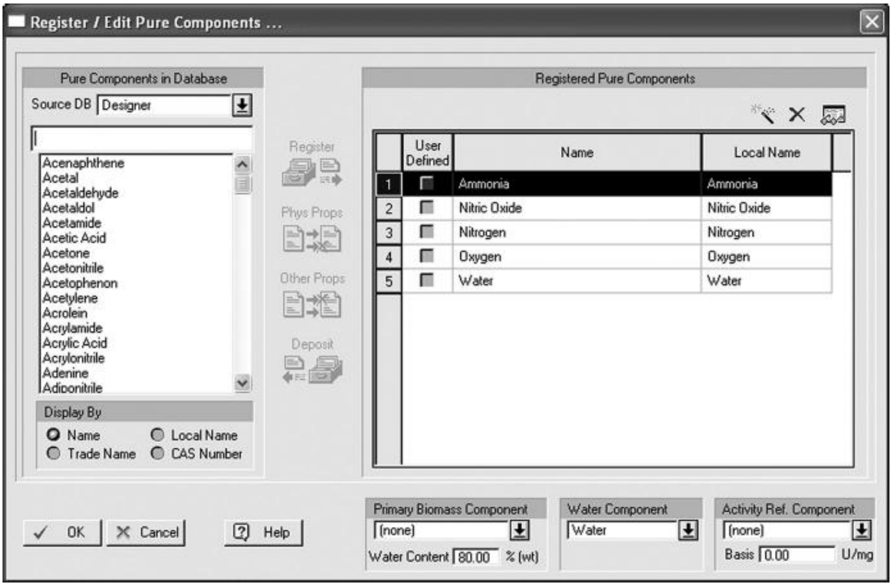


FIGURE 3.15
Selection of stoichiometric CSTR.



Source DB Designer

Display By: ● Name ○ Local Name ○ Trade Name ○ CAS Number

	User Defined	Name	Local Name
1	☐	Ammonia	Ammonia
2	☐	Nitric Oxide	Nitric Oxide
3	☐	Nitrogen	Nitrogen
4	☐	Oxygen	Oxygen
5	☐	Water	Water

Primary Biomass Component (none)
Water Content 80.00 % (wt)
Water Component Water
Activity Ref. Component (none)
Basis 0.00 U/mg

FIGURE 3.16
Component selection page in SuperPro.

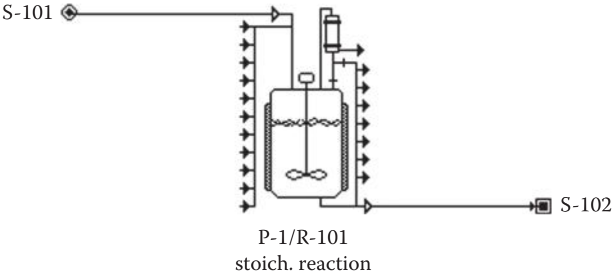
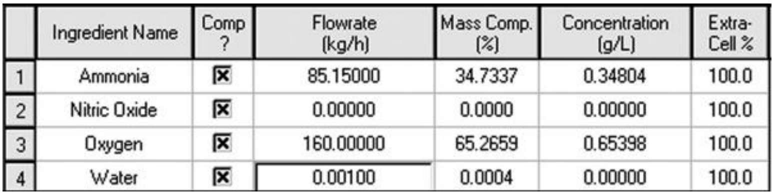


FIGURE 3.17
Stoichiometric continuous CSTR in SuperPro.



	Ingredient Name	Comp ?	Flowrate (kg/h)	Mass Comp. (%)	Concentration (g/L)	Extra-Cell %
1	Ammonia	☒	85.15000	34.7337	0.34804	100.0
2	Nitric Oxide	☒	0.00000	0.0000	0.00000	100.0
3	Oxygen	☒	160.00000	65.2659	0.65398	100.0
4	Water	☒	0.00100	0.0004	0.00000	100.0

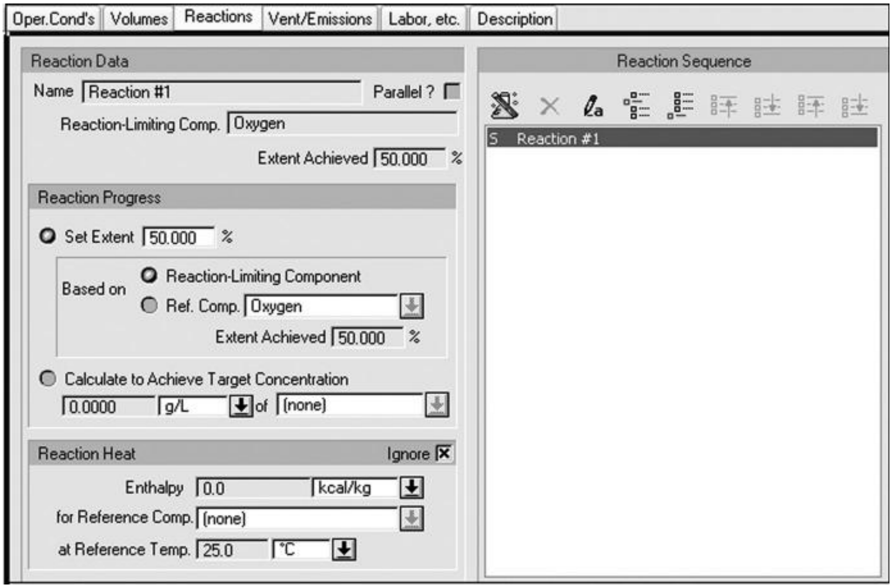
FIGURE 3.18
Feed stream conditions.

Double click on the line of the feed stream and set the feed stream conditions as shown in Figure 3.18. Note that the small amount of water is added to bypass the error generated by the CSTR reactor because there was no liquid or solid in the feed stream.

Insert the reaction data; assume a 50% completion for the limiting reactant (Figure 3.19).

Solve the mass and energy balances and generate the stream table, under *View*, select *Stream Summary Table*, right click on the empty area and select *Edit Content*, select inlet and exit streams. The generated table appears like that shown in Figure 3.20.

The PFR can also be used to generate the same results. In the operating conditions page, it must be set that the reaction is taking place in the vapor phase (Figure 3.21), otherwise an error message will be displayed: *No material is available for reaction*.



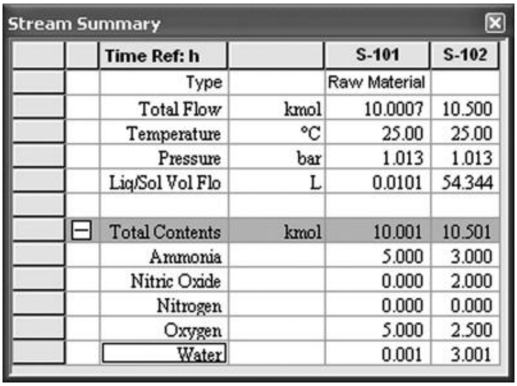
Reaction Data
Name: Reaction #1
Parallel ? ☐
Reaction-Limiting Comp.: Oxygen
Extent Achieved: 50.000 %

Reaction Progress
● Set Extent: 50.000 %
Based on: ● Reaction-Limiting Component ○ Ref. Comp. Oxygen
Extent Achieved: 50.000 %
○ Calculate to Achieve Target Concentration: 0.0000 g/L of (none)

Reaction Heat
Ignore ☒
Enthalpy: 0.0 kcal/kg
for Reference Comp.: (none)
at Reference Temp.: 25.0 °C

Reaction Sequence: S Reaction #1

FIGURE 3.19
Reaction stoichiometric and the extent of reaction.



Stream Summary

Time Ref: h		S-101	S-102
Type		Raw Material	
Total Flow	kmol	10.0007	10.500
Temperature	°C	25.00	25.00
Pressure	bar	1.013	1.013
Liq/Sol Vol Flo	L	0.0101	54.344
⊟ Total Contents	kmol	10.001	10.501
Ammonia		5.000	3.000
Nitric Oxide		0.000	2.000
Nitrogen		0.000	0.000
Oxygen		5.000	2.500
Water		0.001	3.001

FIGURE 3.20
Stream summary generated by SuperPro.

The process of solving for mass balance the generated results is shown in Figure 3.22.

Conclusions

For conversion reactors, hand calculations and simulation results using Hysys, PRO/II, Aspen Plus, and SuperPro Designer were exactly the same.

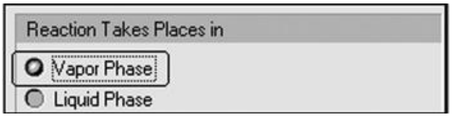
Example 3.3: Multiple Reactions

Consider the following two reactions taking place in an isothermal reactor:

$$CH_4 + H_2O \longrightarrow 3H_2 + CO$$

$$CO + H_2O \longrightarrow CO_2 + H_2$$

Feed enters the reactor at 350°C, 30 atm, and 2110 mol/s with feed mole fractions, 0.098 CO, 0.307 H_2O, 0.04 CO_2, 0.305 hydrogen, 0.1 methane, and 0.15 nitrogen. The reactions take place simultaneously. Assume that 100% conversion of methane and carbon monoxide (CO), neglect pressure drop across the reactor. Calculate the molar flow rates of the product components.

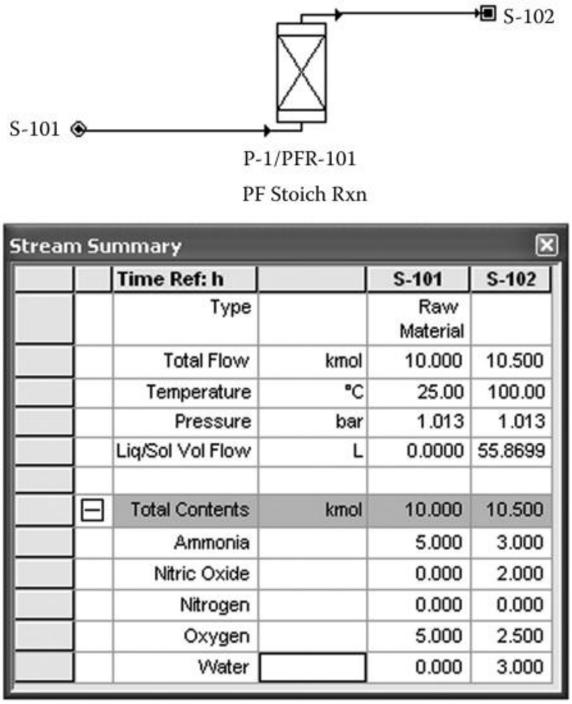


Reaction Takes Places in

● Vapor Phase

○ Liquid Phase

FIGURE 3.21
Selection of a reaction phase in SuperPro.



Stream Summary ☒

	Time Ref: h		S-101	S-102
	Type		Raw Material	
	Total Flow	kmol	10.000	10.500
	Temperature	°C	25.00	100.00
	Pressure	bar	1.013	1.013
	Liq/Sol Vol Flow	L	0.0000	55.8699
⊟	Total Contents	kmol	10.000	10.500
	Ammonia		5.000	3.000
	Nitric Oxide		0.000	2.000
	Nitrogen		0.000	0.000
	Oxygen		5.000	2.500
	Water		0.000	3.000

FIGURE 3.22
Process flow sheet and stream table properties.

SOLUTION

Hand Calculations

The labeled process flow sheet is shown in Figure 3.23; the material balance using the extent of reaction method:

$$CH_4 + H_2O \longrightarrow 3H_2 + CO \quad \xi_1$$

$$CO + H_2O \longrightarrow CO_2 + H_2 \quad \xi_2$$

Material Balance

$$n_{CH_4} = 0.1(2110\ \text{mol/s}) - \xi_1$$

$$n_{H_2O} = 0.307\ (2110\ \text{mol/s}) - \xi_1 - \xi_2$$

$$n_{H_2} = 0.305\ (2110\ \text{mol/s}) + 3\xi_1 + \xi_2$$

$$n_{CO} = 0.098\ (2110\ \text{mol/s}) + \xi_1 - \xi_2$$

$$n_{CO_2} = 0.04\ (2110\ \text{mol/s}) + \xi_2$$

$$n_{N_2} = 0.15\ (2110\ \text{mol/s})$$

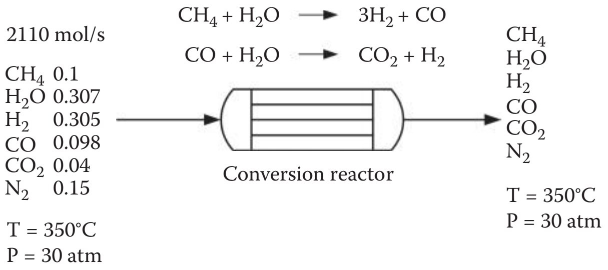


FIGURE 3.23
Process flowsheet of Example 3.3.

Relations

Complete conversion of methane (CH_4):

$$1 = \frac{0.1(2110\ \text{mol/s}) - n_{CH_4}}{0.1(2110\ \text{mol/s})}$$

Complete conversion of CO:

$$1 = \frac{0.098\ (2110\ \text{mol/s}) - n_{CO}}{0.098\ (2110\ \text{mol/s})}$$

From the first relation, the exit molar flow rate of methane is zero ($n_{CH_4} = 0$), and substituting this value in methane material balance equations,

$$0 = 0.1(2110\ \text{mol/s}) - \xi_1$$
$$\xi_1 = 211\,\text{mol/s}$$

The first and the second reactions take place at the same time and the percent conversions of both reactions are 100%.

$$1 = \frac{0.098\ (2110\ \text{mol/s}) - n_{CO}}{0.098\ (2110\ \text{mol/s})_1} = \frac{\xi_2}{0.098\ (2110\ \text{mol/s})} = \frac{\xi_2}{0.098\ (2110\ \text{mol/s})}$$

The second extent of reaction: $\xi_2 = 0.098(2110) = 206.78$ mol/s

Substituting calculated values of ξ_1 and ξ_2 in the material balance equations gives the following exit molar flow rates:

$$n_{CH_4} = 0.0$$
$$n_{H_2O} = 0.307(2110\ \text{mol/s}) - 211 - 206.78 = 230\ \text{mol/s}\left(827.96\ \text{kmol/h}\right)$$
$$n_{H_2} = 0.305\ (2110\ \text{mol/s}) + 3 \times 211 + 206.78 = 1483.33\ \text{mol/s}\left(5340\ \text{kmol/h}\right)$$
$$n_{CO} = 0.098\ (2110\ \text{mol/s}) + 211 - 206.78 = 211\,\text{mol/s}\left(759.6\ \text{kmol/h}\right)$$
$$n_{CO_2} = 0.04\ (2110\ \text{mol/s}) + 206.78 = 291.18\ \text{mol/s}(1048.25\ \text{kmol/h})$$
$$n_{N_2} = 0.15\ (2110\ \text{mol/s}) = 316.5\ \text{mol/s}\left(1139.4\ \text{kmol/h}\right)$$

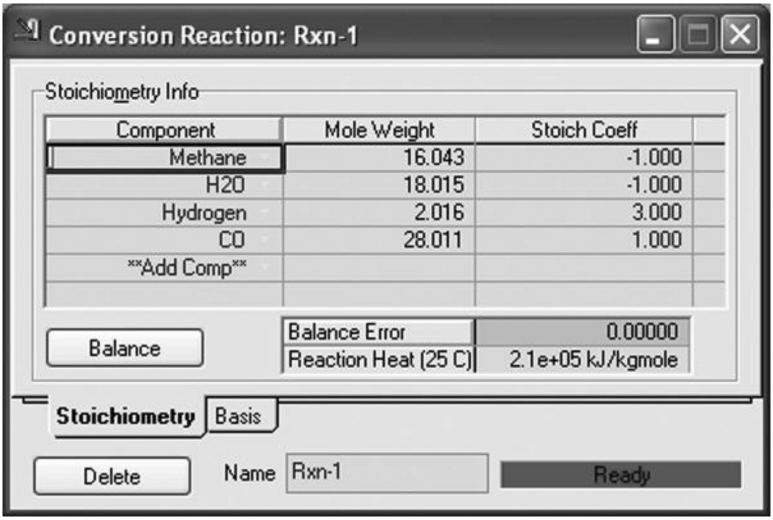
HYSYS SIMULATION

In a new case in Hysys, click the *Components* tab and add all components involved (reactants and products). Click on the *Fluid PKgs* tab and select Peng–Robinson as the fluid package. Select *Reactions packages* under *Flowsheet* and on the *Reactions* page of the *Simulation Basis Manager*, click on *Add Rxn* and select conversion, then click on *Add Reaction*. Select the components: methane, H_2O, H_2, and CO, under *stoich. Coeff* enter –1 for methane and water as the reactant, 3 for hydrogen and 1 for CO as the product components (Figure 3.24). The balance error should be 0.00.

Click on the *Basis* tab and set the conversion to 100% (Figure 3.25).

The stoichiometric coefficients of the second reaction are entered in the same way as the coefficients of the first reaction. Click on *Basis*; select CO as the base component, for Rxn Phase: overall, for CO: 100, and 0.0 for C1 and C2. Click on *Add to FP* and then on *Add set to Fluid Package*; note that 'Basis-1' should appear under *Assoc. Fluid Pkgs*. Press *Return to Simulation Environment* to return to the simulation environment. You may have noticed a button that was never there before when we looked at the reaction sets. Click on *Ranking* and change the default setting to 1 so that those reactions occur simultaneously in the parallel reactions (Figure 3.26).

After adding the two reactions, using the default set name (i.e., *Global Rxn Set*) add the set to *Current Reactions Sets*; the reaction package page appears like that shown in Figure 3.27. The reaction set should appear under *Current Reaction Sets* with the *Associated Reactions*, otherwise it will not appear when returning to the simulation environment.



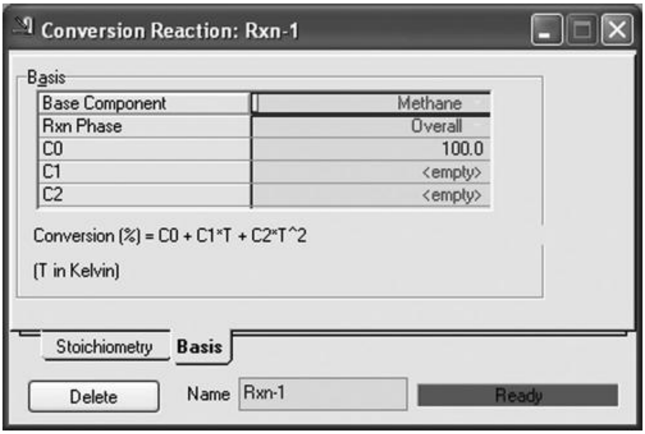
Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
Hydrogen	2.016	3.000
CO	28.011	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	2.1e+05 kJ/kgmole

Name Rxn-1

Ready

FIGURE 3.24
Conversion reactions of stoichiometry page.



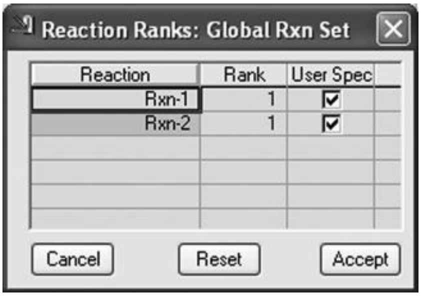
Base Component	Methane
Rxn Phase	Overall
C0	100.0
C1	<empty>
C2	<empty>

Conversion (%) = C0 + C1*T + C2*T^2

(T in Kelvin)

Name Rxn-1

FIGURE 3.25
Conversion windows.



Reaction	Rank	User Spec
Rxn-1	1	☑
Rxn-2	1	☑

FIGURE 3.26
Reaction ranks for a parallel reaction.

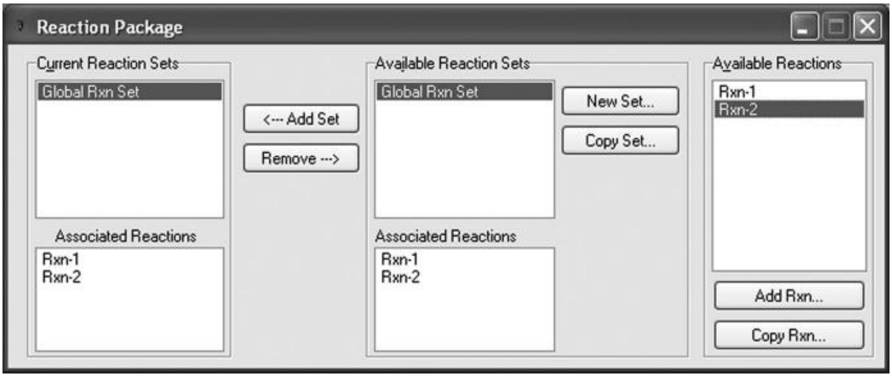


FIGURE 3.27
Simulation basis managers.

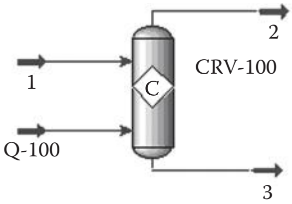
Enter the simulation environment by clicking on *Return to Simulation Environment*. To set up the conversion reactor, select a conversion reactor from the object palette and place it on the PFD. Connect feed and product streams and then double click on stream 1 and enter the temperature, 350°C; pressure, 30.4 bar; and molar flow, 7596 kgmol/h. Click on *Composition* and enter the molar fraction and then close the inlet stream window and double click on the conversion reactor; then press the *Reaction* tab from the pull-down menu in front of *Reaction Set* and chose the reaction set.

When the heat stream is not attached, it is assumed adiabatic; to make it isothermal, attach a heat stream and set the temperature on the product stream the same as the inlet stream temperature. On the *Parameters* page, a pressure drop across the reactor is set to zero.

Hysys requires you to attach another product stream. Go ahead and attach a liquid product stream and call it 3. The PFD of the conversion reactor is shown in Figure 3.28.

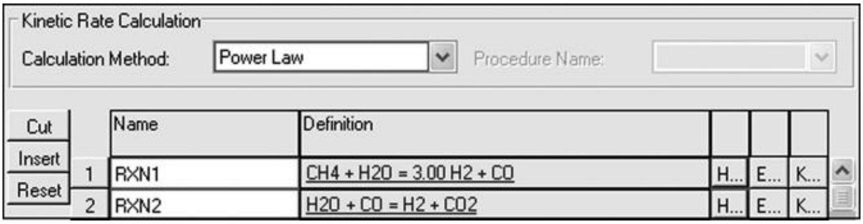
PRO/II SIMULATION

PRO/II is capable of handling multiple reactions. The same procedure of Example 3.2 is used here. First, perform the process flow sheet of the conversion reactor and specify the feed stream with the given total flow rate and compositions, Temperature is 350°C and pressure is 30 atm. Under the *Reactions input* menu, select *Reaction Data* and enter the two reactions as shown in Figure 3.29. Select reaction set R1 from the *Reaction set Name* of the pull-down menu. Click on *Extent of Reaction* and specify 100% conversion (fractional conversion is 1) for



Streams				
		1	2	3
Temperature	C	350.00	350.0	350.0
Pressure	kPa	3040	3040	3040
Molar flow	kgmol/h	7596	9115	0.0000
Comp molar flow (Methane)	kgmol/h	760	0	0
Comp molar flow (Hydrogen)	kgmol/h	2317	5340	0
Comp molar flow (CO)	kgmol/h	744	760	0
Comp molar flow (CO_2)	kgmol/h	304	1048	0
Comp molar flow (Nitrogen)	kgmol/h	1139	1139	0
Comp molar flow (H_2O)	kgmol/h	2332	828	0

FIGURE 3.28
Process flowsheet and the molar flow rate of the product stream.



Kinetic Rate Calculation

Calculation Method: Power Law

Procedure Name:

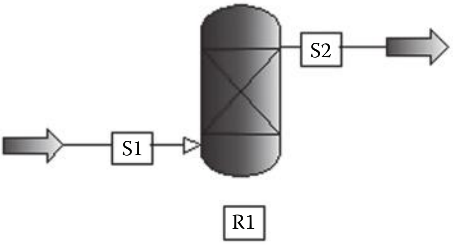
	Name	Definition			
1	RXN1	CH4 + H2O = 3.00 H2 + CO	H...	E...	K...
2	RXN2	H2O + CO = H2 + CO2	H...	E...	K...

FIGURE 3.29
Reaction data of Example 3.3.

both reactions. After running the system, the process flow sheet and the stream property table appear like that shown in Figure 3.30.

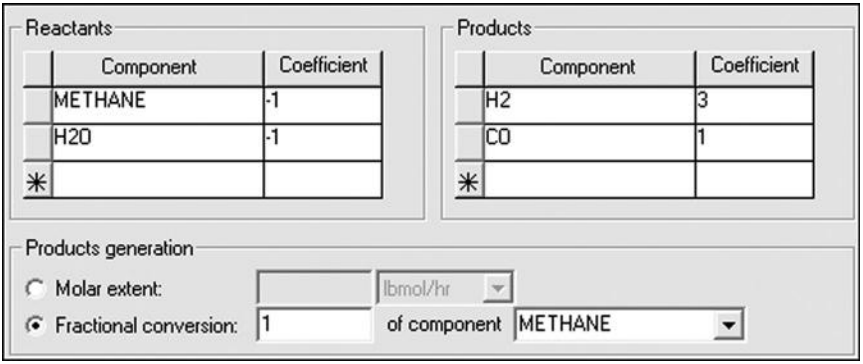
ASPEN SIMULATION

Aspen can handle multiple reactions. For material balance on multiple reactions, select a stoichiometric reactor (*Rstoic*) from the reactors' subdirectory



Stream name Stream description Phase		S1 Vapor	S2 Mixed
Temperature	K	623.1500	298.1500
Pressure	kPa	3039.7500	3039.7500
Enthalpy	M*kJ/h	197.0091	18.1428
Molecular weight		16.4572	13.7144
Mole fraction vapor		1.0000	0.9101
Mole fraction liquid		0.0000	0.0899
Rate	kgmol/h	7596.000	9115.200
Fluid rates	kgmol/h		
CH_4		759.6000	0.0000
H_2O		2331.9719	827.9641
H_2		2316.7800	5339.9883
CO		744.4080	759.6000
CO_2		303.8400	1048.2479
N_2		1139.4000	1139.4000

FIGURE 3.30
Generate text report of Example 3.3.



Reactants

Component	Coefficient
METHANE	-1
H2O	-1
*	

Products

Component	Coefficient
H2	3
CO	1
*	

Products generation

○ Molar extent: lbmol/hr

● Fractional conversion: 1 of component METHANE

FIGURE 3.31
Stoichiometric coefficient and fractional conversion of the first reaction.

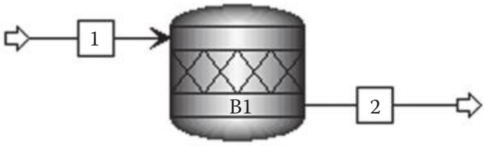
and place it in the PFD area. Click on *Material Stream*, and connect feed and product streams. Click on *Components* and enter all components (reactants and products). Select Peng–Robinson as the fluid package. Double click on the reactors block diagram. In the opened Data Browser window, click on the *Specification* tab; enter 1 atm for pressure and 25°C for temperature. Then click on the *Reactions* tab. Press *New* and enter components involved in the first reaction, enter the stoichiometric coefficient, and then the fractional conversion as shown in Figure 3.31. Repeat the same procedure for adding the second reaction. Close the stoichiometry page. Double click on stream 1 and enter the temperature, pressure, flow rate, and composition. Repeat the same for the second reaction; then click *Ok* to close. Click *Run* to generate the stream table as shown in Figure 3.32.

SUPERPRO DESIGNER SIMULATION

For multiple reactions, the procedure is done for a single reaction, but in this case another reaction needs to be added. The two reactions take place in parallel. The process of solving the material balance is shown in Figure 3.33. The limiting component is defined by the SuperPro; however, the radio button of the limiting component should be selected for each reaction and the parallel should be checked for each reaction. The stream summary is shown in Figure 3.34.

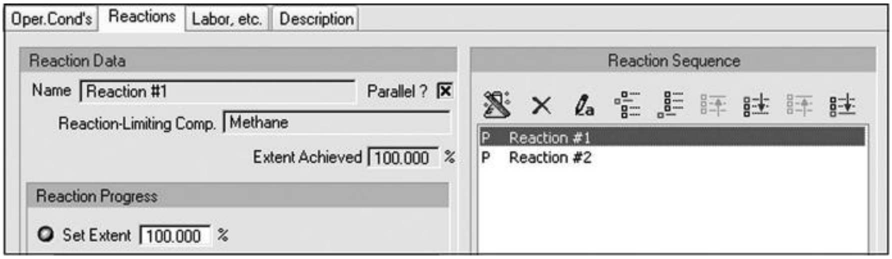
CONCLUSION

The results of material balance calculations obtained with hand calculations, Hysys, PRO/II, Aspen, and SuperPro Designer simulation package are the same.



Example 3.3			
Stream ID		1	2
Temperature	K	623.1	623.1
Pressure	atm	30.00	30.00
Vapor frac		1.000	1.000
Mole flow	kmol/h	7596.000	9115.200
Mass flow	kg/h	125009.221	125009.221
Volume flow	L/min	215695.070	261027.749
Enthalpy	MMBtu/h	–703.008	–572.114
Mole flow	kmol/h		
Methane		759.600	
CO_2		744.408	759.600
CO_2		303.840	1048.248
H_2O		2331.972	827.964
H_2		2316.780	5339.988
N_2		1139.400	1139.400

FIGURE 3.32
Process flow sheet and the stream table of Example 3.3.



Reaction Data

Name: Reaction #1

Parallel ? ☒

Reaction-Limiting Comp.: Methane

Extent Achieved: 100.000 %

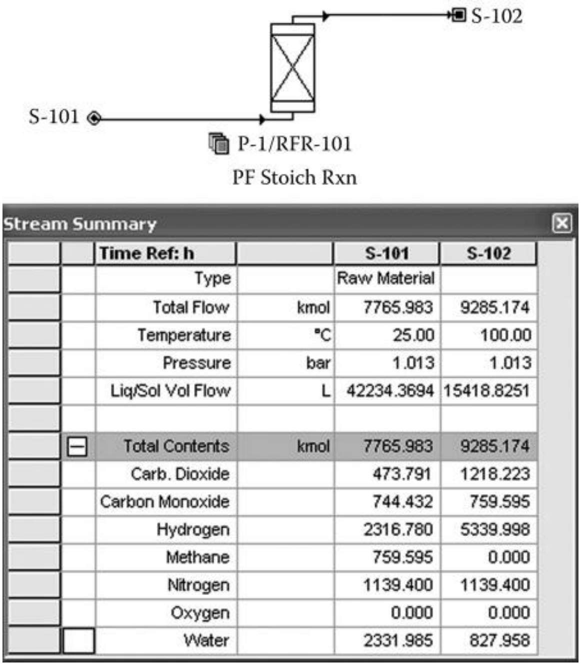
Reaction Progress

● Set Extent: 100.000 %

Reaction Sequence

P Reaction #1
P Reaction #2

FIGURE 3.33
Reactions data.



		Time Ref: h		S-101	S-102
		Type		Raw Material	
		Total Flow	kmol	7765.983	9285.174
		Temperature	°C	25.00	100.00
		Pressure	bar	1.013	1.013
		Liq/Sol Vol Flow	L	42234.3694	15418.8251
	⊟	Total Contents	kmol	7765.983	9285.174
		Carb. Dioxide		473.791	1218.223
		Carbon Monoxide		744.432	759.595
		Hydrogen		2316.780	5339.998
		Methane		759.595	0.000
		Nitrogen		1139.400	1139.400
		Oxygen		0.000	0.000
	☐	Water		2331.985	827.958

FIGURE 3.34
Streams summary.

3.4 Energy Balance without Reaction

The general balance equation for an open continuous system at steady state in the absence of generation/consumption term is

$$\text{Energy input} = \text{Energy output}$$

$$\text{Energy input} = \dot{U}_{\text{in}} + \dot{E}_{k,\text{in}} + \dot{E}_{p,\text{in}} + P_{\text{in}}\dot{V}_{\text{in}}$$

$$\text{Energy output} = \dot{U}_{\text{out}} + \dot{E}_{k,\text{out}} + \dot{E}_{p,\text{out}} + P_{\text{out}}\dot{V}_{\text{out}}$$

$$\text{Energy transferred} = \dot{Q} - \dot{W}_s$$

$$\text{Energy transferred} = \text{Energy out} - \text{Energy in}$$

$$\dot{Q} - \dot{W}_s = (\dot{U}_{\text{out}} + \dot{E}_{k,\text{out}} + \dot{E}_{p,\text{out}} + P_{\text{out}}\dot{V}_{\text{out}})$$
$$-(\dot{U}_{\text{in}} + \dot{E}_{k,\text{in}} + \dot{E}_{p,\text{in}} + P_{\text{in}}\dot{V}_{\text{in}})$$

$$\dot{Q} - W_s = \Delta\dot{U}_{\text{in}} + \Delta\dot{E}_k + \Delta\dot{E}_p + \Delta(P\dot{V})$$

$$\dot{H} = \dot{U} + P\dot{V}$$

$$\Delta\dot{H} = \Delta\dot{U} + \Delta(P\dot{V})$$

Rearranging the above equations leads to the first Law of Thermodynamics for an open system at steady state.

$$\dot{Q} - \dot{W}_s = \Delta\dot{H} + \Delta\dot{E}_k + \Delta\dot{E}_p, \quad \text{where } (\Delta = \text{output–input})$$

where $\dot{Q}$ is the heat transferred to or from the system, $\dot{W}_s$ is the shaft work, $\Delta\dot{H}$ is the rate of change in enthalpy of the system, $\Delta\dot{E}_k$ is the rate in change of the kinetic energy, $\Delta\dot{E}_p$ is the rate of change in potential energy, and $\Delta\dot{U}$ is the rate of change in the internal energy of the system.

Example 3.4: Energy Balance on a Heat Exchanger

A shell and tube heat exchanger is used to cool hot water with cold water. Hot water enters through the tube side of a heat exchanger with a mass flow rate 0.03 kg/s and 80°C to be cooled to 30°C. Cold water in the shell side flows with a mass flow rate of 0.06 kg/s at a temperature of 20°C. Determine the outlet temperatures of the cold water.

SOLUTION

HAND CALCULATIONS

Heat transfer rate can be calculated using energy balance equation:

$$\dot{Q} = \dot{m}C_p\Delta T$$

For this case, the total heat transfer may be obtained from the energy balance equation considering adiabatic heat exchanger.

$$\dot{m}_c \, Cp_c\Delta T_c = \dot{m}_h Cp_h \Delta T_h$$

So the heat transfer rate was calculated as

$$Q_h = \dot{m}_h Cp_h \Delta T_h$$

$$\dot{m}_h = 0.03\text{kg/s}$$

$$\Delta T_h = 80 - 30 = 50°\text{C}$$

Cp_h is the average specific heat value

For water at

$$T = 80°\text{C}, \quad Cp_\text{h} = 4.198 \text{ KJ/kg°C}$$
$$T = 30°\text{C}, \quad Cp_\text{h} = 4.179 \text{ KJ/kg°C}$$
$$Cp_\text{avg} = \frac{(4.198 + 4.179)}{2} = 4.1885 \text{ KJ/kg°C}$$

The heat transfer rate from hot stream to cold stream:

$$\dot{Q}_\text{h} = \dot{m}_\text{h} Cp_\text{h} \Delta T_\text{h} = 0.03 \frac{\text{kg}}{\text{s}} \left(4.188 \frac{\text{kJ}}{\text{kg°C}} \right) (80 - 30)°\text{C} = 6.28 \text{ kJ/s}$$

Calculate the temperature of water at the outlet of the shell side ($T_{\text{c, out}}$, °C). The exit temperature of the hot water is calculated from

$$Q_\text{c} = \dot{m}_\text{c} Cp_\text{c} \Delta T_\text{c}$$
$$\dot{m}_\text{c} = 0.06 \text{ kg/s}$$

Cp_c at $T_{\text{c,in}} = 20°\text{C}$ and atmospheric pressure since the outlet temperature is unknown

Cp at $20°\text{C} = 4.183$ kJ/kg°C

$$\Delta T_\text{c} = \frac{\dot{Q}_\text{h}}{\dot{m}_\text{c} \times Cp_\text{C}}$$

Substituting values,

$$\Delta T_\text{c} = \frac{6.28(\text{kJ/s})}{0.06 \text{ (kg/s)} \times 4.183 \text{ (kJ/kJ°C)}} = 25°\text{C}$$

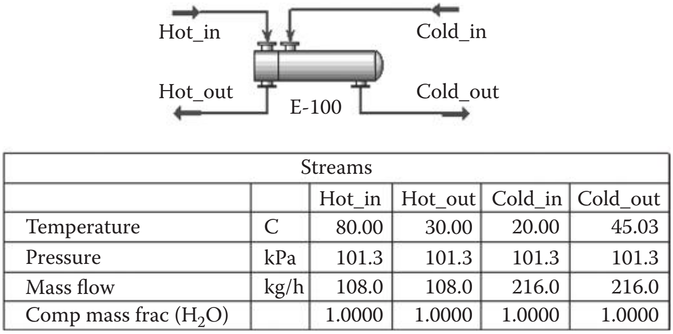
Hence,

$$T_{\text{c,out}} = T_{\text{c,in}} + \Delta T_\text{c} = 25 + 20 = 45°\text{C}$$

HYSYS SIMULATION

In a Hysys new case, all the components involved in the problem is selected; for this case, it is water. For fluid package, *ASME Stream* is selected, then *Enter Simulation Environment*.

From the object palette, a shell and tube heat exchanger is selected followed by specifying the required stream and parameters for the heat exchanger, information of streams, such as temperature, pressure, flow rate, and compositions, should be specified in order to make the software work. After specifying all the necessary information to the cold and hot inlet streams and the hot exit temperature, pressure drop in the tube and shell sides are set to zero. Hysys calculates automatically, once enough information is received. The solution for this problem is shown in Figure 3.35. To avoid the warning message *Ft Correction Factor is Low*, while



Streams					
		Hot_in	Hot_out	Cold_in	Cold_out
Temperature	C	80.00	30.00	20.00	45.03
Pressure	kPa	101.3	101.3	101.3	101.3
Mass flow	kg/h	108.0	108.0	216.0	216.0
Comp mass frac (H_2O)		1.0000	1.0000	1.0000	1.0000

FIGURE 3.35
Exit temperature of the cold stream.

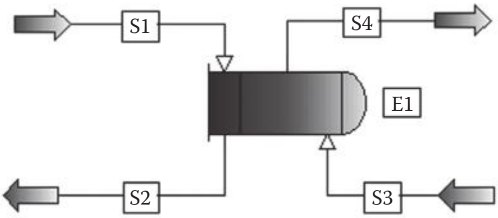
in the *Design/Parameters* page, set the cell below *Shells in Series* at the bottom of the screen to 2 instead of 1.

PRO/II SIMULATION

Open a new case in PRO/II; click *File* and then *New*. Then click *Component Selection* on the toolbar. Select water. Next, click on *Thermodynamic Data*. Once inside, click on *Most Commonly Used* and then click on *Peng–Robinson*. Then click *Add* and then *OK* to return back to the PFD screen. Now it is ready to insert units and streams. The unit that we want to put in the simulation is the mixer. Scroll down the toolbar until you see the shell and tube heat exchanger, *Rigorous HX*. Next, click on *Streams*. First create a feed stream, S1, entering into the tube side. Next, create stream S2 from the other side of the heat exchanger, the exit of the tube side. The next stream, S3, should go into the shell side and S4 should leave the shell side. Double click on S1 and specify the tube side mass flow rate (0.03 kg/s). The inlet temperature is 80°C and the pressure is 1 atm. Double click on stream S3 and specify the mass flow rate of the cold stream as 0.06 kg/s; temperature, 20°C; and pressure 1 atm. Double click on the heat exchanger icon and specify the calculation type such that the tube outlet temperature is 30°C. Set the Area/Shell to an arbitrary value, 2 m^2. Now it is time to run the simulation. Click on *Run* on the toolbar. The simulation should turn to blue. The next is to view the result. To view the results from each stream, right click on the stream and then choose *View Results*. Sample results can be seen in Figure 3.36. The result in Figure 3.36 is displayed by clicking *Output* in the toolbar and then select *Stream Property Table*. Note that *Simple Hx* exchanger can also be used for the same purpose.

ASPEN PLUS SIMULATION

A shell and tube heat exchanger is selected from the *Heat Exchangers* submenu. *Steam-TA* is selected for the property method. The inlet heat stream and inlet cold streams were fully specified. In the heat exchanger specifications, the hot stream outlet temperature is selected and specified as 30°C. Specifying the two feed streams and the outlet temperature of the cold stream, the system is ready to run. The results should appear like that shown in Figure 3.37. The cold stream outlet temperature is 318.2 K (45°C).



Stream name Stream description		S1	S2	S3	S4
Phase		Water	Water	Water	Water
Temperature pressure	C kg/cm^2	80.000 1.033	30.000 1.033	20.000 1.033	45.027 1.033
Flowrate	kgmol/h	5.995	5.995	11.990	11.990
Composition Water		1.000	1.000	1.000	1.000

FIGURE 3.36
Process flow sheet and the stream summary of the shell and tube heat exchanger.

SuperPro Designer

Water is a default component in SuperPro; consequently, there is no need for component selection. The heat exchanger is selected as follows:

Unit Procedures ≫ Heat Exchanger ≫ Heat exchanging

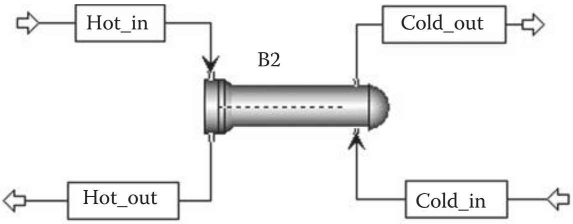
The two inlets are connected and fully specified (temperature, pressure, flow rates, and compositions). Two exit streams are connected. Double click on the exchanger block in the PFD area, and under *Performance Options*; and select the hot stream outlet temperature button and enter the hot stream exit temperature as 30°C. Results are shown in Figure 3.38.

Conclusions

According to manual calculation, the cold water outlet temperature was 45°C. The results obtained match with the values obtained from Hysys, PRO/II, Aspen Plus, and SuperPro software. Selection of a suitable fluid package is very important to obtain the correct results. Also, providing the sofware with correct values of temperature, pressure, flow rate, and composition will lead to obtain the right solution.

3.5 Energy Balance on Reactive Processes

Material balances could be done by either writing balances on either compounds (which required the extent of reaction) or elements (which required only balances without generation terms for each element); we can also do



Examble 3.4					
Stream ID		Cold_in	Cold_out	Hot_in	Hot_out
Temperature	K	293.1	318.2	353.1	303.1
Pressure	atm	1.000	1.000	1.000	1.000
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	kmol/h	11.990	11.990	5.995	5.995
Mass flow	kg/h	216.000	216.000	108.000	108.000
Volume flow	L/min	3.606	3.635	1.852	1.808
Enthalpy	MMkcal/h	−0.820	−0.814	−0.403	−0.409
Mass frac					
Water		1.000	1.000	1.000	1.000

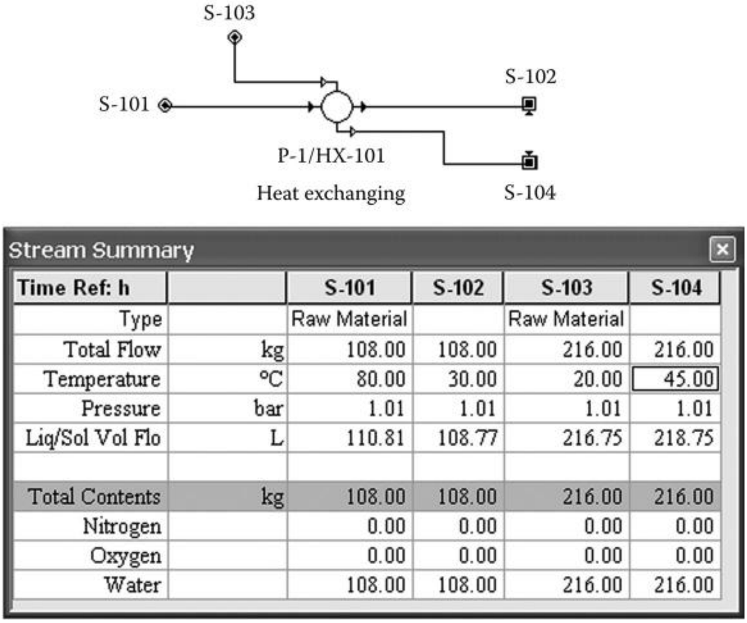
FIGURE 3.37
Shell and tube PFD and the stream summary.

energy balances using either compounds or elements. For energy balances with reaction, we have two methods for solving these types of problems [2,3]:

1. Heat of reaction method.
2. Heat of formation method.

These two methods differ in the choice of the reference state. The heat of reaction method is ideal when there is a single reaction for which $\Delta\hat{H}_r^\circ$ is known. This method requires calculation of the extent of reaction, $\dot{\xi}$, on any reactant or product for which the feed and product flow rates are known. The reference state is such that all reactant and product species are at 25°C and 1 atm in the states for which the heat of reaction is known. $\hat{H}_i$ accounts for change in enthalpy with T and phase (if necessary). Hence, the rate of change in enthalpy of a single reactive process is

$$\Delta\dot{H} = \dot{\xi}\Delta H_r^o + \sum_{\text{out}} \dot{n}_i\hat{H}_i - \sum_{\text{in}} \dot{n}_i\hat{H}_i$$



Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material		Raw Material	
Total Flow	kg	108.00	108.00	216.00	216.00
Temperature	°C	80.00	30.00	20.00	45.00
Pressure	bar	1.01	1.01	1.01	1.01
Liq/Sol Vol Flo	L	110.81	108.77	216.75	218.75
Total Contents	kg	108.00	108.00	216.00	216.00
Nitrogen		0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00
Water		108.00	108.00	216.00	216.00

FIGURE 3.38
Heat exchanger summary.

For multiple reactions,

$$\Delta\dot{H} = \sum_{\text{reactors}} \dot{\xi}_i \Delta H^{\circ}_{rj} + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

The reference state is such that the reactants and products are at 25°C and 1 atm. A reference temperature other than 25°C can be considered in this case, and the heat of reaction should be calculated at the new reference state

$$\Delta\dot{H} = \sum_{\text{reactors}} \dot{\xi}_i \Delta H_{rj(Tref)} + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

where

$$\Delta\dot{H}_r(T) = \Delta\dot{H}^{\circ}_{\text{rxn}}(T = 25^{\circ}\text{C}) + \int_{25^{\circ}\text{C}}^{T} \Delta Cp\,\mathrm{d}T$$

$$\Delta Cp = \sum v_i Cp_i$$

Example 3.5: Oxidation of Ammonia

The standard heat of reaction for the oxidation of ammonia is given below:

$$NH_3 + \frac{5}{4}O_2 \rightarrow NO + \frac{6}{4}H_2O$$

One hundred kmol/h of NH_3 and 200 kmol/h of O_2 at 25°C are fed into a reactor in which the ammonia is completely consumed. The product gas emerges at 300°C. Calculate the rate at which heat must be transferred to or from the reactor [4].

SOLUTION

HAND CALCULATIONS

Neglecting change in kinetic and potential energy, the change in the enthalpy of single reaction taking place in a stoichiometric reactor is

$$Q - W = \Delta\dot{H}$$

$$\Delta\dot{H} = \dot{\xi}\Delta\hat{H}_r^o + \sum_{\text{out}} \dot{n}_i\hat{H}_i - \sum_{\text{in}} \dot{n}_i\hat{H}_i$$

Material Balance (extent of reaction)
Basis: 100 kmol/s of NH_3

$$n_{NH_3} = 100 - \xi$$

$$n_{O_2} = 200 - \frac{5}{4}\xi$$

$$n_{NO} = 0 + \xi$$

$$n_{H_2O} = 0 + \frac{6}{4}\xi$$

Complete conversion of ammonia ($x_c = 1$):

$$\frac{\xi}{100} = 1 \Rightarrow \xi = 100$$

SOLUTIONS

$n_{NH_3} = 0$ kmol/s, $n_{O_2} = 75$ kmol/s, $n_{NO} = 100$ kmol/s, and $n_{H_2O} = 150$ kmol/s.

Energy Balance (reference temperature: 25°C):

$$\Delta\dot{H} = \xi\Delta H_r^o + \sum_{\text{out}} \dot{n}_i\hat{H}_i - \sum_{\text{in}} \dot{n}_i\hat{H}_i$$

$$\Delta\hat{H}_r^o = \frac{6}{4}(-241{,}800) + (90{,}370) - (-46{,}190) = -226{,}140 \text{ kJ/kmol}$$

The overall change in the system sensible heat of all components:

$$\Delta\dot{H}_s = \left[75\int_{25}^{300} Cp_{O_2}\,dT + 100\int_{25}^{300} Cp_{NO}\,dT + 150\int_{25}^{100} Cp_{H_2O,g}\,dT\right]_{out} - 0$$

$$\Delta\dot{H}_s = \left[(75\times 8.47 + 100\times 8.453 + 150\times 9.57\right]\ \text{kJ/mol}\ 1000\ \text{mol/kmol} = 2.92\times 10^6\ \text{kJ/h}$$

The change in the process enthalpy equals the change in the sensible heat plus the heat of reaction:

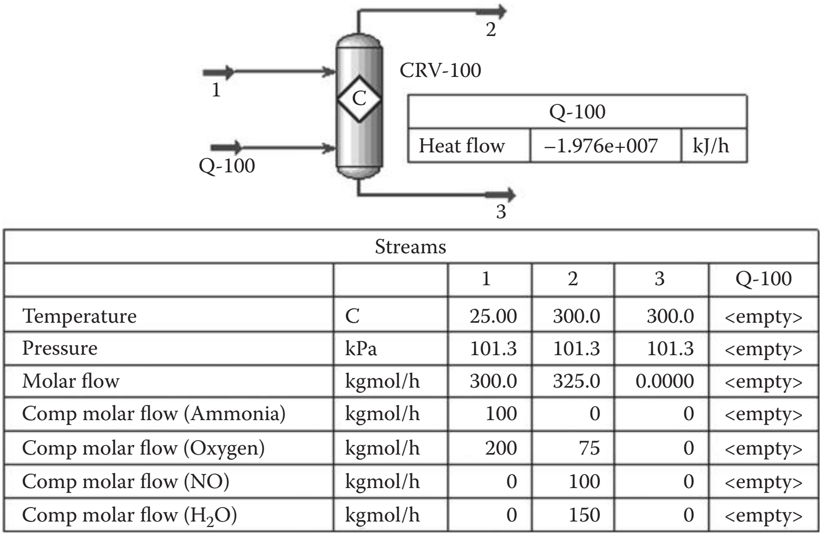
$$\Delta\dot{H} = 100\,\frac{\text{kmol}}{\text{h}}\left(-226{,}140\,\frac{\text{kJ}}{\text{kmol}}\right) + 2.92\times 10^6\,\frac{\text{kJ}}{\text{h}} = -1.97\times 10^6\,\frac{\text{kJ}}{\text{h}}$$

Hysys Method

The conversion reactor is selected from the object palette in Hysys. The percent conversion of ammonia is set to 100% as stated in the problem statements. The heat flow from the conversion reactor is shown in Figure 3.39. Peng–Robinson EOS is used for property measurement.

PRO/II Simulation

In a new case in PRO/II, the components involved are selected: ammonia, oxygen, nitric oxide, and water. From the *Thermodynamic Data* in the toolbar, Peng–Robinson EOS is selected from the *Most Commonly Used* property calculation system. The *Conversion Reactor* is selected from the palettes in the PFD. A feed



Q-100		
Heat flow	−1.976e+007	kJ/h

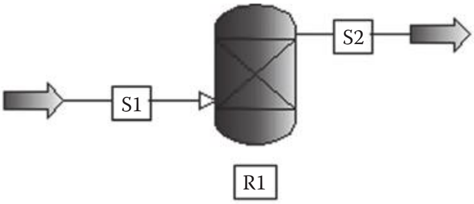
Streams					
		1	2	3	Q-100
Temperature	C	25.00	300.0	300.0	<empty>
Pressure	kPa	101.3	101.3	101.3	<empty>
Molar flow	kgmol/h	300.0	325.0	0.0000	<empty>
Comp molar flow (Ammonia)	kgmol/h	100	0	0	<empty>
Comp molar flow (Oxygen)	kgmol/h	200	75	0	<empty>
Comp molar flow (NO)	kgmol/h	0	100	0	<empty>
Comp molar flow (H_2O)	kgmol/h	0	150	0	<empty>

FIGURE 3.39
Heat released from the conversion reaction.

stream S1 is connected and fully specified and an exit stream S2 is connected. Once the process flow sheet is completed, it is time to enter the reaction. Click on *Reaction Data*, in the pop-up menu, and name the reaction set and reaction description. Click on *Enter Data*, name the reaction, and then click on *Reactants = Products*. Set the reaction stoichiometry based on the balanced reaction. Click *Ok* three times to return to the PFD. Click on the reactor block diagram. Select the reaction set from the down arrow in front of the *Reaction Set Name*. Click on *Reaction Extent*, select ammonia as the base component and set fraction conversion to 1. ($A = 1$, B and $C = 0$). The system is ready to run. Click on *Run*, the block color changes to blue. The result appears like that shown in Figure 3.40. To generate results and place it just below the process flow sheet as shown in Figure 3.40, click on *Output* in the toolbar and then select *Stream Property Table*. Double click on the table block. Under the *Property list to be used* select *Comp. Molar Rates*. Click *Add All* to add the property of all streams. The heat duty can be found from the generated text report. The heat duty is –19.8 M kJ/h. The value is close to that obtained by hand calculations.

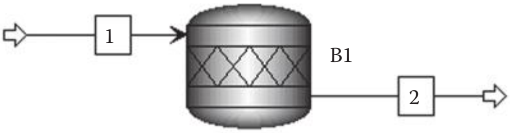
ASPEN PLUS SIMULATION

The stoichiometeric reactor in Aspen Plus is being used to estimate the rate of heat of transfer from the reactor. The components' molar flow rates are shown in Figure 3.41. The heat released is shown in Figure 3.42. The results are within the range of hand calculations.



Stream name Stream description Phase		S1 Vapor	S2 Vapor
Temperature	K	298.1500	573.1500
Pressure	kPa	101.3250	101.3250
Enthalpy	M*kJ/h	2.3611	10.2874
Molecular weight		27.0094	24.9317
Mole fraction vapor		1.0000	1.0000
Mole fraction liquid		0.0000	0.0000
Rate	kgmol/h	300.000	325.000
Fluid rates	kgmol/h		
Ammonia		100.0000	0.0000
NO		0.0000	100.0000
Water		0.0000	150.0000
Oxygen		200.0000	75.0000

FIGURE 3.40
Process flow sheet and the stream summary.



Example 3.5			
Stream ID		1	2
Temperature	K	298.1	573.1
Pressure	atm	1.00	1.00
Vapor frac		1.000	1.000
Mole flow	kmol/h	300.000	325.000
Mass flow	kg/h	8102.816	8102.816
Volume flow	L/min	121988.456	254629.564
Enthalpy	MMBtu/h	−4.356	−23.092
Mole flow	kmol/h		
Water			150.000
NO			100.000
Oxygen		200.000	75.000
Ammonia		100.000	

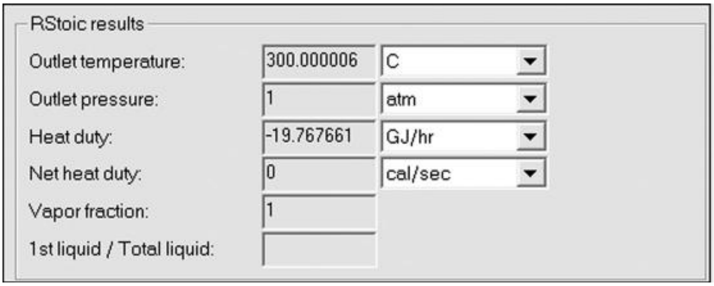
FIGURE 3.41
Stream summary and the process flow sheet.

SuperPro Designer

Selecting conversion reactor:

Unit procedures >> Continuous reactions >> Stoichiometric >> in PFR

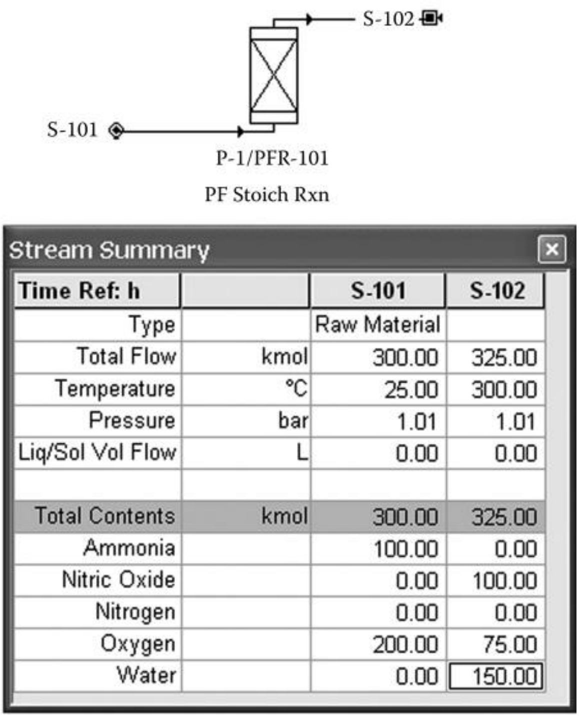
The limiting reactant is ammonia with complete conversion. The reaction takes place in the vapor phase and the heat of reaction should be provided. Results are shown in Figure 3.43 and the heat duty is shown in Figure 3.44.



RStoic results

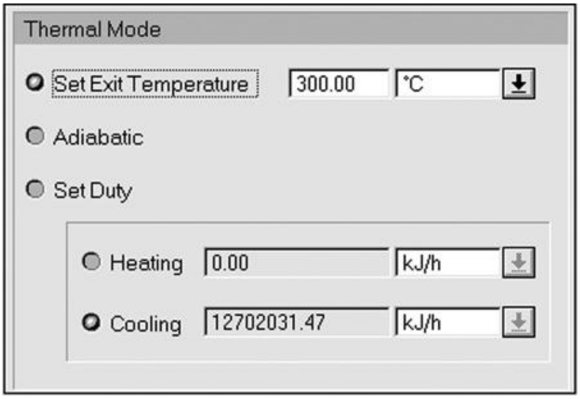
Outlet temperature:	300.000006	C
Outlet pressure:	1	atm
Heat duty:	-19.767661	GJ/hr
Net heat duty:	0	cal/sec
Vapor fraction:	1	
1st liquid / Total liquid:		

FIGURE 3.42
Heat duty of a stoichiometric reaction.



Time Ref: h		S-101	S-102
Type		Raw Material	
Total Flow	kmol	300.00	325.00
Temperature	°C	25.00	300.00
Pressure	bar	1.01	1.01
Liq/Sol Vol Flow	L	0.00	0.00
Total Contents	kmol	300.00	325.00
Ammonia		100.00	0.00
Nitric Oxide		0.00	100.00
Nitrogen		0.00	0.00
Oxygen		200.00	75.00
Water		0.00	150.00

FIGURE 3.43
Stream summary and process flow sheet.



● Set Exit Temperature 300.00 °C

○ Adiabatic

○ Set Duty

○ Heating 0.00 kJ/h

● Cooling 12702031.47 kJ/h

FIGURE 3.44
Reactor heat duty.

CONLUSIONS

Hysys, SuperPro Designer, and Aspen Plus results are exactly the same. There is discrepancy between hand calculations and the result obtained with SuperPro mainly due to physical properties such as specific heat.

PROBLEMS

3.1 Cumene Reaction

Cumene is produced from the reaction of benzene and propylene at 25°C and 1 atm. The inlet mass flow rate of benzene is 1000 kg/h and that of propylene is 180 kg/h. Assume 45% completion of the limiting reactant. Calculate molar flow rates of the product stream.

$$C_6H_6(\text{benzene}) + C_3H_6(\text{propene}) \longrightarrow C_9H_{12}(\text{cumene})$$

3.2 Nitric Oxide Production

Ammonia is burnt to produce nitric oxide. The fractional conversion of the limiting reactant is 0.6. NH_3 and O_2 are in equimolar proportion, and the total inlet flow rate is 100 kmol/h. The operating temperature and pressure are 25°C and 1 atm, respectively. Calculate the exit component molar flow rates. Assume that the reactor is operating adiabatically.

3.3 Multiple Reactions

A feed enters a conversion reactor at 350°C, 30 atm, and a molar flow rate of 7600 kmol/h. The feed molar fractions are 0.098 CO, 0.307 H_2O, 0.04 CO_2, 0.305 hydrogen, and 0.25 methane. The reactions take place in series. Assume 100% conversion of methane and CO, neglect pressure drop across the reactor. Calculate the molar flow rates of the product components. The reactions take place in an isothermal conversion reactor

$$CH_4 + H_2O \longrightarrow 3H_2 + CO$$

$$CO + H_2O \longrightarrow CO_2 + H_2$$

3.4 Gas-Phase Reaction

The gas-phase reaction proceeds with 80% conversion. Estimate the heat that must be provided or removed, if the gases enter at 400°C and leave at 500°C. The following reaction takes place: $CO_2 + 4H_2 \rightarrow 2H_2O + CH_4$.

3.5 Burning of CO

CO at 10°C is completely burnt at 1 atm pressure with 50% excess air that is fed to a burner at a temperature of 540°C. The combustion products leave the burner chamber at a temperature of 425°C. Calculate the heat evolved, *Q*, from the burner.

3.6 Production of Ketene from Acetone

Pure acetone reacts isothermally to form ketene and methane at 2 atm and 650°C. The percent conversion of acetone is 70%. Calculate the reactor exit molar flow rate of acetone, ketone, and methane. Calculate the heat added or removed from the reactor. As a basis assume 100 kmol/h of pure acetone. Note that 1 mol of acetone reacts to form 1 mol of ketene and 1 mole of methane.

References

1. Ghasem, N. M. and R. Hend, 2009. *Principles of Chemical Engineering Processes*, CRC Press, New York, NY.
2. Felder, R. M. and R. W. Rousseau, 1999. *Elementary Principles of Chemical Processes*, 3rd edn, John Wiley, New York, NY.
3. Reklaitis, G. V., 1983. *Introduction to Material and Energy Balances*, John Wiley & Sons, New York, NY.
4. Himmelblau, D. M., 1996. *Basic Principles and Calculations in Chemical Engineering*, 6th edn, Prentice-Hall, Englewood Cliffs, NJ.

4

Shell and Tube Heat Exchangers

At the end of this chapter you should be able to

1. Know the major types of available heat-exchange equipment, with particular emphasis on shell-and-tube heat exchangers.
2. Estimate overall heat transfer coefficients for a shell-and-tube heat exchanger.
3. Compute the pressure drops on both sides of a shell-and-tube heat exchanger.
4. Perform mechanical design of the most appropriate shell-and-tube heat exchanger to meet desired heat duty and pressure drops.
5. Verify the heat exchanger designed by hand computations with four software packages, Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer.

4.1 Introduction

The process of heat exchange between two fluids that are at different temperatures, separated by a solid wall, occurs in many engineering applications. The device used to implement this exchange is called a heat exchanger, and specific applications may be found in space heating and air conditioning, power production, waste heat recovery and chemical processing. Heat exchangers are typically classified according to flow arrangement and type of construction. In the first classification, flow can be countercurrent or cocurrent. There are different types of heat exchangers; double pipe heat exchanger, shell and tube heat exchanger, plate heat exchanger, and phase change heat exchangers (boilers and condensers). Shell and tube heat exchanger is the most common type of heat exchangers in oil refineries and other large chemical processes [1,2]. The tube side is for corrosive, fouling, scaling, hazardous, high temperature, high-pressure, and more expensive fluids. The shell side is for more viscous, cleaner, lower flow-rate, evaporating and condensing fluids. When a gas or vapor is used as a heat exchange fluid, it is typically introduced on the shell side. Also, high viscosity liquids, for which the pressure drop for flow through the tubes might be prohibitively large, can be introduced in shell side.

4.2 Design of Shell and Tube Heat Exchanger

When two fluids of different temperatures flow through the heat exchanger, one fluid flows in the tube side (the set of tubes is called a tube bundle) and the other fluid flows in the shell side outside the tubes. Heat is transferred from hot fluid to the cold fluid through the tube walls, either from tube side to shell side or vice versa. The fluids can be either liquids or gases on either the shell or the tube side. Heat transfer coefficients, pressure drops and heat transfer area depend on the design's geometric configuration of heat exchanger which needs to be determined. Computation of shell-and-tube heat exchangers involves iteration. The geometric design to be determined includes shell diameter, tube diameter, tube length, tube configuration, and number of tubes and shell passes [3–5].

4.2.1 Required Heat Duty, Q_{req}

The starting point of any heat transfer calculation is the overall energy balance and the rate equation. Assuming only sensible heat is transferred, the required heat duty Q_{req} can be written as follows:

$$Q_{req} = m_h Cp_h (T_{h,in} - T_{h,out}) = m_c Cp_c (T_{c,out} - T_{c,in}) \tag{4.1}$$

The heat exchanger has to meet or exceed this requirement, the basic design equation:

$$Q_{req} = U_i A_i F(\Delta T_{lm}) \tag{4.2}$$

where U_i is the overall heat transfer coefficient, A_i is the inside heat transfer area, the symbol F stands for a correction factor that must be used with the log mean temperature difference for a countercurrent heat exchanger, ΔT_{lm}:

$$\Delta T_{lm} = \frac{\left(T_1 - t_2\right) - \left(T_2 - t_2\right)}{\ln\left(T_1 - t_2/T_2 - t_2\right)} \tag{4.3}$$

where T_1 and t_1 are the hot side and cold side inlet temperature, respectively, and T_2 and t_2 are the corresponding outlet temperatures. The value of F depends upon the exact arrangement of the streams within the exchangers. The range of hot side fluid to the cold side fluid temperatures, R,

$$R = \frac{T_1 - T_2}{t_2 - t_1} = \frac{T_{hot,in} - T_{hot,out}}{t_{cold,out} - t_{cold,in}} \tag{4.4}$$

The range of cold fluid to maximum temperature difference,

$$S = \frac{t_2 - t_1}{T_1 - t_1} = \frac{t_{\text{cold,out}} - t_{\text{cold,in}}}{T_{\text{hot,in}} - t_{\text{cold,in}}} \tag{4.5}$$

The mathematical relationship between F, R, and S can be found from graphical representation or calculated as follows [4,5]. The formula for one shell pass and 2, 4, tube passes or any multiple of 2, $F_{1\text{–}2}$,

$$F_{1-2} = \frac{\left[\sqrt{R^2+1}\big/(R-1)\right]\ln\left[(1-S)/(1-SR)\right]}{\ln\left[A+\sqrt{R^2+1}\big/A-\sqrt{R^2+1}\right]}, \quad A = \frac{2}{S} - 1 - R \tag{4.6}$$

The formula for two shell pass and 4, 8, tube passes or any multiple of 4, $F_{2\text{–}4}$

$$F_{2-4} = \frac{\left[\sqrt{R^2+1}\big/2(R-1)\right]\ln\left[(1-S)/(1-SR)\right]}{\ln\left[\left(A+B+\sqrt{R^2+1}\right)\Big/\left(A+B-\sqrt{R^2+1}\right)\right]} \tag{4.7}$$

where

$$B = \frac{2}{S}\sqrt{(1-S)(1-SR)}$$

The value of F should be greater than 0.8 because low values of F means that substantial additional area must be supplied in the heat exchanger to overcome the inefficient thermal profile. The approximate heat transfer area A can be calculated using reasonable guess for the overall heat transfer coefficient; selected values are available in Table 4.1 [2]. The next step is to determine the approximate number of tubes N_t, needed to do the job.

4.2.2 Tube Selection

The tube length is selected as 8, 10, 12, 16, and 20 ft. Likewise, and the most common tube OD is $\frac{1}{4}$, $\frac{3}{8}$, $\frac{1}{2}$, $\frac{5}{8}$, $\frac{3}{4}$, 1, $1\frac{1}{4}$, or $1\frac{1}{2}$ in. The tube wall thickness is defined by the Birmingham wire gage (BWG). The tubes are typically specified to be 14 BWG. The most common tube lengths are 16 and 20 ft and the most common tube OD values are $\frac{3}{4}$ and 1 in. The velocity through a single tube should be between 3 and 10 ft/s to keep the pressure under reasonable constraints and to maintain turbulent flow, and minimize fouling. The number of tube passes can be adjusted to get the velocity to fall in this range. The

TABLE 4.1

Selected Overall Heat Transfer Coefficient (*U*) for Shell and Tube Heat Exchangers

Shell Side	Tube Side	Design (Btu/°F ft^2 h)	Included Total Dirt
Ethanol amine solutions	Water, or amine solutions	140–200	0.003
Organic solvents	Water	50–150	0.003
Demineralized water	Water	300–500	0.001
Water	Water	140–260	0.003
Low boiling hydrocarbon	Water	80–200	0.003
Air, N_2, compressed	Water	40–80	0.005
Propane, butane	Steam condensing	200–300	0.0015
Water	Steam condensing	250–400	0.0015

most commonly used heat exchanger tube data are shown in Table 4.2. Further information can be found elsewhere [3,6–10].

4.2.3 Shell Inside Diameter, D_s

Once the number of tubes is known, pitch (square or triangle) and number of tube passes is known, the shell size can be defined. A square pitch is chosen for reasons of convenience in cleaning the outside of the tubes because when the tubes are in-line, cleaning is relatively easy. Tubes on a triangular pitch cannot be cleaned by tools, but rather by passing a chemical solution through on the shell side. The standard choice is square pitch; 1.25 in. for 1-in. OD tubes, and 1 in. square pitch for $\frac{3}{4}$ in. OD tubes. Knowing the number of tubes and number of passes the required inside diameter (ID) of the shell can

TABLE 4.2

Heat Exchanger Tube Data

OD (in.)	BWG	ID (in.)
$\frac{1}{2}$	12	0.282
	14	0.334
	16	0.370
	18	0.402
$\frac{3}{4}$	10	0.482
	11	0.510
	12	0.532
	13	0.560
1	8	0.670
	9	0.704
	10	0.732
	11	0.760

be used from standard tables. Shells are made from commercial steel pipes up to an outside diameter (OD) of 24 in. Table 4.3 shows the selected tube sheet layouts. More information can be obtained from Kern [3].

4.2.4 Number of Baffles

Normally, baffles are equally spaced. The minimum baffle spacing is one-fifth of the shell diameter, but not less than 2 in. and maximum baffle spacing is $74D_o^{0.75}$, where D_o is the outside tube diameter in inches [3].

$$\text{Number of baffles} = \frac{L}{\text{Baffle spacing}} - 1$$

where L is the tube length.

4.2.5 Heat Transfer Coefficients

The thermal performance of the designed heat exchanger can be checked by calculating the overall heat transfer coefficient. This required calculating the tube side and shell side heat transfer coefficients, the tube wall contribution to the resistance, and the appropriate fouling resistance. The overall heat transfer coefficient, U_o based on the outside surface area of the tubes is

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{\Delta x}{k_W}\left(\frac{A_o}{A_{Lm}}\right) + \frac{1}{h_i}\left(\frac{A_o}{A_i}\right) + R_{fi}\left(\frac{A_o}{A_i}\right) + R_{fo} \tag{4.8}$$

where h_o is the outside film heat transfer coefficient, h_i the inside film heat transfer coefficient, Δx the tube wall thickness, k_W is the tube metal

TABLE 4.3

Shell Side ID

$\frac{3}{4}$ in. OD Tubes on 1 in. Square Pitch				1 in. OD Tubes on $1\frac{1}{4}$ in. Square Pitch			
Shell ID (in.)	**1-Pass**	**2-Pass**	**4-Pass**	**Shell ID (in.)**	**1-Pass**	**2-Pass**	**4-Pass**
8	32	26	20	8	21	16	14
10	52	52	40	10	32	32	26
12	81	76	68	12	48	45	40
$13\frac{1}{4}$	97	90	82	$13\frac{1}{4}$	61	56	52
$15\frac{1}{4}$	137	124	116	$15\frac{1}{4}$	81	76	68
$19\frac{1}{4}$	224	220	204	$19\frac{1}{4}$	138	132	128
$21\frac{1}{4}$	277	270	246	$21\frac{1}{4}$	177	166	158
25	413	394	370	25	260	252	238
31	657	640	600	31	406	398	380

conductivity, R_{fi} and R_{fo} are the inside and outside fouling resistances, respectively. A_{o} is the tube outside area, A_{i} is the tube inside area, and A_{LM} is the log mean of A_{i} and A_{o}. The wall thickness, Δx,

$$\Delta x = \frac{D_{\mathrm{o}} - D_{\mathrm{i}}}{2}, \quad A_{\mathrm{LM}} = \frac{A_{\mathrm{o}} - A_{\mathrm{i}}}{\ln\left(A_{\mathrm{o}} / A_{\mathrm{i}}\right)} \tag{4.9}$$

The overall heat transfer coefficient based on the inside area as a function of D_{o} and D_{i} is

$$\frac{1}{U_{\mathrm{i}}} = \left(\frac{D_{\mathrm{i}}}{D_{\mathrm{o}}}\right)\frac{1}{h_{\mathrm{o}}} + \frac{D_{\mathrm{i}}\Delta x}{D_{\mathrm{LM}}k_{\mathrm{w}}} + \frac{1}{h_{\mathrm{i}}} + R_{\mathrm{fi}} + \left(\frac{D_{\mathrm{i}}}{D_{\mathrm{o}}}\right)R_{\mathrm{fo}} \tag{4.10}$$

where the log mean diameter, D_{LM}

$$D_{\mathrm{LM}} = \frac{D_{\mathrm{o}} - D_{\mathrm{i}}}{\ln(D_{\mathrm{o}}/D_{\mathrm{i}})} \tag{4.11}$$

4.2.5.1 Tube Side Heat Transfer Coefficient, h_i

The heat transfer coefficient for inside tubes (h_{i}) can be calculated using Sieder–Tate equation for laminar flow [3]:

$$\mathrm{Nu}_{\mathrm{i}} = \frac{h_{\mathrm{i}}D_{\mathrm{i}}}{k_{\mathrm{i}}} = 1.86\left[\left(N_{\mathrm{Rei}}\right)\left(N_{\mathrm{Pri}}\right)\left(\frac{D_{\mathrm{i}}}{L}\right)\right]^{1/3}\left(\frac{\mu_{\mathrm{i}}}{\mu_{\mathrm{w}}}\right)^{0.14} \tag{4.12}$$

for turbulent flow, the heat transfer coefficient inside tubes (h_{i}) can be calculated using Sieder–Tate equation for the flow in a constant diameter pipe:

$$\mathrm{Nu}_{\mathrm{i}} = \frac{h_{\mathrm{i}}D_{\mathrm{i}}}{k_{\mathrm{i}}} = 0.027N_{\mathrm{Rei}}^{0.8}\,N_{\mathrm{Pri}}^{1/3}\left(\frac{\mu_{\mathrm{i}}}{\mu_{\mathrm{w}}}\right)^{0.14} \tag{4.13}$$

where

$$N_{\mathrm{Rei}} = \frac{\rho_{\mathrm{i}}u_{\mathrm{i}}D_{\mathrm{i}}}{\mu_{\mathrm{i}}} \quad \text{and} \quad N_{\mathrm{Pri}} = \frac{C_{p_{\mathrm{i}}}\mu_{\mathrm{i}}}{k_{\mathrm{i}}}$$

where ρ_{i}, u_{i}, D_{i}, μ_{i}, C_{pi}, and k_{i} are density, velocity, ID, viscosity, specific heat, and thermal conductivity of tube side fluid, respectively [7].

4.2.5.2 Shell Side Heat Transfer Coefficient, h_o

For turbulent flow, the kern method can be used [3]:

$$\mathrm{Nu}_o = \frac{h_o D_e}{k} = 0.36\, N_{\mathrm{Reo}}^{0.55}\, N_{\mathrm{Pro}}^{1/3} \left(\frac{\mu_o}{\mu_w}\right)^{0.14} \tag{4.14}$$

The Reynolds number, $N_{\mathrm{Reo}} = D_e V_{\max} \rho_o / \mu_o$, where D_e is the hydraulic effective diameter. $V_{\max}$ is the maximum velocity of the fluid through the tube bank which equals the shell side fluid volumetric flow rate divided by the shell side cross flow area. Among the physical properties (ρ, μ, k, and C_p), μ demonstrates the strongest dependence on temperature and has the largest effect on the transfer process. The hydraulic effective diameter,

$$D_e = \frac{4 \times \text{free area}}{\text{Wetted perimeter}} = \frac{4\left(P_t^2 - \pi D_o^2 / 4\right)}{\pi D_o} \tag{4.15}$$

To calculate the mass velocity normal to tubes at the centerline of the exchanger, G_o, first, the cross-sectional area between baffles and shell axis, A_{cf} is calculated,

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times b \tag{4.16}$$

where

$$\text{Clearance} = P_t - D_o \tag{4.17}$$

Since the flow entering the shell distributes itself into the space in which tubes are located, and then the flow turns around each baffle. An alternative method is used called the Donohue equation [3], the equation is based on the weighted average of the mass velocity of the shell-side fluid flowing parallel to the tubes (G_b) and the mass velocity of the shell-side fluid flowing across the tubes (G_c):

$$\left(\frac{h_o D_o}{k_o}\right) = 0.2\left(\frac{D_o G_e}{\mu_o}\right)^{0.6} \left(\frac{C_{p_o} \mu_o}{k_o}\right)^{0.33} \left(\frac{\mu_o}{\mu_w}\right)^{0.14} \tag{4.18}$$

where

$$G_e = (G_b\ G_c)^{1/2}$$

$$G_b = \dot{m}/S_b, \quad S_b = f_b \frac{\pi D_s^2}{4} - N_b \frac{\pi D_o^2}{4} \tag{4.19}$$

$$G_c = \dot{m}/S_c, \quad S_c = b \times D_s\left(1 - \frac{D_o}{p_t}\right) \tag{4.20}$$

f_b = fraction of the shell cross-section occupied by the baffle window, commonly 0.1995 for 25% baffle
N_b = number of tubes in baffle window = f_b × number of tubes
$\dot{m}$ = the mass flow rate of the shell-side fluid
D_o = OD of tubes
D_s = ID of the shell
b = baffle spacing
P_t = tube pitch

4.2.6 Pressure Drop

Allowable pressure drop for both streams is an important parameter for heat exchanger design. Generally, for liquids, a value of 7–10 psi is permitted per shell. A higher pressure drop is usually warranted for viscous liquids, especially in the tubeside. For gases, the allowed value is generally 0.7–3.0 psi, with 1.5 psi being typical [8].

4.2.6.1 Pressure Drop in the Tube Side

The pressure drop for flow of a liquid or gas without phase change through straight tubes can be calculated using the following equation:

$$-\Delta P_i = P_{in} - P_{out} = 1.2\frac{N_P f_D G_i^2 L}{2 g_c \rho_i D_i \phi} \tag{4.21}$$

where N_p is the number of tube passes and L is the tube length,

$$f_D = \left(1.82 \log_{10} N_{Rei} - 1.64\right)^{-2} \tag{4.22}$$

the tube side mass velocity, $G_i = \rho_i u_i$.

ϕ is the correction factor for the nonisothermal turbulent flow = 1.02 (μ/μ_w).

4.2.6.2 Pressure Drop in the Shell Side

The pressure drop for the flow of liquid without phase change across the tubes in the shell side is given by following equations [6]:

$$-\Delta P_o = P_{in} - P_{out} = K_s \frac{2 N_R f' G_o^2}{g_c \rho_c \phi} \tag{4.23}$$

$$N_{\text{reversals}} = \frac{L}{b} = \frac{\text{Length of tube}}{\text{Baffle spacing}} \tag{4.24}$$

The correction factor,

$$K_s = 1.1 \times N_{\text{reversals}} \tag{4.25}$$

The number of tubes at centerline

$$\cong D_s/P_t \tag{4.26}$$

The number of tube rows across which the shell fluid flows, N_R, which equals the total number of tubes at the center plane minus the number of tube rows that pass through the cut portions of the baffles. For 25% cut baffles, N_R may be taken as 50% of the number of the tubes at the center plane.

$$N_R = 0.5 \times \frac{D_s}{P_t} \tag{4.27}$$

The modification friction factor, f'

$$f' = b_f \left(\frac{D_o G_o}{\mu_o} \right)^{-0.15} \tag{4.28}$$

where b for square pitch is

$$b_f = 0.044 + \frac{0.08 x_L}{(x_T - 1)^{0.43 + 1.13/x_L}} \tag{4.29}$$

where the ratio of the pitch is transverse to the flow of the tube OD which is x_T, the ratio of pitch parallel to the tube OD is x_L.

For square pitch $x_L = x_T$; hence,

$$x_L = x_T = \frac{P_t}{D_o} \tag{4.30}$$

4.2.7 Alternative Pressure Drop Method

An alternative method is presented in the following sections which can be used to determine pressure drop in the tube side and the shell side of the shell and tube heat exchanger.

4.2.7.1 Pressure Drop in the Tube Side

The pressure drop in the tube side can be calculated using the following equation:

$$\Delta P_i = f\frac{L}{D}\left(\frac{1}{2}\rho V^2\right) \times N_p \tag{4.31}$$

where L is the length of the tubes, D is the ID of the tubes, ρ is the density of the tube side fluid, and V is the average flow velocity through a single tube, N_p is the number of tube passes. The fanning friction factor, f, can be calculated from Darcy friction factor, f_D

$$f_D = (1.82\log_{10} N_{Re} - 1.64)^{-2} \tag{4.32}$$

The Darcy friction factor is related to the Fanning friction factor by $f_D = 4f$.

4.2.7.2 Pressure Drop in the Shell Side

The pressure drop in the shell side can be calculated using the following equation:

$$\Delta P_{shell} = \frac{2f\,G_s^2 D_s\left(N_B + 1\right)}{\rho D_e\left(\mu/\mu_s\right)} \tag{4.33}$$

where f is the fanning friction factor for flow on the shell side [5], G_s the mass velocity on the shell side, D_s the ID of the shell, N_B the number of baffles, ρ the density of the shell-side fluid, and D_e an equivalent diameter. The mass velocity $G_s = m/S_m$, where m is the mass flow rate of the fluid, and S_m is the cross flow area measured close to the central symmetry plane of the shell containing its axis. The cross flow area, S_m

$$S_m = D_s \times L_B \times \frac{\text{clearance}}{\text{pitch}} \tag{4.34}$$

where L_B is the baffle spacing, the equivalent diameter, D_e, is defined as follows:

$$D_e = \frac{4\left(C_p S_n^2 - \pi D_o^2/4\right)}{\pi D_o} \tag{4.35}$$

where D_o is the OD of the tubes, and S_n is the pitch, center to center distance of the tube assembly. The constant $C_p = 1$ for a square pitch, and $C_p = 0.86$ for a triangular pitch [5]. The fanning friction factor is calculated using Reynolds number based on equivalent diameter as

$$R_e = \frac{D_e G_s}{\mu_o} \tag{4.36}$$

4.2.8 Summary of Design Steps

The following steps are used in designing a shell and tube heat exchanger:

1. The required heat duty Q_{req} is usually fixed by the required service and the designed heat exchanger has to meet or exceed this requirement.
2. Select the streams that should be placed on the tube side and shell side.
3. Calculate the heat transfer area required using a reasonable guess for the overall heat transfer coefficient.
4. Select suitable tube specifications (OD/ID/Pt and length).
5. Calculate tube cross-sectional area by assuming appropriate velocity inside tubes.
6. Estimate number of tubes and tube passes.
7. Estimate outside and inside film heat transfer coefficient.
8. Calculate the overall heat transfer coefficient and compare with assumed overall value.
9. If assumed U and estimated U are different, repeat the calculation by changing baffle spacing and re-estimating shell side film heat transfer coefficient.

4.3 Boilers and Condensers

Condensers are typically multipass shell and tube exchangers with floating heads. The heat is removed by contacting vapor with a cold surface (the tube wall). The liquid then flows off the tube under the influence of gravity, collects, and flows out of the exchanger. In some cases, vapor flow rates may be high enough to sweep the liquid off the tubes. Boilers are closed vessels in which water or other fluid is heated. The heated or vaporized fluid exits the boiler for use in various processes or heating applications. The correlation for predicting heat transfer coefficients are presented by Hewitt [10].

Example 4.1 DEA Solution and Water Exchanger

Design a shell and tube heat exchanger to cool 50,000 lb/h of diethanolamine (DEA) solution (0.2 mass fractions DEA/0.8 water) from 144°F to 113°F by using water at 77°F heated to 100°F. Assume tube inside fouling resistance, $R_{fi} = 0.004$ ft^2 h °F/Btu, ignoring shell side fouling resistance.

SOLUTION

HAND CALCULATIONS

The schematic diagram of the 1–4 shell-tube passes the heat exchanger is shown in Figure 4.1 and the physical properties of the shell side and tube side at average pass temperature is depicted in Table 4.4.

The required heat duty, Q_{req}

$$Q_{req} = \dot{m}_h Cp_h (T_{h,in} - T_{h,out}) = \dot{m}_c Cp_c (T_{c,out} - T_{c,in})$$

$$Q_{req} = 50{,}000 \frac{\text{lb}}{\text{h}} \times 0.92 \frac{\text{Btu}}{\text{lb}\,°\text{F}} \times (144 - 113)°\text{F} = 1.426 \times 10^6 \frac{\text{Btu}}{\text{h}}$$

The mass flow rate of cold stream

$$Q_{req} = m_c Cp_c (T_{c,in} - T_{c,out})$$

$$\dot{m}_c = \frac{Q_{req}}{Cp_c (T_{c,out} - T_{c,in})} = \frac{1.426 \times 10^6\,(\text{Btu/h})}{1.0(\text{Btu/lb}\,°\text{F}) \times (100 - 77)°\text{F}} = 62{,}000 \frac{\text{lb}}{\text{h}}$$

Assume an appropriate value of the overall heat transfer coefficient (U), the suitable designed overall heat transfer coefficient for DEA solution–water system, U is between 140 and 200 Btu/ft^2 h °F (Table 4.1).

$$\text{Assume} \quad U_i = 150 \frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

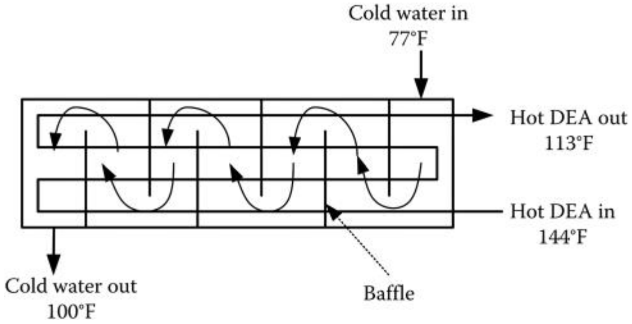


FIGURE 4.1
Process flowsheet for 1–4 DEA-water shell and tube heat exchanger.

TABLE 4.4

Physical Properties

Parameters	Tube Side (Hot) DEA Solution (128.5°F)	Shell Side (Cold) Water (88.5°F)
ρ (lb/ft^3)	59.76	59.87
C_p (Btu/lb °F)	0.92	1.0
μ (cP)	0.75	0.77
k (Btu/h ft °F)	0.30	0.36

The overall heat transfer area based on the tube outside area, A_i

$$A_\mathrm{i} = \frac{Q}{U_\mathrm{i} F \Delta T_\mathrm{LM}}$$

The overall heat transfer area based on the tube outside area, A_o

$$A_\mathrm{o} = \frac{Q}{U_\mathrm{o} F \Delta T_\mathrm{LM}}$$

The log means temperature difference, ΔT_LM

$$\Delta T_\mathrm{LM} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln\left[(T_1 - t_2)/(T_2 - t_1)\right]} = \frac{(144 - 100) - (113 - 77)}{\ln\left[(144 - 100)/(113 - 77)\right]} = 40°\mathrm{F}$$

The temperature range between hot and cold fluid, R,

$$R = \frac{T_1 - T_2}{t_2 - t_1} = \frac{144 - 113}{100 - 77} = 1.35$$

The range of cold fluid temperature to maximum temperature difference, S,

$$S = \frac{t_2 - t_1}{T_1 - t_1} = \frac{100 - 77}{144 - 77} = 0.343$$

The configuration factor, F can be found from figures in [4–8] or using the following equation:

$$F = \frac{\sqrt{R^2 + 1}\ln\left\{1 - S / 1 - R.S\right\}}{(R - 1)\ln\left[2 - S\left(R + 1 - \sqrt{R^2 + 1}\right)\Big/ 2 - S\left(R + 1 + \sqrt{R^2 + 1}\right)\right]}$$

Substituting values in the configuration factor, F

$$F = \frac{\sqrt{1.35^2+1}\ln\left\{\dfrac{1-0.343}{1-1.35\times 0.343}\right\}}{(1.35-1)\ln\left[\dfrac{2-0.343\left(1.35+1-\sqrt{1.35^2+1}\right)}{2-0.343\left(1.35+1+\sqrt{1.35^2+1}\right)}\right]} = \frac{1.68\times 0.2}{0.362} = 0.93$$

The inside heat transfer area, A_i,

$$A_i = \frac{Q}{U_i F \Delta T_{LM}} = \frac{1.426\times 10^6\,(\text{Btu/h})}{150\,(\text{Btu/ft}^2\,\text{h°F})\times 0.93\times 40°\text{F}} = 255\ \text{ft}^2$$

The velocity inside tubes should be assumed to maintain turbulent flow, an appropriate value is between 3 and 10 ft/s, let the velocity inside tubes be $u_i = 5$(ft/s). The total cross-sectional area per pass (DEA solution in the tube side), A_{ci}

$$A_{ci} = \frac{m_i}{\rho_i u_i} = \frac{50{,}000(\text{lb/h})}{\left(59.76\ \text{lb/ft}^3\right)\times 5(\text{ft/s})\times 3600(\text{s/h})} = 0.0465\ \text{ft}^2$$

Selecting tube length, $L = 14$ ft, OD = $\frac{3}{4}$, 11 BWG (ID = 0.482 in.)
The number of tubes per pass, N_t

$$N_t = \frac{A_{c_i}}{\pi D_i^2/4} = \frac{0.0465\ \text{ft}^2}{\pi(0.482\ \text{in.})^2/4}\times\frac{144\ \text{in.}^2}{\text{ft}^2} = 36.68\frac{\text{tube}}{\text{pass}} \cong 37\frac{\text{tube}}{\text{pass}}$$

Heat transfer area per tube, $A_t = \pi D_i L$

$$A_t = \pi D_i L = \pi(0.482\ \text{in.})\frac{\text{ft}}{12\ \text{in.}}\times 14\ \text{ft} = 1.75\frac{\text{ft}^2}{\text{tube}}$$

The number of tube passes, N_p

$$N_p = \frac{A_i}{A_t N_t} = \frac{255\ \text{ft}^2}{1.75(\text{ft}^2/\text{tube})\times 37(\text{tube/pass})} = 3.94\ \text{passes}$$

Let $N_p = 4$, then A_i, based on the new number of tube passes,

$$A_i = N_p N_t(\pi D_i)L = 4\times 37\times\pi\times\frac{0.482}{12}\times 14 = 262\ \text{ft}^2$$

The corrected overall heat transfer coefficient based on the corrected internal heat transfer area, U_i

$$U_i = \frac{1.426\times 10^6\,(\text{Btu/h})}{262\ \text{ft}^2\times 0.93\times 40°\text{F}} = 146\frac{\text{Btu}}{\text{ft}^2\,\text{h°F}}$$

The shell ID (D_s) is estimated using tabulated data [6] or using the relation given by Coulson and Richardson [8], D (tube bundle) = OD × $(N_t/k)^{1/n}$, where OD is the outside diameter of single tube, N_t is the number of tubes, and k and n are constants depending on the number of tube passes (for two passes $k = 0.249$ and $n = 2.207$). The calculation gives the size of the tube bundle and not the shell diameter. The shell diameter is now obtained from adding the tube bundle diameter and the clearance between the tube bundle and the shell. The clearance typical ranges from 10 to 90 mm [8]. Using Table 4.3 [6], in four tube passes exchanger and 148 tubes the shell ID, $D_s = 17\frac{1}{4}$ in.

An approximate number of baffles are twice the length of tubes in meters; if the tube length is 5 m, then the number of baffles is 10. More baffles can be added to increase the heat transfer coefficients, but the increase in number of baffles increases pressure drop, which must be kept within acceptable limits. The range of baffle spacing, b is

$$\left(\frac{D_s}{5}\right) < b < D_s$$

So, b is in the range: $\left(12\text{ in.}/5\right) < b < 17\frac{1}{4}$ in., let $b = 10$ in.

The shell side heat transfer coefficient, h_o, is estimated using the heat transfer equation from Kern [3].

$$\text{Nu}_o = \frac{h_o D_e}{k} = 0.36\, N_{\text{Reo}}^{0.55}\, N_{\text{Pro}}^{1/3} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

where $N_{\text{Reo}} = D_e G_o / \mu_o$ and $N_{\text{Pro}} = Cp_o \mu_o / k_o$.

The hydraulic effective diameter, D_e

$$D_e = \frac{4\left(P_t^2 - \pi D_o^2/4\right)}{\pi D_o} = \frac{4 \times \left(1^2 - \pi\left(0.75\right)^2/4\right)}{\pi \times 0.75} = 0.948\text{ in.}$$

The shell side mass velocity normal to tubes at centerline of exchanger is calculated by dividing the shell side mass flow rate to the cross-sectional area of the shell area between baffle and shell axis. The cross-sectional area between baffles and shell axis, A_{cf},

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times b$$

Substituting values to calculate the cross-sectional area between baffles and the shell axis, A_{cf}

$$A_{cf} = \frac{17.25\text{ in.}}{1\text{ in.}} \times \left(0.25\text{ in.}\frac{1\text{ ft}}{12\text{ in.}}\right) \times \left(10\text{ in.}\frac{\text{ft}}{12\text{ in.}}\right) = 0.30\text{ ft}^2$$

The shell side mass velocity, G_o

$$G_o = \frac{m_o}{A_{cf}} = \frac{62{,}000(\text{lb/h})}{0.30\ \text{ft}^2} = 207{,}026\frac{\text{lb}}{\text{ft}^2\ \text{h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{Reo} = \frac{D_e G_o}{\mu_o} = \frac{0.948\ \text{in.}(1\ \text{ft}/12\ \text{in.})207{,}026(\text{lb/ft}^2\ \text{h})}{0.77\ \text{cP} \times 1(\text{lb/ft s})(3600\ \text{s/h})/1488\ \text{cP}} = 8779$$

The Shell side Prandtl number, N_{Pro}

$$N_{Pro} = \frac{C_{p_o}\mu_o}{k_o} = \frac{1.0(\text{Btu/lb}\ ^\circ\text{F}) \times 0.77\ \text{cP}\ 1[(\text{lb/ft s})(3600\ \text{s/h})]/(1488\ \text{cP})}{0.36(\text{Btu/ft}^2\ \text{h}\ ^\circ\text{F})} = 5.2$$

Substituting values of Reynolds number and Prandtl number in the heat transfer equations and neglecting the effect of change in viscosity,

$$\text{Nu}_o = \frac{h_o D_e}{k_o} = 0.36\left(8779\right)^{0.55}\left(5.2\right)^{1/3}\left(1\right)^{0.14} = 92$$

The shell side heat transfer coefficient, h_o

$$h_o = \text{Nu}_o \frac{k_o}{D_e} = 92\frac{\left(0.36(\text{Btu/ft}^2\ \text{h}\ ^\circ\text{F})\right)}{0.948\ \text{in.} \times 1(\text{ft}/12\ \text{in.})} = 419\frac{\text{Btu}}{\text{ft}^2\ \text{h}\ ^\circ\text{F}}$$

The tube side heat transfer coefficient h_i is calculated using Sieder–Tate equation [6]:

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027 N_{Rei}^{0.8} N_{Pri}^{1/3}\left(\frac{\mu_i}{\mu_w}\right)^{0.14}$$

The tube side Reynolds number, N_{Rei}

$$N_{Rei} = \frac{D_i \rho_i u_i}{\mu_i} = \frac{0.482\ \text{in.}(1\ \text{ft}/12\ \text{in.})\left(59.76(\text{lb/ft}^3)\right)\left(5\ \text{ft/s}\right)}{0.75\ \text{cP} \times 1(\text{lb/ft s})/1488\ \text{cP}} = 23{,}812$$

The tube side Prandtl number, N_{Pri}

$$N_{Pri} = \frac{C_{p_i}\mu_i}{k_i} = \frac{0.92(\text{Btu/lb}\ ^\circ\text{F}) \times 0.75\ \text{cP}\left(1\ \text{lb/ft s}/1488\ \text{cP}\right) \times \left(3600\ \text{s/h}\right)}{0.30(\text{Btu/ft}^2\ \text{h}\ ^\circ\text{F})} = 5.56$$

Substituting estimated values of Reynolds number and Prandtl number in tube side film heat transfer coefficient,

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027\left(23{,}812\right)^{0.8}\left(5.56\right)^{1/3} \times 1 = 152$$

The tube side film heat transfer coefficient, h_i

$$h_\text{i} = \text{Nu}_\text{i}\frac{k}{D_\text{i}} = 152\frac{0.3(\text{Btu/ft h °F})}{0.482\text{ in.} \times (1\text{ ft}/12\text{ in.})} = 1133\frac{\text{Btu}}{\text{h ft}^2\text{ °F}}$$

The overall heat transfer coefficient based on internal area, U_i

$$\frac{1}{U_\text{i}} = \frac{D_\text{i}}{D_\text{o}h_\text{o}} + \frac{D_\text{i}\Delta x}{D_\text{LM}k_\text{w}} + \frac{1}{h_\text{i}} + R_\text{fi} + \left(\frac{D_\text{i}}{D_\text{o}}\right)R_\text{fo}$$

The tube thickness, Δx

$$\Delta x = \frac{D_\text{o} - D_\text{i}}{2} = \frac{0.75 - 0.482}{2} = 0.134\text{ in.}$$

The log mean diameter, D_LM,

$$D_\text{LM} = \frac{D_\text{o} - D_\text{i}}{\ln\left(D_\text{o}/D_\text{i}\right)} = \frac{0.75 - 0.482}{\ln\left(0.75\ /\ 0.482\right)} = 0.606\text{ in.}$$

The thermal conductivity of carbon steel is 30 Btu/h ft °F. The overall heat transfer coefficient based on the design specifications.

$$\frac{1}{U_\text{i}} = \frac{0.482\text{ in.}}{0.75\text{ in.} \times (419\text{Btu/ft}^2\text{ h°F})} + \frac{0.482\text{ in.} \times 0.134\text{ in.}(1\text{ ft}/12\text{ in.})}{0.606\text{ in.} \times 30(\text{Btu/h ft °F})}$$

$$+ \frac{1}{1133(\text{Btu/ft}^2\text{ h°F})} + 0.004\frac{\text{ft}^2\text{ h°F}}{\text{Btu}}$$

The overall heat transfer coefficient, U_i

$$\frac{1}{U_\text{i}} = 1.534 \times 10^{-3} + 2.96 \times 10^{-4} + 8.825 \times 10^{-4} + 0.004\frac{\text{ft}^2\text{ h°F}}{\text{Btu}}$$

$$= 4.71 \times 10^{-3}\frac{\text{ft}^2\text{ h°F}}{\text{Btu}}$$

The calculated U-value based on the exchanger designed specifications is

$$U_\text{i} = 149\frac{\text{Btu}}{\text{ft}^2\text{ h°F}}$$

Consequently,

$$U_\text{o} = U_\text{i}\frac{D_\text{i}}{D_\text{o}} = 149\frac{\text{Btu}}{\text{ft}^2\text{ h°F}} \times \frac{0.482}{0.75} = 95.6\frac{\text{Btu}}{\text{ft}^2\text{ h°F}}$$

The calculated overall heat transfer coefficient based on tube inside area (U_i = 149 Btu/h ft^2 °F), is close to the assumed designed value (U_i = 146 Btu/h ft^2 °F), consequently the specifications of the designed exchanger is satisfactory. If the calculated heat transfer coefficient based on the exchanger specifications is lower than the initially assumed value, then the heat provided by the designed exchanger is less than the required heat. The estimated heat transfer coefficient based on the exchanger design qualifications should be close to the assumed design value; the simplest way is to calculate the shell side heat transfer coefficient, h_o, based on assumed corrected value (i.e., U_i = 146 Btu/ft^2 h °F):

$$h_o = \frac{1}{D_o/D_i\left[1/U_i - 1/h_i - (D_i\Delta x/D_{LM}k) - R_{fi}\right]}$$

$$h_o = \frac{1}{(0.75/0.482)\left[(1/146) - (1/1133) - 2.96\times10^{-4} - 0.004\right]} = 385\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

The shell side Nusselt number, Nu_o

$$\text{Nu}_o = \frac{h_o D_e}{k_o} = \frac{385\,\text{Btu}/\text{ft}^2\,\text{h}\,°\text{F}\times(0.948\text{ in.})/(12\text{ in./ft})}{0.36\,\text{Btu/ft}\,\text{h}\,°\text{F}} = 84.36$$

The shell side Reynolds number, N_{Reo}

$$N_{Reo} = \left[\frac{\text{Nu}_o}{0.36\,N_{Pro}^{1/3}}\right]^{1/0.55} = \left[\frac{84.36}{0.36(5.2)^{1/3}}\right]^{1/0.55} = 7496$$

The shell side mass velocity,

$$G_o = \frac{N_{Reo}\mu_o}{D_e} = \frac{7496\times0.77\,\text{cP}\dfrac{\text{lb}}{1488\,\text{cP}}\bigg|\dfrac{\text{lb}}{\text{ft s}}\bigg|\dfrac{3600}{\text{h}}}{(0.948\text{ in.}/12\text{ in./ft})} = 176{,}758\frac{\text{lb}}{\text{ft}^2\,\text{h}}$$

The new shell side cross-sectional area, A_{cfo}

$$A_{cfo} = \frac{m_o}{G_o} = \frac{62{,}000\,\text{lb/h}}{176{,}758\,\text{lb/ft}^2\,\text{h}} = 0.35\,\text{ft}^2$$

The new baffle spacing b,

$$b = \frac{A_{cfo}}{D_s/P_t\times\text{Clearance}} = \frac{0.35\,\text{ft}^2\bigg|\dfrac{144\text{ in.}}{\text{ft}^2}}{\dfrac{17.25\text{ in.}}{1\text{ in.}}\times0.25\text{ in.}} = 11.75\text{ in.}$$

The new baffle spacing is 11.75 in., which is higher than the previously assumed value (b = 10 in.), the increase in baffle spacing, decreases shell side heat transfer coefficient. The pressure drop for the flow of liquid without phase change through a circular tube is given by the following equations [6]:

$$-\Delta P_o = P_{in} - P_{out} = K_s \frac{2N_R f' G_o^2}{g_c \rho_c \phi}$$

$$N_{reversals} = \frac{L}{b} = \frac{14\ \text{ft}}{11.75\ \text{in.}} \frac{12\ \text{in.}}{\text{ft}} = 14.30$$

The value of

$$K_s = 1.1 \times N_{reversals} = 1.1 \times 14.3 = 15.73$$

Number of tubes at centerline

$$\cong \frac{D_s}{P_t} = \frac{17.25\ \text{in.}}{1\ \text{in.}} = 17.25$$

The number of tube rows across which the shell fluid flows, N_R, equals the total number of tubes at the center plane minus the number of tube rows that pass through the cut portions of the baffles. For 25% cut baffles, N_R may be taken as 50% of the number of the tubes at the center plane.

$$N_R = 0.5 \times 17.25 = 8.625 \cong 9$$

The modification friction factor, f'

$$f' = b\left(\frac{D_o G_o}{\mu_o}\right)^{-0.15}$$

where b for square pitch is

$$b = 0.044 + \frac{0.08 x_L}{(x_T - 1)^{0.43 + 1.13/x_L}}$$

where x_T is the ratio of the pitch transverse to flow to tube OD and x_L is the ratio of pitch parallel to tube OD. For square pitch $x_L = x_T$

$$x_L = x_T = \frac{P_t}{D_o} = \frac{1}{0.75} = 1.33$$

Hence,

$$b = 0.044 + \frac{0.08 \times 1.333}{(1.333 - 1)^{0.43 + 1.13/1.333}} = 0.48$$

$$f' = b\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15} = 0.48\left(\frac{(0.75\text{ in./12 in./ft}) \times (176{,}758\text{ lb/ft}^2\text{ h})}{0.325\text{ cP} \times (\text{lb/ft s/1488 cP}) \times (3600\text{ s/h})}\right)^{-0.15}$$

$$= 0.1146$$

Substituting in the shell side pressure drop equation:

$$-\Delta P_o = K_s\frac{2N_Rf'G_o^2}{g_c\rho_c\varphi} = 15.73\frac{2 \times 9 \times 0.1146\left(\frac{176{,}758\text{ lb}}{\text{ft}^2\text{ h}}\bigg|\frac{\text{h}}{3600\text{ s}}\right)^2}{32.2(\text{ft lb/lb}_f\text{ s}^2) \times 59.87(\text{lb/ft}^3) \times 1} \times \frac{1\text{ ft}^2}{144\text{ in.}^2}$$

$$= 0.28\text{ psi}$$

Estimating the pressure drop in the tube side is much easier than calculated pressure drop in the shell side. The pressure drop in the tube side is calculated using the following equations [6]:

$$-\Delta P_i = 1.2\frac{N_Pf_DG_i^2L}{2g_c\rho_iD_i\phi}$$

where

$$f_D = \left(1.82\log_{10}N_{\text{Re i}} - 1.64\right)^{-2}$$

$$f_D = \left(1.82\log_{10}23{,}812 - 1.64\right)^{-2} = 0.025$$

Tube side mass velocity

$$G_i = \rho_iu_i = 59.76\frac{\text{lb}}{\text{ft}^3} \times 5\frac{\text{ft}}{\text{s}} = 298.8\frac{\text{lb}}{\text{ft}^2\text{ s}}$$

Substituting in pressure drop equation, $-\Delta P_i$

$$-\Delta P_i = 1.2\frac{N_Pf_DG_i^2L}{2g_c\rho_iD_i\phi}$$

$$= 1.2\frac{4 \times 0.025 \times \left(298.8(\text{lb/ft}^2\text{ s})\right)^2 \times 14\text{ ft}}{2 \times 32.2(\text{ft lb/lb}_f\text{ s}^2) \times 59.76(\text{lb/ft}^3) \times (0.482\text{ in./12 in./ft}) \times 1} \times \frac{1\text{ ft}^2}{144\text{ in.}}$$

$$= 6.74\text{ psi}$$

The summary of the resultant designed heat exchanger specifications is shown in Table 4.5.

HYSYS SIMULATION

The difference in the heat duty between hand calculations and Hysys and/or UniSim is due to the value of specific heat calculated using both softwares.

TABLE 4.5

Design Specifications

	Shell Side	Tube Side
Components	Water (100%)	DEA/water (0.2/0.8)
Mass flow rate (lb/h)	100,000	50,000
Temperature (°F)	77/100	144/113°F
Pressure (bar)	1.0	1.0
Pass	1	4
Shell ID (in.)	$17\frac{1}{4}$	
Tubes: OD/ID/P_t (in.)		0.75/0.482/1
Tube configuration		Square pitch
Length (ft)		14
Total number of tubes		148
Number of baffles		13
Baffle spacing (in.)	11.75	11.75
Fouling factor (ft^2 h °F/Btu)		0.004
Pressure drop (psi)	0.256	6.74
LMTD (°F)	40	
F factor	0.93	
U_o (Btu/h ft^2 °F)	93.83	
Duty (Btu/h)	1,426,000	

Hysys/Unisim has no features to calculate heat transfer coefficients of shell and tube sides. Start by opening new case in Hysys; add the component; water and DEA amine. NRTL was selected as the fluid package. In the connection page, S1, S2 are assigned for tube side streams and S3, S4 are for inlet and exit shell side streams, respectively.

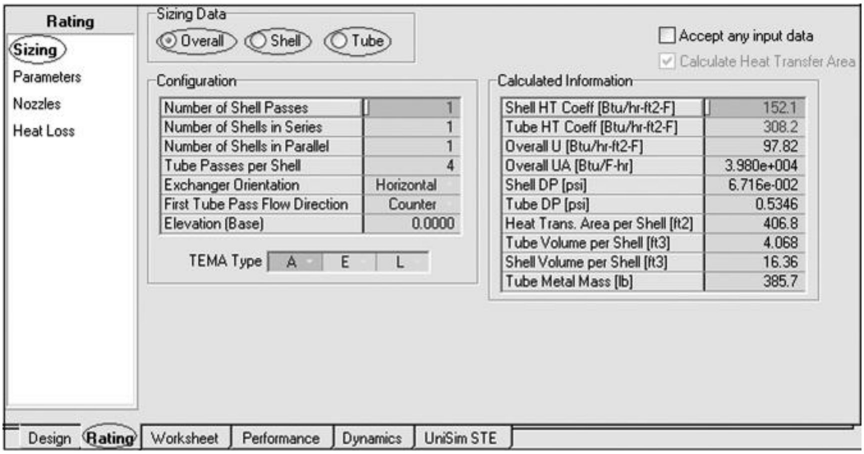
Double click on the exchanger icon in the PFD area, while in *Design*, *Parameters* page, *steady state rating* is selected from the pull down menu of *Heat Exchanger Model.* In the *Rating*, then *Sizing* page (Figure 4.2).

Overall: Tube passes per shell is 4 and number of shell passes is 1.

Shell: Shell diameter is 17.25 in., number of tubes per shell is 148 tubes, tube pitch is 1 in., tube layout is square, baffle cut is 25% and baffle spacing is 11.75 in. are provided.

Tube windows, OD/ID, tube length and tube fouling must be supplied (0.75/0.482 in., 14 ft, and 0.004 Btu/h ft^2 °F, respectively.

The final results could be seen in the performance page or a table can be generated by right click on the exchanger block, and then select show table. The table content can be modified by double clicking on the table and then adding or removing variables as shown in Figure 4.3. The Hysys calculated over all heat transfer coefficient is based on the area provided in the tube page, and is by dividing UA/A.



Sizing Data: ● Overall ○ Shell ○ Tube

☐ Accept any input data
☑ Calculate Heat Transfer Area

Configuration

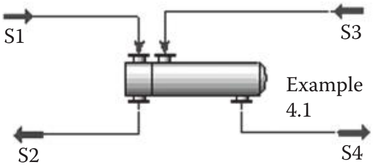
Number of Shell Passes	1
Number of Shells in Series	1
Number of Shells in Parallel	1
Tube Passes per Shell	4
Exchanger Orientation	Horizontal
First Tube Pass Flow Direction	Counter
Elevation (Base)	0.0000

TEMA Type: A E L

Calculated Information

Shell HT Coeff [Btu/hr-ft2-F]	152.1
Tube HT Coeff [Btu/hr-ft2-F]	308.2
Overall U [Btu/hr-ft2-F]	97.82
Overall UA [Btu/F-hr]	3.980e+004
Shell DP [psi]	6.716e-002
Tube DP [psi]	0.5346
Heat Trans. Area per Shell [ft2]	406.8
Tube Volume per Shell [ft3]	4.068
Shell Volume per Shell [ft3]	16.36
Tube Metal Mass [lb]	385.7

FIGURE 4.2
Sizing data menu.



Example 4.1		
Duty	1.454e+006	Btu/h
Shell side feed mass flow	6.200e+004	lb/h
Tube inlet temperature	144.0	F
Tube outlet temperature	113.0	F
Shell inlet temperature	77.00	F
Shell outlet temperature	100.2	F
Control UA	3.980e+004	Btu/F-h
LMTD	36.53	F
Overall U	97.82	Btu/h-ft^2-F
Uncorrected LMTD	39.77	F
Ft factor	0.9187	
Heat trans. area per shell	406.8	ft^2
Tube side pressure drop	0.5346	psi
Shell side pressure drop	6.716e–002	psi

FIGURE 4.3
Process flowsheet of exchanger specifications.

PRO/II SIMULATION

PRO/II has a rigorous model available for complex heat exchangers to help understand how this piece of equipment can be designed by manipulating different parameters. Use of the rigorous model allows for more accurate simulations to be run on the unit with a more detailed report of the findings. Many parameters were taken into consideration when designing the heat exchanger. These parameters include: number of tubes per shell, number of passes, tube configuration and length, heat transfer coefficients, area per shell, shell diameter, pitch, baffles, material type, and pressure drop. After approaching the heat exchanger design by hand, all specifications were retrieved and inputted into PRO/II to run a simulation on the design. The results of the simulation were compared against those obtained by hand to make sure there was reasonable agreement between the two.

The process flowsheet is performed by selecting the block *Rigorous HX* and connecting inlet and exit stream as shown in Figure 4.4. If the label of inlet streams and heat exchanger are in red color that means data is required. Click on the component selection icon and select water and diethanolamine. From the thermodynamic data, NRTL is used for this example. Double click on tube side stream S1 (DEA solution) and shell side inlet stream S3 (water) and specify flow rate, composition, temperature and pressure. Once these two streams are fully specified the label for stream S1 and S2 color changed to black.

Double clicking on the *Rigorous HX* block; a window will popup as shown in Figure 4.5. The data of the tubes, configuration, film coefficients, baffle, nozzles, and pressure drop should be provided (to fill in data click on the button of each item):

Tubes: ID 0.482 in., length 14 ft, OD 0.75 in., pitch 1 in., pattern square 90°.

Configuration: Number of tube passes/shell is 4.

Film coefficients: Overall *U*-value estimate is 100 Btu/h ft^2 °F, tubeside fouling resistance is 0.004 h ft^2 °F/Btu, shell side fouling resistance is 0 and scale factor is 1.

Baffle: Cut is 0.25 and the center spacing 11.75 in.

Nozzles: Tube side nozzle ID inlet and outlet is 4 in. and 3 in. for inlet and outlet of the shell side.

Pressure drop: Calculated using Pro II default setting.

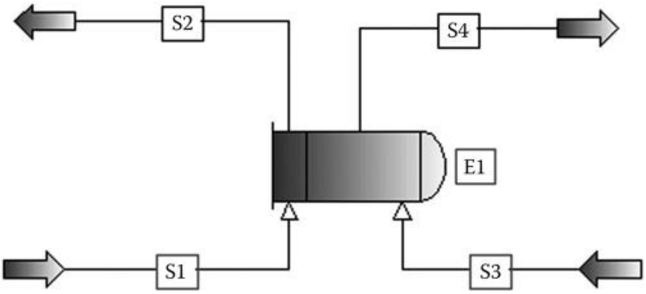
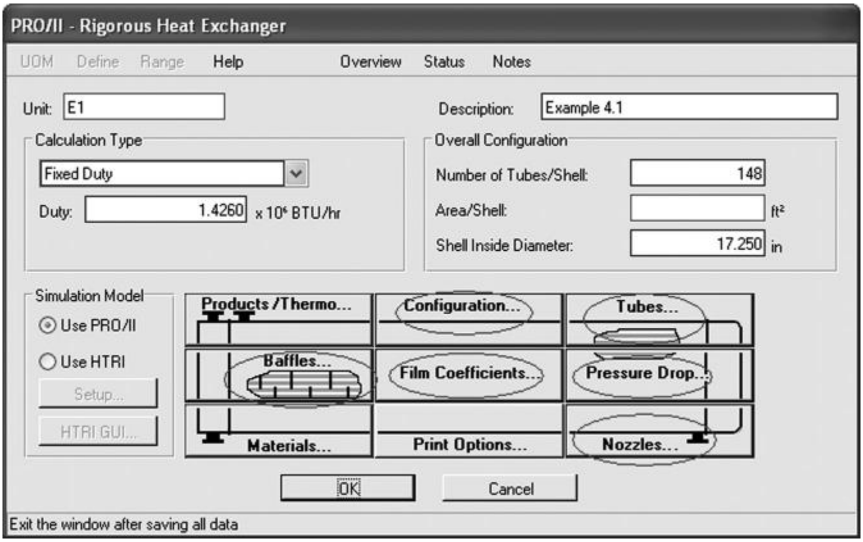


FIGURE 4.4
Process flowsheet of Rigorous HX in provision.



Unit: E1

Description: Example 4.1

Fixed Duty

Duty: 1.4260 x 10^6 BTU/hr

Number of Tubes/Shell: 148

Area/Shell: ft²

Shell Inside Diameter: 17.250 in

● Use PRO/II

○ Use HTRI

Exit the window after saving all data

FIGURE 4.5
Rigorous heat exchanger calculation type and overall configuration.

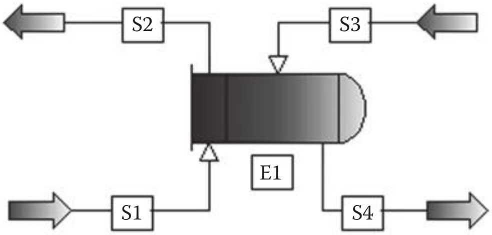
Filling in all the required data makes simulation ready to run. The process flowsheet, the stream table parameters and exchanger description is shown in Figure 4.6.

Aspen Plus Simulation

The flowing procedure can be used to simulate shell and tube heat exchanger with Aspen as follows: Log on to the Aspen Plus system and start a blank simulation. Click on *Heat Exchanger* tab in the model library and select *HeatX* which is used in rigorous design, it will calculate energy balance, pressure drop, exchanger area, velocities. *HeatX* exchanger requires two process streams; a hot and cold stream. This block will be used in design calculation for this example. Click anywhere in the PFD area to place exchanger icon. Click on the *Material streams* and connect the tube side and shell side streams with the red arrows on the exchanger block. Double click on inlet streams (tube side and shell side) and specify temperature, pressure, flow rate, and compositions.

Double click on the exchanger block, in the *Setup* page (Figure 4.7), under *Calculation* select *Detailed*. The *LMTD* and *Pressure Drop* are calculated from the exchanger design geometry. The overall heat transfer coefficient needs to specify how Aspen will calculate the *U*-value for the exchanger. There are several options, for this example, the *U*-value will be calculated from *Film coefficient*, which is calculated from individual heat transfer coefficient (h_o, h_i), more input is needed on another page for this option.

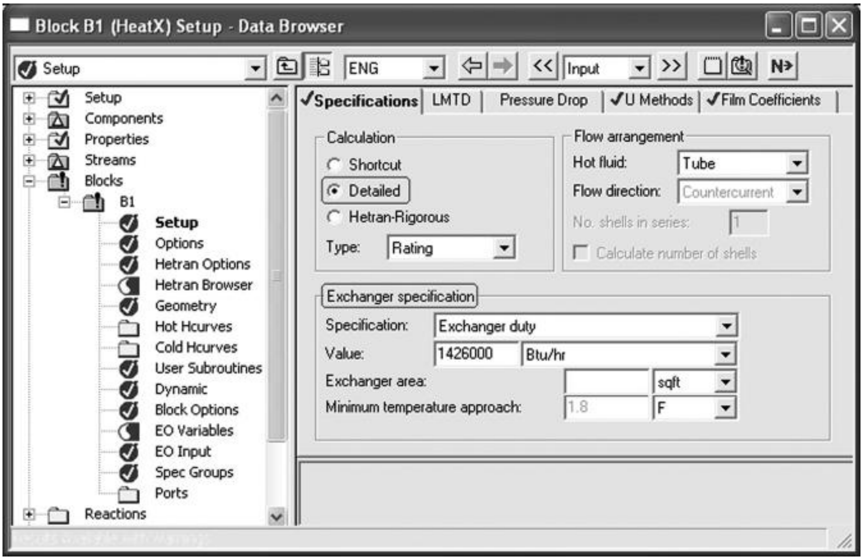
In this example, the Film coefficients are calculated from *Exchanger geometry* option, for both sides (hot and cold) of exchanger need to be specified. The fouling factors for each stream need to be provided in the space area. After the heat transfer coefficient calculations are specified, the next step is to set out the geometry



HxRig name HxRig description		E1 Example 4.1
Duty	MM Btu/h	1.4260
Area	ft^2	442.0124
U-Value	Btu/h-ft^2-F	193.4623
U-Value (Fouling)	Btu/h-ft^2-F	87.7729
LMTD	F	39.9295
FT factor		0.9205

Stream name		S1	S2	S3	S4
Temperature	F	144.000	113.151	77.000	100.037
Pressure	psia	14.700	6.421	14.700	14.195
Flowrate	lb-mol/h	2315.452	2315.452	3441.523	3441.523

FIGURE 4.6
PRO/II simulation results for Example 4.1.



Calculation
○ Shortcut
● Detailed
○ Hetran-Rigorous
Type: Rating

Flow arrangement
Hot fluid: Tube
Flow direction: Countercurrent
No. shells in series: 1
☐ Calculate number of shells

Exchanger specification
Specification: Exchanger duty
Value: 1426000 Btu/hr
Exchanger area: sqft
Minimum temperature approach: 1.8 F

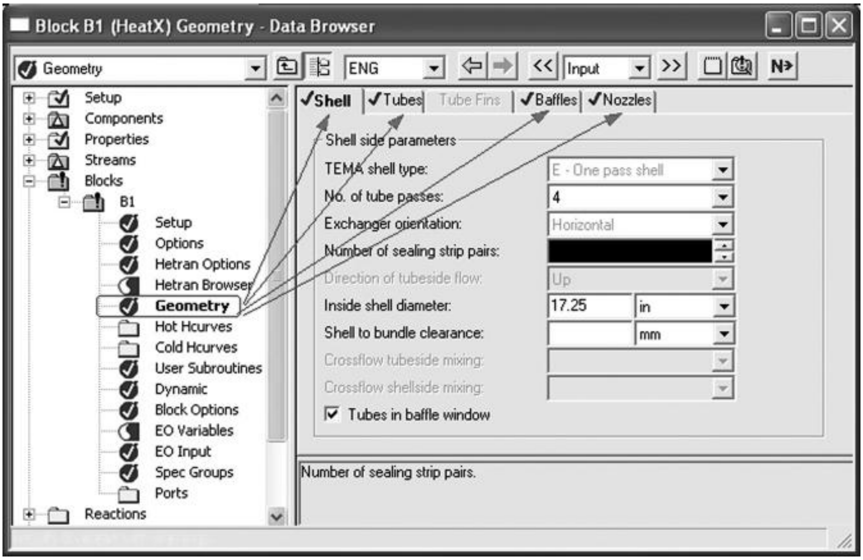
FIGURE 4.7
Setup page of the shell and tube heat exchanger.

of the heat exchanger. Since Aspen does not do every calculation, hand computation will be needed. User needs to supply the number of tube passes, the shell diameter, the number of tubes, the length of the tubes (typical values are 8–20 ft), and the inside and ODs of the tubes, the pitch, the material of tubes, the number of baffles and the baffle spacing.

The *Geometry* page is shown in Figure 4.8. On the *Shell* page, the number of tube passes and the shell ID need to be specified. On the *Tube* page, the number of tubes, outside/inside tube diameter, tube layout, and pitch needs to be provided. On the Baffles page, baffle type, number of baffles, baffle cut, and baffle spacing need to be provided. For the *baffle type*, segmental baffles are typical. In the *No. of baffles, all passes*, specify the number of baffles in the exchanger. More baffles can be added to increase the heat transfer coefficients, the pressure drop must be kept within acceptable limits. For the *Baffle cut*, specify the fraction of cross-sectional area for the shell fluid flow. For example, 0.25 means that one baffle covers 75% of the shell cross-sectional area while 25% is left for fluid flow. The *baffle cut* must be between 0 and 0.5. *Baffle to Baffle spacing*, if the baffle spacing is not known at the start of the simulation, the best way is to choose spacing between the tube sheet and the first/last baffle. Then Aspen will automatically calculate the inner baffle spacing [10]. In the *Nozzle* page, Shell side inlet and outlet nozzle diameter (approximately one-fourth shell ID) and tube side inlet and outlet nozzle diameter (approximately one-fifth shell ID) need to be supplied. The data used in carrying out this example are:

Shell: Number of tube passes is 4; inside shell diameter is 17.25 in.

Tubes: Tube number is 148, pattern square, length 14 ft, pitch 1 in., inner diameter 0.482, and outer diameter 0.75.



TEMA shell type: E - One pass shell

No. of tube passes: 4

Exchanger orientation: Horizontal

Number of sealing strip pairs:

Direction of tubeside flow: Up

Inside shell diameter: 17.25 in

Shell to bundle clearance: mm

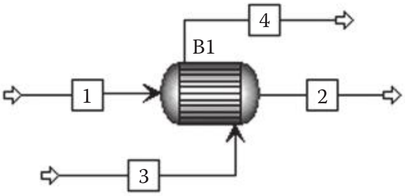
Crossflow tubeside mixing:

Crossflow shellside mixing:

☑ Tubes in baffle window

Number of sealing strip pairs.

FIGURE 4.8
Geometry page.



Example 4.1					
Stream ID		1	2	3	4
Temperature	F	144.0	111.4	77.0	101.7
Pressure	psi	14.70	8.82	14.70	14.45
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	lbmol/h	2315.452	2315.452	3441.523	3441.523
Mass flow	lb/h	50000.000	50000.000	62000.000	62000.000
Volume flow	cuft/h	833.567	817.620	999.628	1013.208
Enthalpy	MMBtu/h	–290.008	–291.434	–422.694	–421.268
Mole flow	lbmol/h				
DIETH-01		95.114	95.114		
WATER		2220.337	2220.337	3441.523	3441.523

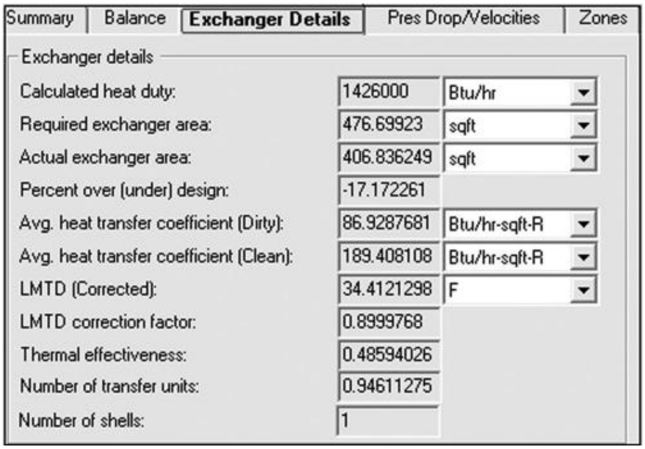
FIGURE 4.9
Exchanger process flow sheet and stream table properties.

Baffles: Number of baffles all passes is 13, baffle cut 0.25, baffle to baffle spacing 12 in.
Nozzles: Shell inlet and outlet nozzle diameter is 4 in. Tube side inlet and outlet nozzle diameter is 3 in.

The simulation is now ready to run. Click on *Next* and run the simulation. If some of the required input is incomplete, then Aspen will point to the appropriate input sheet where the input is needed. Process flow sheet and stream table properties are shown in Figure 4.9. The summary of results page for the heat exchanger is shown on the *Exchanger Details* page (Figure 4.10).

SuperPro Designer Simulation

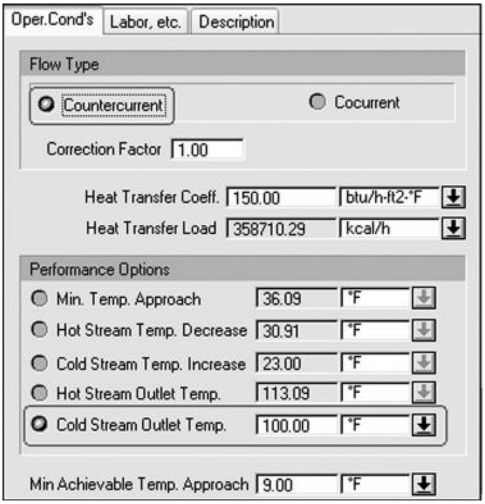
The heat exchange in the SuperPro designer calculates only simple energy balance. Once the inlet stream conditions are provided, the product stream is calculated. From the *Unit Procedure* in the tool bar menu, *Heat exchange*, and then *Heat exchanging* is selected. While in the Connection Mode, inlet and exit streams are connected. From the *Tasks* Menu, *Edit Pure component* is selected, exchanger components are registered. After feed stream temperature, pressure, flow rates, and compositions are specified. By double clicking on the heat exchanger, the operation conditions page is displayed where the *Flow type* (counter current) and the Performance options (cold stream outlet temperature = 100°F) are selected as shown in Figure 4.11.



Exchanger details

Calculated heat duty: 1426000 Btu/hr
Required exchanger area: 476.69923 sqft
Actual exchanger area: 406.836249 sqft
Percent over (under) design: -17.172261
Avg. heat transfer coefficient (Dirty): 86.9287681 Btu/hr-sqft-R
Avg. heat transfer coefficient (Clean): 189.408108 Btu/hr-sqft-R
LMTD (Corrected): 34.4121298 F
LMTD correction factor: 0.8999768
Thermal effectiveness: 0.48594026
Number of transfer units: 0.94611275
Number of shells: 1

FIGURE 4.10
Exchanger detailed design specifications.



Flow Type

● Countercurrent ○ Cocurrent

Correction Factor 1.00

Heat Transfer Coeff. 150.00 btu/h-ft2-°F
Heat Transfer Load 358710.29 kcal/h

Performance Options

○ Min. Temp. Approach 36.09 °F
○ Hot Stream Temp. Decrease 30.91 °F
○ Cold Stream Temp. Increase 23.00 °F
○ Hot Stream Outlet Temp. 113.09 °F
● Cold Stream Outlet Temp. 100.00 °F

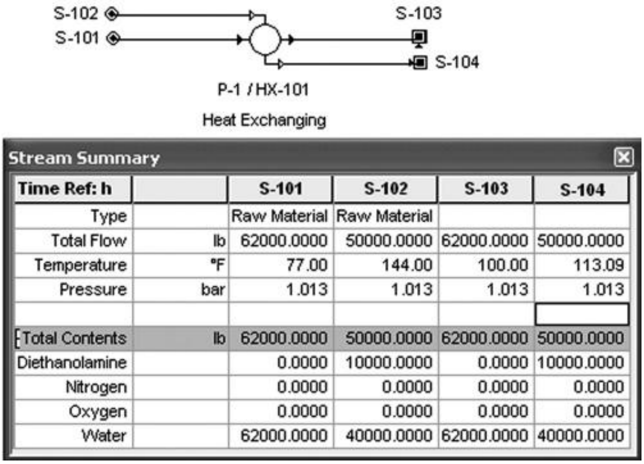
Min Achievable Temp. Approach 9.00 °F

FIGURE 4.11
Heat exchanger operating conditions.

The material balance icon can be clicked to run the simulation. The output can be presented by stream table summary shown in Figure 4.12.

Example 4.2 Design of a Propanol Condensor

Saturated vapor of *n*-propanol is flowing at 165,000 lb/h is to be condensed in an existing shell and tube heat exchanger. The exchanger contains 900 steel tubes



Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	lb	62000.0000	50000.0000	62000.0000	50000.0000
Temperature	°F	77.00	144.00	100.00	113.09
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	lb	62000.0000	50000.0000	62000.0000	50000.0000
Diethanolamine		0.0000	10000.0000	0.0000	10000.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		62000.0000	40000.0000	62000.0000	40000.0000

FIGURE 4.12
Heat exchanger process flow sheet and stream summary.

(18 BWG, 12 ft long, $\frac{3}{4}$ in. OD on a $\frac{15}{16}$ triangular pitch in a 37 in. ID shell). The exchanger is 1 shell and 2 pass. The *n*-propanol flows in the shell side and cooling water flows in the tube side. If the cooling water enters at 75°F and exits at 115°F, will the exchanger work?

Data:

Boiling point of *n*-propanol at 2.3 bar = 244°F
Latent heat of vaporization = 257 Btu/lb
Thermal conductivity of the tubes = 26 Btu/h ft °F
Shell side heat transfer coefficient = 1200 Btu/h ft^2 °F
Tube side heat transfer coefficient = 200 Btu/h ft^2 °F
Fouling resistance for water = 0.004 h ft^2 °F/kJ

SOLUTION

HAND CALCULATIONS

The schematic diagram of the *n*-propanol–water exchanger is shown in Figure 4.13.

The required heat duty to condense *n*-propanol at 2.3 bar,

$$Q_{\text{required}} = \dot{m}\lambda = 165{,}000\,\frac{\text{lb}}{\text{h}} \times 257\,\frac{\text{Btu}}{\text{lb}} = 4.24 \times 10^7\,\frac{\text{Btu}}{\text{h}}$$

where m is the mass flow rate of propanol and λ is the latent heat of vaporization at condenser operating pressure. The cold stream mass flow rate, $\dot{m}_c$

$$\dot{m}_c = \frac{4.24 \times 10^7\,\text{Btu/h}}{1.0\,\text{Btu/lb}\,°\text{F} \times (115 - 75)°\text{F}} = 1.06 \times 10^6\,\frac{\text{lb}}{\text{h}}$$

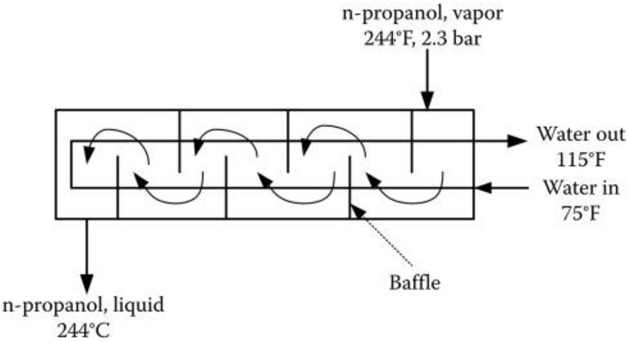


FIGURE 4.13
Schematic diagram of propanol–water exchanger.

The amount of heat with the existing heat exchanger is calculated as follows:

$$Q = U_o A_o F \Delta T_{LM}$$

The correction factor for condensation, $F = 1$

$$\Delta T_{LM} = \frac{(244 - 75) - (244 - 115)}{\ln\left(244 - 75 / 244 - 115\right)} = 148°\text{F}$$

The tubes outside total heat transfer surface area, A_o

$$A_o = N_t\left(\pi D_o L\right) = 900\left(\pi \times 0.75\,\text{in.} \frac{1\,\text{ft}}{12\,\text{in.}} \times 12\,\text{ft}\right) = 2120\,\text{ft}^2$$

The tubes inside heat transfer surface area, A_i

$$A_i = N_t\left(\pi D_i L\right) = 900\left(\pi \times 0.652\,\text{in.} \frac{1\,\text{ft}}{12\,\text{in.}} \times 12\,\text{ft}\right) = 1843\,\text{ft}^2$$

The thickness of the tube wall, Δx

$$\Delta x = \frac{0.75 - 0.652}{2} = 0.049\,\text{in.}$$

The log means area, A_{LM}

$$A_{LM} = \frac{A_o - A_i}{\ln(A_o / A_i)} = \frac{2120 - 1843}{\ln(2120/1843)} = 1978\,\text{ft}^2$$

The overall heat transfer coefficient based on outside area, U_o

$$\frac{1}{U_o} = \frac{A_o}{A_i h_i} + \frac{A_o \Delta x}{A_{LM} k_w} + \frac{1}{h_o} + R_{fi}\frac{A_o}{A_i} + R_{fo}$$

Substituting required values in the above equations,

$$\frac{1}{U_o} = \frac{2120\,\text{ft}^2}{1843\,\text{ft}^2\left(\dfrac{200\,\text{Btu}}{\text{h}\,\text{ft}^2\,°\text{F}}\right)_i} + \frac{2120\,\text{ft} \times 0.049\,\text{in.}(1\,\text{ft}/12\,\text{in.})}{1978\,\text{ft}^2 \times (26\,\text{Btu}/\text{h}\,\text{ft}\,°\text{F})} + \frac{1}{\left(\dfrac{1200\,\text{Btu}}{\text{h}\,\text{ft}^2\,°\text{F}}\right)}$$

$$+\, 0.004\frac{\text{h}\,\text{ft}^2\,°\text{F}}{\text{Btu}}\left|\frac{2120\,\text{ft}^2}{1843\,\text{ft}^2}\right.$$

Solving for the overall heat transfer coefficient.

$$\frac{1}{U_o} = 5.75 \times 10^{-3} + 1.68 \times 10^{-4} + 8.33 \times 10^{-4} + 4.6 \times 10^{-3} = 0.0113\frac{\text{h}\,\text{ft}^2\,°\text{F}}{\text{Btu}}$$

The calculated overall heat transfer coefficients,

$$U_o = 88.1\frac{\text{Btu}}{\text{h}\,\text{ft}^2\,°\text{F}}$$

The heat provided by the system design, Q_{design}

$$Q_{\text{design}} = U_o A_o F \Delta T_{\text{LM}} = 88.1\frac{\text{Btu}}{\text{h}\,\text{ft}^2\,°\text{F}} \times 2120\,\text{ft}^2 \times 1 \times 148°\text{F} = 2.76 \times 10^7\,\frac{\text{Btu}}{\text{h}}$$

The heat required is more than heat provided by the system design ($Q_{\text{required}} > Q_{\text{design}}$), and therefore, the existence heat exchanger is not satisfactory. The summary of the designed exchanger specifications are shown in Table 4.6.

HYSYS SIMULATION

The process flow sheet is constructed by selecting the *Heat Exchanger* icon in the object pallet. NRTL fluid package was used. While in *Design/Parameters* page, for *Heat Exchanger Model*, the *Exchanger Design (weighed)* is selected from the pull-down menu. Pressure drop needs to be specified or set to zero for both shell and tube side. In the *Rating/Sizing* page the overall UA is supplied from the hand calculation section (1.866×10^5 Btu/h°F) as shown in Figure 4.14. Shell side and tube side data were taken from the hand calculations. Once the required data are filled in, the results should appear as those in Figure 4.15.

The heat duty obtained by Unisim is higher than the value obtained with hand calculations. This is due to the value of the latent heat of vaporization calculated by Unisim.

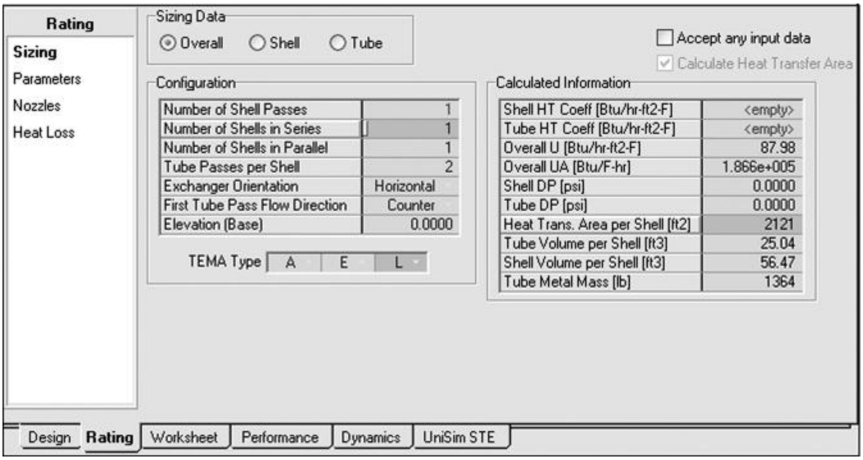
PRO/II SIMULATION

Using the *Rating* mode under the calculation type and specifying tube side and shell side film coefficients. The Pro II simulated results are in good agreement with hand calculations. Results show that the heat provided by the designed exchanger is less than the required heat duty. The process flow sheet and stream table properties obtained using Pro II software is shown in Figure 4.16.

TABLE 4.6

Design Specifications

	Shell Side	Tube Side
Components	*n*-Propanol	Water
Mass flow rate (lb/h)	165,000	1,060,000
Temperature (°F)	244(vapor)/244(liquid)	75/115°F
Pressure (bar)	1.0	1.0
Pass	1	2
Shell ID (in.)	37	
Tubes: OD/ID/P_t (in.)		0.75/0.652/0.9375
Tube configuration		Triangle pitch
Length (ft)		12
Total number of tubes		900
Number of baffles		2
Baffle spacing (in.)		55
Fouling factor (ft^2 h °F/Btu)		0.004
LMTD (°F)	148	
F factor	1.0	
U_o (Btu/h ft^2 °F)	88.1	
Duty (Btu/h)	2.76×10^7	



Sizing Data: ● Overall ○ Shell ○ Tube

☐ Accept any input data

☑ Calculate Heat Transfer Area

Configuration

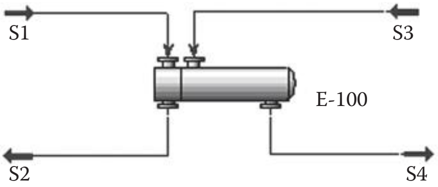
Number of Shell Passes	1
Number of Shells in Series	1
Number of Shells in Parallel	1
Tube Passes per Shell	2
Exchanger Orientation	Horizontal
First Tube Pass Flow Direction	Counter
Elevation (Base)	0.0000

TEMA Type A E L

Calculated Information

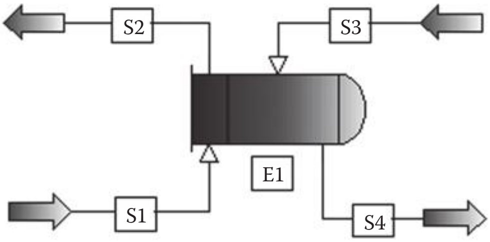
Shell HT Coeff [Btu/hr-ft2-F]	<empty>
Tube HT Coeff [Btu/hr-ft2-F]	<empty>
Overall U [Btu/hr-ft2-F]	87.98
Overall UA [Btu/F-hr]	1.866e+005
Shell DP [psi]	0.0000
Tube DP [psi]	0.0000
Heat Trans. Area per Shell [ft2]	2121
Tube Volume per Shell [ft3]	25.04
Shell Volume per Shell [ft3]	56.47
Tube Metal Mass [lb]	1364

FIGURE 4.14
Sizing data of heat exchanger.



E-100		
Duty	2.893e+007	Btu/h
Tube side feed mass flow	1.060e+006	lb/h
Shell side feed mass flow	1.650e+005	lb/h
Tube inlet temperature	75.00	F
Tube outlet temperature	102.0	F
Shell inlet temperature	244.0	F
Shell outlet temperature	244.0	F
Control UA	1.866e+005	Btu/F-h
Overall U	87.98	Btu/h-ft2-F
LMTD	155.1	F

FIGURE 4.15
Process flow sheet streams summary.



HxRig name		E1
HxRig description		Example 4.2
Duty	MMBtu/h	27.6977
Area	ft^2	2026.9386
U-Value	Btu/h-ft^2-F	148.0547
U-Value (Fouling)	Btu/h-ft^2-F	88.0632
LMTD	F	155.1914
FT factor		0.9999

Stream name		S1	S2	S3	S4
Temperature	F	75.000	101.171	244.000	243.247
Pressure	psia	14.700	12.817	50.720	50.065
Flowrate	lbmol/h	58838.941	58838.941	2745.611	2745.611

FIGURE 4.16
Process flow sheet and stream table conditions.

ASPEN SIMULATION

In the block setup page, Detailed, *Simulation* mode is selected. The method of calculating overall heat transfer coefficient is *Film coefficients*, and then in the film coefficient page, the constant value is selected. Value of tube side film coefficient and shell side is specified. In the geometry page:

Shell: Shell ID is 37 in., tube number is 900, tube length is 12 ft, tubes outside/ID is 0.75 in./0652 in. triangle pitch 15/16 in.

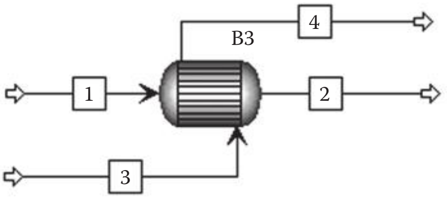
Baffle: Baffle cut is 0.25, baffle spacing is 40 in., and baffle number is 2.

Nozzle: Shell side inlet nozzle and outlet nuzzle diameter is 9 in., tube side inlet and outlet nuzzle is 7 in.

Specifying all necessary data, the process flow sheet and stream table properties is shown in Figure 4.17. Detailed exchanger description is shown Figure 4.18.

SUPERPRO SIMULATION

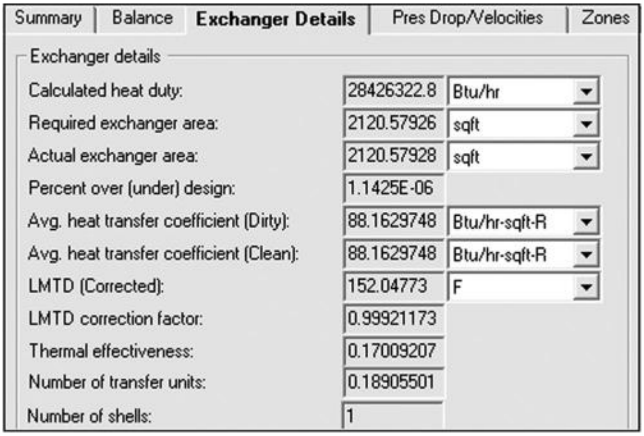
With SuperPro only simple energy balance is done. The process is carried out by providing temperature, pressure, flow rates, and compositions of the two inlet streams and providing the temperature of one of the exit streams. The results are shown in Figure 4.19.



Example 4.2

Stream ID		1	2	3	4
Temperature	F	75.0	103.8	244.0	239.8
Pressure	psi	14.50	9.48	30.37	28.09
Vapor frac		0.000	0.000	1.000	0.404
Mole flow	lbmol/h	58838.941	58838.941	2745.611	2745.611
Mass flow	lb/h	1.06000E+6	1.06000E+6	165000.000	165000.000
Volume flow	cuft/h	17072.015	17342.735	682767.868	298456.096
Enthalpy	MMBtu/h	−7228.654	−7200.227	−290.708	−319.134
Mole flow	lbmol/h				
WATER		58838.941	58838.941		
1-PRO-01				2745.611	2745.611

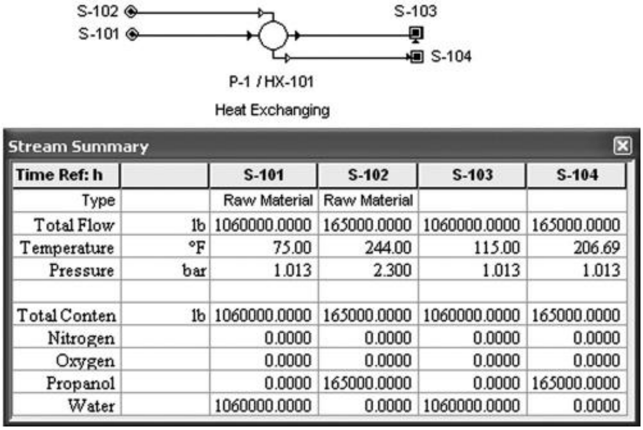
FIGURE 4.17
Process flow sheet and stream table properties.



Exchanger details

Calculated heat duty:	28426322.8	Btu/hr
Required exchanger area:	2120.57926	sqft
Actual exchanger area:	2120.57928	sqft
Percent over (under) design:	1.1425E-06	
Avg. heat transfer coefficient (Dirty):	88.1629748	Btu/hr-sqft-R
Avg. heat transfer coefficient (Clean):	88.1629748	Btu/hr-sqft-R
LMTD (Corrected):	152.04773	F
LMTD correction factor:	0.99921173	
Thermal effectiveness:	0.17009207	
Number of transfer units:	0.18905501	
Number of shells:	1	

FIGURE 4.18
Exchanger detailed results simulated with Aspen.



Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	lb	1060000.0000	165000.0000	1060000.0000	165000.0000
Temperature	°F	75.00	244.00	115.00	206.69
Pressure	bar	1.013	2.300	1.013	1.013
Total Conten	lb	1060000.0000	165000.0000	1060000.0000	165000.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Propanol		0.0000	165000.0000	0.0000	165000.0000
Water		1060000.0000	0.0000	1060000.0000	0.0000

FIGURE 4.19
Stream summary generated with SuperPro designer.

CONCLUSIONS

Hand calculations and Software simulations were in good agreement in the sense that the existing exchanger is not able to provide the required heat duty to condense the shell side saturated vapor n-propanol. Exit streams shows that the propanol is partially liquefied. Comparing software results with hand calculations shows that results obtained with Pro II is the closest to the hand computations.

Example 4.3 Ethylene Glycol–Water Heat Exchanger

Design a shell and tube heat exchanger for 100,000 lb/h of ethylene glycol (EG) at 250°F cooled to 130°F using cooling water heated from 90°F to 120°F. Assume that the tube side fouling resistance is 0.004 (h ft^2 °F)/Btu and neglecting shell side fouling resistance.

SOLUTION

Hand Calculations

The schematic diagram of the exchanger process flow sheet is shown in Figure 4.20.

The physical properties of the shell side and tube side fluids determined at average temperatures are shown in Table 4.7.

Assuming that ethylene glycol enters the shell side of the heat exchanger and cooling water is flowing inside the tubes, the required heat duty, Q_{req}

$$Q_{\text{req}} = m_o Cp_o \Delta T_o = 100{,}000 \frac{\text{lb}}{\text{h}} \times 0.65 \frac{\text{Btu}}{\text{lb °F}} \left(250 - 130\right)\text{°F} = 7.8 \times 10^6 \frac{\text{Btu}}{\text{h}}$$

The mass flow rate of the cooling stream (tube side), $\dot{m}_i$

$$\dot{m}_i = \frac{Q_{\text{req}}}{Cp_i \Delta T_i} \frac{7.8 \times 10^6 \,\text{Btu/h}}{1.01 \,\text{Btu/lb °F} \left(120 - 90\right)\text{°F}} = 260{,}000 \frac{\text{lb}}{\text{h}}$$

The log means temperature difference, ΔT_{LM}

$$\Delta T_{\text{LM}} = \frac{(250 - 120) - (130 - 90)}{\ln\left(250 - 120/130 - 90\right)} = 76.4\text{°F}$$

The correction factor, F

$$F = \frac{\left[\sqrt{R^2 + 1}/R - 1\right] \ln\left[1 - S/1 - SR\right]}{\ln\left[A + \sqrt{R^2 + 1}/A - \sqrt{R^2 + 1}\right]}$$

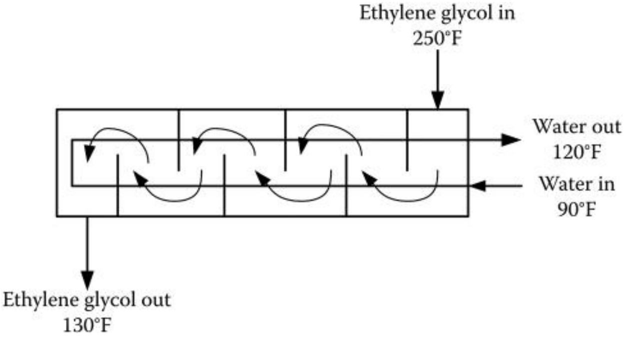


FIGURE 4.20
Schematic diagram of ethylene glycol–water countercurrent exchanger.

TABLE 4.7

Physical Properties at Average Temperatures

	Shell Side	Tube Side
Parameters	Ethylene glycol (190°F)	Water (105°F)
ρ (lb/ft^3)	68.6	62.4
C_p (Btu/lb °F)	0.65	1.01
μ (cP)	3.50	0.67
k (Btu/h ft °F)	0.16	0.363

where

$$R = \frac{T_{\mathrm{h,in}} - T_{\mathrm{h,out}}}{T_{\mathrm{c,out}} - T_{\mathrm{c,in}}} = \frac{250 - 130}{120 - 90} = 4.0$$

$$S = \frac{T_{\mathrm{c,out}} - T_{\mathrm{c,in}}}{T_{\mathrm{h,in}} - T_{\mathrm{c,in}}} = \frac{120 - 90}{250 - 90} = 0.188$$

$$A = \frac{2}{S} - 1 - R = \frac{2}{0.188} - 1 - 4 = 5.64$$

Substituting values of R, S, and A to calculate F:

$$F = \frac{\left[\sqrt{4^2 + 1}/4 - 1\right] \ln\left[1 - 0.188/1 - 0.188 \times 4\right]}{\ln\left[5.64 + \sqrt{4^2 + 1}/5.64 - \sqrt{4^2 + 1}\right]} = 0.85$$

Assuming a reasonable guess for the overall heat transfer coefficient, let $U_{\mathrm{i}} = 100$ Btu/ft^2 h °F; consequently, the inside overall heat transfer area, A_{i} is

$$A_{\mathrm{i}} = \frac{Q_{\mathrm{req}}}{U_{\mathrm{i}} F \Delta T_{\mathrm{LM}}} = \frac{7.8 \times 10^6 \,\mathrm{Btu/h}}{100 \,\mathrm{Btu/ft^2\,h\,°F} \times 0.85 \times 76.4\,\mathrm{°F}} = 1200 \,\mathrm{ft}^2$$

Assuming that the tube side fluid velocity is 5 ft/s, the total inside tubes cross-sectional area/pass, A_{ci}

$$A_{\mathrm{ci}} = \frac{F_{\mathrm{i}}}{u_{\mathrm{i}}} = \frac{m_{\mathrm{i}}/\rho_{\mathrm{i}}}{u_{\mathrm{i}}} = \frac{260{,}000 \,\mathrm{lb/h} \ / \ 62.4 \,\mathrm{lb/ft^3}}{5 \,\mathrm{ft} \ / \ \mathrm{s} \times \mathrm{h} \ / \ 3600 \,\mathrm{s}} = 0.2315 \,\mathrm{ft}^2/\mathrm{pass}$$

The approximate number of tubes required for the job must be determined. For this purpose, tube dimensions should be selected. For this example the selected tubes have an OD of $\frac{3}{4}$ in., 16 BWG tubing (ID = 0.62 in.) arranged on a 1-in. square pitch and length of tube 18 ft. The inside cross-sectional area per tube, A_{tc}

$$A_{\mathrm{tc}} = \frac{\pi D_{\mathrm{i}}^2}{4} = \frac{\pi \times (0.62 \,\mathrm{in.})^2}{4} = 0.302 \,\mathrm{in.}^2/\mathrm{tube}$$

The total number of tubes per pass, N_t

$$N_t = \frac{A_{ci}}{A_{tc}} = \frac{0.2315\ \text{ft}^2}{0.302\ \text{in.}^2/\text{tube}}\frac{144\ \text{in.}^2}{\text{ft}^2} = 110\ \text{tube/pass}$$

The inside surface area per tube, A_t

$$A_t = \pi D_i L = \pi \times 0.62\frac{\text{in.}}{12\ \text{in./ft}} \times 18\ \text{ft} = 2.925\ \text{ft}^2$$

The total number of tube passes, N_p

$$N_p = \frac{A_i}{N_t\,A_t} = \frac{1200\ \text{ft}^2}{2.925(\text{ft}^2/\text{tube}) \times 110\ \text{tubes/pass}} = 3.73\ \text{passes}$$

Since there is no 3.73 passes the number of tube passes is rounded to 4 ($N_p = 4$); consequently, the total heat transfer area, A_i, must be corrected,

$$A_i = N_p N_t\left(\pi D_i L\right) = 4 \times 110 \times \pi \times 0.62\,\text{in.}\frac{1\,\text{ft}}{12\,\text{in.}} \times 18\,\text{ft} = 1285\,\text{ft}^2$$

Since the inside heat transfer area is changed, the overall heat transfer coefficient must be corrected accordingly.

$$U_i = \frac{Q_{req}}{A_i F \Delta T_{lm}} = \frac{7.8 \times 10^6\ \text{Btu/h}}{1285\ \text{ft}^2 \times 0.85 \times 76.4^\circ\text{F}} = 93.46\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,^\circ\text{F}}$$

The overall heat transfer coefficient of the designed heat exchanger must be calculated to be compared with the guessed corrected value; for this purpose, the tube side (h_i) and shell side (h_o) film heat transfer coefficient must be determined. The tube side film heat transfer coefficient h_i is calculated using the following equation [6]:

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027\,N_{\text{Rei}}^{0.8} N_{\text{Pri}}^{1/3}\left(\frac{\mu}{\mu_w}\right)^{0.14}$$

where $N_{\text{Rei}} = D_i\rho_i u_i / \mu_i$ and $N_{\text{Pri}} = C_{pi}\,\mu_i / k_i$.

Reynolds number, N_{Rei}

$$N_{\text{Rei}} = \frac{D_i\rho_i u_i}{\mu_i} = \frac{(0.62\ \text{in./12 in./ft}) \times 62.4(\text{lb/ft}^3) \times 5(\text{ft/s})}{0.67\,\text{cP} \times (1\,\text{lb/ft}\,\text{s})/(1488\ \text{cP})} = 35{,}800$$

Prandtl number, N_{Pri}

$$N_{\text{Pri}} = \frac{C_{p_i}\mu_i}{k_i} = \frac{1(\text{Btu/lb}\,^\circ\text{F}) \times 0.67\,\text{cP} \times 2.42(1\text{lb/ft}\,\text{h}/1\text{cP})}{0.363(\text{Btu/ft}\,\text{h}\,^\circ\text{F})} = 4.47$$

Substituting calculated values of Reynolds number and Prandtl number in the film heat transfer equation. The Nusselt number, $\mathrm{Nu_i}$,

$$\mathrm{Nu_i} = \frac{h_i D_i}{k_i} = 0.027 N_{\mathrm{Rei}}^{0.8} N_{\mathrm{Pri}}^{1/3} \left(\frac{\mu}{\mu_w}\right)^{0.14} = 0.027(35{,}800)^{0.8}(4.47)^{1/3} \times 1 = 195.5$$

The film side heat transfer confident, h_i

$$h_i = \frac{195.5 \times k_i}{D_i} = 195.54 \times \frac{0.363(\mathrm{Btu/ft\,h\,°F})}{(0.62\ \mathrm{in./12\ in./ft})} = 1374 \frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

The shell side heat transfer coefficient, h_o, is calculated using the heat transfer equation from Kern [3]:

$$\mathrm{Nu_o} = \frac{h_o D_e}{k_o} = 0.36 N_{\mathrm{Reo}}^{0.55} N_{\mathrm{Pro}}^{1/3} \left(\frac{\mu_o}{\mu_w}\right)^{0.14}$$

where $N_{\mathrm{Reo}} = D_e G_o/\mu_o$ and $N_{\mathrm{Pro}} = C_{p_o}\mu_o/k_o$.

$$\text{The hydraulic effective diameter} = D_e = \frac{4\left(P_t^2 - (\pi D_o^2/4)\right)}{\pi D_o}$$

$$D_e = \frac{4 \times \left(1^2 - (\pi(0.75)^2/4)\right)}{\pi \times 0.75} = 0.948\ \mathrm{in.}$$

The mass velocity normal to tubes at the centerline of the exchanger, G_o, depends on the cross-sectional area between baffles and shell axis, A_{cf}. The shell side diameter for 4 tube passes and 440 tubes, $\frac{3}{4}$ in. OD, 1 in. square pitch, can be found from tube sheet layouts tables [6]. Since the number is between 432 and 480 tubes, the shell side packed with 480 tubes is chosen. Assuming that the shell ID is 29 in., and the baffle spacing is 8 in.

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times b$$

$$A_{cf} = \frac{29\ \mathrm{in.}}{1\ \mathrm{in.}} \times \left(0.25\ \mathrm{in.}\frac{1\ \mathrm{ft}}{12\ \mathrm{in.}}\right) \times \left(8\ \mathrm{in.}\frac{\mathrm{ft}}{12\ \mathrm{in.}}\right) = 0.404\ \mathrm{ft^2}$$

The shell side mass velocity, G_o

$$G_o = \frac{m_o}{A_{cf}} = \frac{100{,}000(\mathrm{lb/h})}{0.404\ \mathrm{ft^2}} = 247{,}525 \frac{\mathrm{lb}}{\mathrm{ft^2\,h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{\mathrm{Reo}} = \frac{D_e G_o}{\mu_o} = \frac{0.948\ \mathrm{in.}(1\ \mathrm{ft}/12\ \mathrm{in.}) \times 247{,}525(\mathrm{lb/ft^2\,h})}{3.5\ \mathrm{cP} \times \dfrac{1(\mathrm{lb/ft\,s}) \times (3600\ \mathrm{s/1h})}{1488\ \mathrm{cP}}} = 2310$$

Shell side Prandtl number, N_{Pro}

$$N_{\mathrm{Pro}} = \frac{C_{p_\mathrm{o}}\mu_\mathrm{o}}{k_\mathrm{o}} = \frac{0.65(\mathrm{Btu/lb\,°F}) \times 3.5\,\mathrm{cP}[1(\mathrm{lb/ft\,s})(3600\,\mathrm{s/h})]/(1488\,\mathrm{cP})}{0.16(\mathrm{Btu/ft^2\,h\,°F})} = 34.4$$

Substituting values of Reynolds number and Prandtl number in the shell side heat transfer equations and neglecting the effect of change in viscosity,

$$\mathrm{Nu_o} = \frac{h_\mathrm{o}D_\mathrm{e}}{k_\mathrm{o}} = 0.36\left(2310\right)^{0.55}\left(34.4\right)^{1/3}\left(1\right)^{0.14} = 83$$

The heat transfer coefficient, h_o

$$h_\mathrm{o} = \mathrm{Nu_o}\frac{k_\mathrm{o}}{D_\mathrm{e}} = 83\frac{\left(0.16(\mathrm{Btu/ft^2\,h\,°F})\right)}{0.948\,\mathrm{in.} \times (1\,\mathrm{ft}/12\,\mathrm{in.})} = 168\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

The designed overall heat transfer coefficient, U_i, based on inside tube surface area.

$$\frac{1}{U_\mathrm{i}} = \frac{D_\mathrm{i}}{D_\mathrm{o}h_\mathrm{o}} + \frac{D_\mathrm{i}\Delta x}{D_\mathrm{LM}k_\mathrm{w}} + \frac{1}{h_\mathrm{i}} + R_\mathrm{fi}$$

The tube thickness, Δx

$$\Delta x = \frac{D_\mathrm{o} - D_\mathrm{i}}{2} = \frac{0.75 - 0.62}{2} = 0.065$$

The tube log means diameter, D_LM

$$D_\mathrm{LM} = \frac{D_\mathrm{o} - D_\mathrm{i}}{\ln\left(D_\mathrm{o}/D_\mathrm{i}\right)} = \frac{0.75 - 0.62}{\ln\left(0.75/0.62\right)} = 0.683$$

Substituting values involved in the overall heat transfer equation,

$$\frac{1}{U_\mathrm{i}} = \frac{0.62}{0.75 \times 168} + \frac{0.62\,\mathrm{in.} \times 0.065(\mathrm{in./12\,in./ft})}{0.683\,\mathrm{in.} \times 30\,\mathrm{Btu/h\,ft\,°F}} + \frac{1}{1374} + 0.004 = 0.098$$

The calculated U-value based on the tube inside area of the designed heat exchanger:

$$U_\mathrm{i} = 102\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,ft}}$$

The calculated over all heat transfer coefficient based on the designed specification is higher than the assumed value consequently the design is successful and the heat exchanger is over specified. To be more accurate, baffle spacing should be increased slightly to decrease the shell side heat transfer coefficient, thus assuming a new baffle spacing, $b = 10$ in. (maximum baffle spacing should not exceed shell side ID, $D_s = 29$ in.).

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times b$$

$$A_{cf} = \frac{29\text{ in.}}{1\text{ in.}} \times \left(0.25\text{ in.}\frac{1\text{ ft}}{12\text{ in.}}\right) \times \left(10\text{ in.}\frac{\text{ft}}{12\text{ in.}}\right) = 0.503\text{ ft}^2$$

The shell side mass velocity, G_o

$$G_o = \frac{m_o}{A_{cf}} = \frac{100{,}000(\text{lb/h})}{0.503\text{ ft}^2} = 198{,}807\frac{\text{lb}}{\text{ft}^2\text{ h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{Reo} = \frac{D_e G_o}{\mu_o} = \frac{0.948\text{ in. }(1\text{ ft}/12\text{ in.}) \times 247{,}525\ (\text{lb/ft}^2\text{h})}{3.5\text{ cP} \times \dfrac{1\text{ lb/ft s} \times 3600\text{ s}/1\text{ h}}{1488\text{ cP}}} = 2310$$

The shell side Prandtl number, N_{Pro}

$$N_{Pro} = \frac{C_{p_o}\mu_o}{k_o} = \frac{0.65(\text{Btu/lb °F}) \times 3.5\text{ cP} \times 2.42[1(\text{lb/ft h})]/(1\text{ cP})}{0.16(\text{Btu/ft}^2\text{ h °F})} = 34.41$$

Substituting values of Reynolds number and Prandtl number in the shell side heat transfer equations and neglecting the effect of change in viscosity,

$$\text{Nu}_o = \frac{h_o D_e}{k_o} = 0.36(1854)^{0.55}(34.4)^{1/3}(1)^{0.14} = 73.45$$

The heat transfer coefficient, h_o

$$h_o = \text{Nu}_o\frac{k_o}{D_e} = 73.45\frac{(0.16(\text{Btu/ft}^2\text{ h °F}))}{0.948\text{ in.} \times (1\text{ ft}/12\text{ in.})} = 148.76\frac{\text{Btu}}{\text{ft}^2\text{ h °F}}$$

The overall heat transfer coefficient,

$$\frac{1}{U_i} = \frac{D_i}{D_o h_o} + \frac{D_i \Delta x}{D_{LM} k_w} + \frac{1}{h_i} + R_{fi}$$

Substituting needed value to the above equation,

$$\frac{1}{U_i} = \frac{0.62}{0.75 \times 148.76} + \frac{0.62\text{ in.} \times (0.065\text{ in.}/12\text{ in./ft})}{0.683\text{ in.} \times 30\text{ Btu/h ft °F}} + \frac{1}{1374} + 0.004 = 0.0105$$

The overall all heat transfer coefficient calculated based on heat exchanger design arrangement is

$$U_i = 95.7\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,\text{ft}}, \quad U_o = \frac{D_i}{D_o} \times U_i = \frac{0.62}{0.75} \times 95.7\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,\text{ft}} = 79.1\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,\text{ft}}$$

The calculated value based on exchanger design specification is close to the assumed corrected value, and so the designed shell and tube heat exchanger is successful.

PRESSURE DROP

The pressure drop for the flow of liquid without phase change through a circular tube is given by the following equations [6]:

$$-\Delta P_o = P_{in} - P_{out} = K_s\frac{2N_R f' G_o^2}{g_c \rho_c \phi}$$

$$N_{\text{reversals}} = \frac{L}{b} = \frac{18\text{ ft}}{10\text{ in.}}\frac{12\text{ in.}}{\text{ft}} = 21.6$$

The value of

$$K_s = 1.1 \times N_{\text{reversals}} = 1.1 \times 21.6 = 23.76$$

Number of tubes at the centerline

$$\cong \frac{D_s}{P_t} = \frac{29\text{ in.}}{1\text{ in.}} = 29$$

The number of tube rows across which the shell fluid flows, N_R, equals the total number of tubes at the center plane minus the number of tube rows that pass through the cut portions of the baffles. For 25% cut baffles, N_R may be taken as 50% of the number of the tubes at the center plane.

$$N_R = 0.5 \times 29 = 14.5 \cong 15$$

The modification friction factor, f'

$$f' = b_2\left(\frac{D_o G_o}{\mu_o}\right)^{-0.15}$$

where b_2 for square pitch is

$$b_2 = 0.044 + \frac{0.08x_L}{(x_T - 1)^{0.43+1.13/x_L}}$$

where x_T is the ratio of the pitch transverse to flow to tube OD and x_L is the ratio of pitch parallel to tube OD. For square pitch $x_L = x_T$

$$x_L = x_T = \frac{P_t}{D_o} = \frac{1}{0.75} = 1.33$$

Hence,

$$b_2 = 0.044 + \frac{0.08 \times 1.333}{(1.333 - 1)^{0.43+1.13/1.333}} = 0.48$$

$$f' = b_2\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15} = 0.48\left(\frac{(0.75\text{ in.}/12\text{ in./ft}) \times (198{,}807\text{ lb/ft}^2\text{ h})}{3.5\text{ cP} \times (\text{lb/ft s}/1488\text{ cP}) \times (3600\text{ s/h})}\right)^{-0.15} = 0.161$$

Substituting into the shell side pressure drop equation:

$$-\Delta P_o = K_s\frac{2N_Rf'G_o^2}{g_c\rho_o\phi} = 23.76\frac{2 \times 15 \times 0.161\left(\frac{198{,}807\text{ lb}}{\text{ft}^2\text{ h}}\left|\frac{\text{h}}{3600\text{ s}}\right.\right)^2}{32.2(\text{ft lb/lb}_f\text{ s}^2) \times 68.6(\text{lb/ft}^3) \times 1} \times \frac{1\text{ ft}^2}{144\text{ in.}^2}$$
$$= 1.1\text{ psi}$$

Estimating the pressure drop in the tube side is much easier than calculated pressure drop in the shell side. The pressure drop in the tube side is calculated using the following equations [6]:

$$-\Delta P_i = 1.2\frac{N_Pf_DG_i^2L}{2g_c\rho_iD_i\phi}$$

where

$$f_D = (1.82\log_{10}N_{Re\,i} - 1.64)^{-2}$$

$$f_D = (1.82\log_{10}35{,}800 - 1.64)^{-2} = 0.0226$$

Tube side mass velocity

$$G_i = \rho_iu_i = 62.4\frac{\text{lb}}{\text{ft}^3} \times 5\frac{\text{ft}}{\text{s}} = 312\frac{\text{lb}}{\text{ft}^2\text{ s}}$$

Substituting in pressure drop equation,

$$-\Delta P_i = 1.2\frac{N_Pf_DG_i^2L}{2g_c\rho_iD_i\phi} = 1.2\frac{4 \times 0.0226 \times \left(312(\text{lb/ft}^2\text{ s})\right)^2 \times 18\text{ ft}}{2 \times 32.2\frac{\text{ft lb}}{\text{lb}_f\text{ s}^2} \times 62.4\frac{\text{lb}}{\text{ft}^3} \times \frac{0.62\text{ in.}}{12\text{ in./ft}} \times 1} \times \frac{1\text{ ft}^2}{144\text{ in.}}$$
$$= 6.36\text{ psi}$$

TABLE 4.8

Design Specifications

	Shell Side	Tube Side
Components	Ethylene glycol (100%)	Water (100%)
Mass flow rate (lb/h)	100,000	260,000
Temperature (°F)	250/130	90/120
Pressure (bar)	1.0	1.0
Pass	1	4
Shell ID (in.)	29	
Tubes: OD/ID/P_t (in.)		0.75/0.62/1
Tube configuration		Square
Length (ft)		18
Total number of tubes		440
Number of baffles		20
Baffle spacing (in.)		8
Fouling factor (ft^2 °F h/Btu)	0.0	0.004
Pressure drop (psi)	1.1	6.36
LMTD (°F)	76.4	
F	0.85	
U_o(Btu/h ft^2 °F)	79	
Duty (Btu/h)	7,800,000	

The summary of the specifications of the designed exchanger is provided in Table 4.8.

HYSYS/UNISIM SIMULATION

In this example, while in *Design/Parameters* page, *Steady State Rating* is selected from the pull-down menu under *Heat Exchanger Model*. For this mode of calculations, pressure drop in the tube side and shell side is calculated by Hysys. The constructed process flow sheet using Hysys/Unisim is shown in Figure 4.21. The overall heat transfer coefficient estimated using Unisim is calculated from the heat duty equation (i.e., $U_o = Q / (A_o °F \Delta T_{LM})$ and not from outside and inside film heat transfer coefficient as the case in Pro II and Aspen Plus. The discrepancy of the exit side shell temperature calculated by Hysys (T for stream S4 = 138) is due to the variation in mass heat capacity (C_p) calculated by Hysys and used in hand estimation (C_p = 1.008 Btu/lb °F).

PRO/II SIMULATION

The data provided to the process flow sheet:

Calculation type: Tube outlet temperature is 120°F, number of tubes per shell is 440, and shell ID is 29 in.

Tubes: Outside tube diameter is 0.75 in., ID is 0.62 in., tube pitch is 1 in square pitch, and tube length is 18 ft.

Baffles: Fractional cut is 0.25, baffle spacing is 10 in.

Configuration: Counter current, horizontal, number of tube passes/shell is 4.

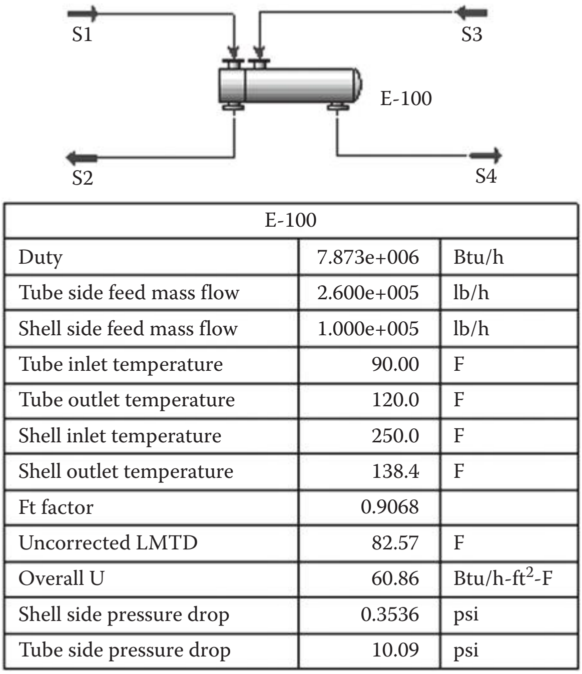
Nozzle: Shell nozzle inlet and outlet diameter is 8 in., tube side nozzle inlet, and outlet diameter is 6 in.

The overall heat transfer coefficient, U_o obtained by hand calculation is different than that obtained by Pro II. Here the *U*-value is based on outside surface area which gives the same results as that based on tubes outside and IDs.

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{A_o \Delta x}{A_{LM} k_w} + \left(\frac{A_o}{A_i}\right)\frac{1}{h_i} + \left(\frac{A_o}{A_i}\right) R_{fi}$$

$$\frac{1}{U_o} = \frac{1}{148.76 \dfrac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}} + \frac{1555\,\text{ft}^2 \times 0.065\,\text{in.}(1\,\text{ft}/12\,\text{in.})}{1413.6\,\text{ft}^2 \times 30\,\text{Btu/ft}\,\text{h}\,°\text{F}}$$

$$+ \left(\frac{1555\,\text{ft}^2}{1286\,\text{ft}^2}\right)\frac{1}{1374(\text{Btu/ft}^2\,\text{h}\,°\text{F})} + \left(\frac{1555\,\text{ft}^2}{1286\,\text{ft}^2}\right) \times 0.004\frac{\text{ft}^2\,\text{h}\,°\text{F}}{\text{Btu}}$$



E-100		
Duty	7.873e+006	Btu/h
Tube side feed mass flow	2.600e+005	lb/h
Shell side feed mass flow	1.000e+005	lb/h
Tube inlet temperature	90.00	F
Tube outlet temperature	120.0	F
Shell inlet temperature	250.0	F
Shell outlet temperature	138.4	F
Ft factor	0.9068	
Uncorrected LMTD	82.57	F
Overall U	60.86	Btu/h-ft^2-F
Shell side pressure drop	0.3536	psi
Tube side pressure drop	10.09	psi

FIGURE 4.21
Process flow sheet of Example 4.3.

Hence,

$$\frac{1}{U_o} = 0.0126 \frac{\text{ft}^2\,\text{h}\,°\text{F}}{\text{Btu}}$$

$$U_o = 79.36 \frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

Using Donohue equation (4.18), the U-value is calculated and compared with Pro II results:

$$\left(\frac{h_o D_o}{k_o}\right) = 0.2\left(\frac{D_o G_e}{\mu_o}\right)^{0.6}\left(\frac{C_{p_o}\mu_o}{k_o}\right)^{0.33}\left(\frac{\mu_o}{\mu_w}\right)^{0.14}$$

The cross-sectional areas for flow are first calculated:

$$D_o = \frac{0.75\text{ in.}}{12\text{ in./ft}} = 0.0625\text{ ft} \quad D_s = \frac{29\text{ in.}}{12\text{ in./ft}} = 2.4167\text{ ft}$$

$$P_t = \frac{1\text{ in.}}{12\text{ in./ft}} = 0.0833\text{ ft} \quad b = \frac{10\text{ in.}}{12\text{ in./ft}} = 0.8333\text{ ft}$$

The area of cross flow, S_c

$$S_c = bD_s\left(1 - \frac{D_o}{P_t}\right) = 0.8333 \times 2.4167\left(1 - \frac{0.0625}{0.0833}\right) = 0.503\text{ ft}^2$$

The number of tubes in the baffle window is approximately equal to the fractional area of the window f_b times the total number of tubes, for a 25% baffle, $f_b = 0.1955$ [3].

$$N_b = 0.1955 \times 440 = 86$$

The area for flow in baffle window,

$$S_b = f_b \frac{\pi D_s^2}{4} - N_b \frac{\pi D_o^2}{4} = 0.1955 \frac{\pi(2.4167\text{ ft})^2}{4} - 86 \frac{\pi(0.0625)^2}{4} = 0.8937\text{ ft}^2$$

The mass velocities are

$$G_c = \frac{\dot{m}_o}{S_c} = \frac{100{,}000\text{ lb/h}}{0.503\text{ ft}^2} = 198{,}807.2 \frac{\text{lb}}{\text{h ft}^2}$$

$$G_b = \frac{\dot{m}_o}{S_b} = \frac{100{,}000\text{ lb/h}}{0.8937\text{ ft}^2} = 111{,}894 \frac{\text{lb}}{\text{h ft}^2}$$

where

$$G_e = \sqrt{G_b G_c} = \sqrt{198{,}807.2 \frac{\text{lb}}{\text{h ft}^2} \times 111{,}894 \frac{\text{lb}}{\text{h ft}^2}} = 149{,}148.68 \frac{\text{lb}}{\text{h ft}^2}$$

The Donohue equation is

$$\left(\frac{h_o D_o}{k_o}\right) = 0.2\left(\frac{D_o G_e}{\mu_o}\right)^{0.6}\left(\frac{C_{po}\mu_o}{k_o}\right)^{0.33}\left(\frac{\mu_o}{\mu_w}\right)^{0.14}$$

Substituting values

$$\left(\frac{h_o \times 0.0625\ \text{ft}}{0.16\dfrac{\text{Btu}}{\text{ft h °F}}}\right) = 0.2\left(\frac{0.0625\ \text{ft} \times 149{,}148.68\dfrac{\text{lb}}{\text{h ft}^2}}{3.5\,\text{cP}\left|\dfrac{2.42\ \text{lb/ft h}}{1\,\text{cP}}\right.}\right)^{0.6}$$

$$\times\left(\frac{0.65\dfrac{\text{Btu}}{\text{lb °F}} \times 3.5\ \text{cP}\left|\dfrac{2.42\ \text{lb/ft h}}{1\,\text{cP}}\right.}{0.16\dfrac{\text{Btu}}{\text{ft h °F}}}\right)^{0.33}$$

$$\left(\frac{h_o \times 0.0625\ \text{ft}}{0.16\ \text{Btu/ft h °F}}\right) = 0.2(1100.57)^{0.6}(34.41)^{0.33}(1)^{0.14}$$

The shell side heat transfer coefficient, h_o

$$h_o = 110\frac{\text{Btu}}{\text{ft}^2\,\text{h °F}}$$

Hence

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{A_o \Delta x}{A_{LM} k_w} + \left(\frac{A_o}{A_i}\right)\frac{1}{h_i} + \left(\frac{A_o}{A_i}\right)R_{fi}$$

$$\frac{1}{U_o} = \frac{1}{110\ \text{Btu/ft}^2\,\text{h °F}} + \frac{1555\ \text{ft}^2 \times 0.065\ \text{in.}(1\ \text{ft/12 in.})}{1416\ \text{ft}^2 \times 30\ \text{Btu/ft h °F}} + \left(\frac{1555\ \text{ft}^2}{1286\ \text{ft}^2}\right)\frac{1}{1374\,\text{Btu/ft}^2\,\text{h °F}}$$

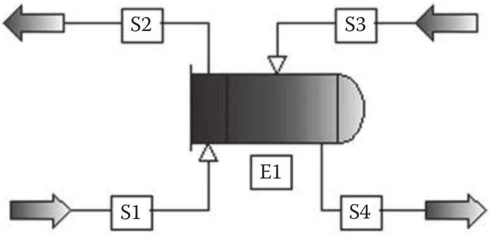
$$+\left(\frac{1555\ \text{ft}^2}{1286\ \text{ft}^2}\right) \times 0.004\frac{\text{ft}^2\,\text{h °F}}{\text{Btu}}$$

$$= 0.0152\frac{\text{ft}^2\,\text{h °F}}{\text{Btu}}$$

$$\frac{1}{U_o} = 9.1 \times 10^{-3} + 1.985 \times 10^{-4} + 8.8 \times 10^{-4} + 4.837 \times 10^{-3} = 0.015(\text{h ft}^2\ \text{°F})/\text{Btu}$$

The overall heat transfer coefficient, U_o

$$U_o = 66.66\ \text{Btu/h ft}^2\ \text{°F}$$



HxRig name		E1
HxRig description		Example 4.1
Duty	MM Btu/h	7.7817
Area	ft^2	1644.8865
U-Value	Btu/h-ft^2-F	106.3943
U-Value (Fouling)	Btu/h-ft^2-F	70.2360
LMTD	F	76.6595
FT factor		0.8786

Stream name		S1	S2	S3	S4
Temperature	F	90.000	120.000	250.000	130.391
Pressure	psia	14.700	8.059	14.700	14.421
Flowrate	lb-mol/h	14432.192	14432.192	1611.125	1611.125

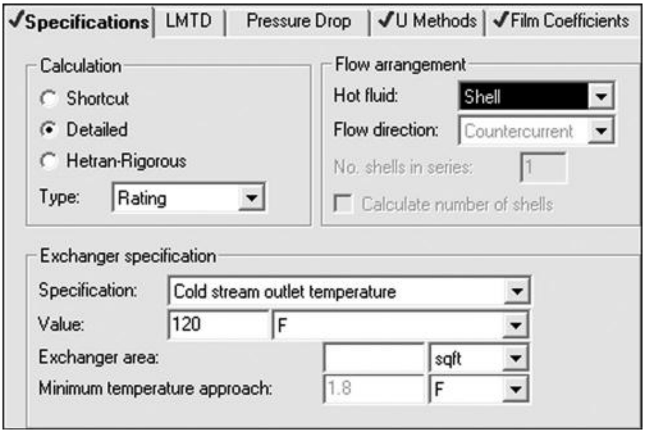
FIGURE 4.22
PRO/II simulation of Example 4.3.

The value obtained by Donohue equation is closer to the *U* (fouling) obtained with Pro II and shown in Figure 4.22. The discrepancy is mainly due to the small dissimilarity in the physical properties used in Pro/II and that used in hand calculations.

ASPEN SIMULATION

The HeatX exchanger is used for this example; HeatX in Aspen Plus is the fundamental heat exchanger algorithm used in rigorous design and calculates energy balance and pressure drop exchanger area. The icon is selected by pressing *Heat Exchangers* tab in the model library. The block requires hot and cold streams. The feed streams are fully specified by double clicking on each stream and filling in, temperature, pressure, flow rate, and compositions. While on the *Setup* page, for the *Calculation* type *Detailed* is selected. Hot fluid is in the shell side. Cold stream outlet temperature is selected as shown in Figure 4.23.

Aspen will calculate the LMTD correction factor for the exchanger. The default setting is the correction based on the geometry and that will not be changed. Now click on the *Pressure drop* tab at the top of the page and a new input page will appear; *Calculate from geometry* is the preferred option. Both the hot and cold side has to be specified for the pressure drop calculations. The input page for the overall heat exchanger appears next. There are several options to calculate the *U*-value, for this example the *U*-value is calculated from *Film coefficients*, the *U*-value is calculated from individual heat transfer coefficient (h_o, h_i). This option requires more input and that page is shown by clicking on the *Film Coefficients* tab at the top of



Calculation
- ○ Shortcut
- ● Detailed
- ○ Hetran-Rigorous

Type: Rating

Flow arrangement
Hot fluid: Shell
Flow direction: Countercurrent
No. shells in series: 1
☐ Calculate number of shells

Exchanger specification
Specification: Cold stream outlet temperature
Value: 120 F
Exchanger area: sqft
Minimum temperature approach: 1.8 F

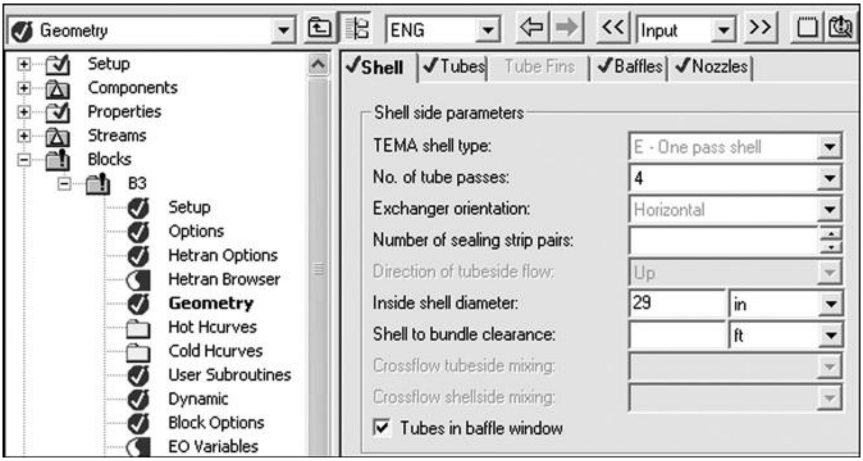
FIGURE 4.23
Setup page of the heat exchanger.

the screen. In the film coefficients page the method to calculate the individual heat transfer coefficients needs to be defined. Here *Calculate from geometry* is selected. Notice, however, that both sides (hot and cold) of the exchanger need to be specified. After the heat transfer coefficient calculation are specified, the next step is to set out the geometry of the heat exchanger (Figure 4.24).

In the geometry page:

Shell: Number of tube passes is 4, inside cell diameter is 29 in.

Tubes: The number of tubes is 440, the length of the tubes 18 ft, the inside and OD of the tubes are 0.75/0.62 in. or nominal diameter (OD = 0.75 in., BWG = 18), the pitch is 1 in.



Shell side parameters
TEMA shell type: E - One pass shell
No. of tube passes: 4
Exchanger orientation: Horizontal
Number of sealing strip pairs:
Direction of tubeside flow: Up
Inside shell diameter: 29 in
Shell to bundle clearance: ft
Crossflow tubeside mixing:
Crossflow shellside mixing:
☑ Tubes in baffle window

FIGURE 4.24
Geometry page of the heat exchanger.

Baffles: The number of baffles is 20, baffle cut 0.25, baffle spacing 10 in.
Nozzle: Shell side nozzle inlet and outlet diameter is 8 in. and tube side nozzle inlet and outlet diameter is 6 in. must be supplied from hand calculations.

When a blue mark appears near the tab, the input sheet is complete.

The simulation is now ready to run. Click on *Next* and run the simulation. The summary result page of the heat is exchanger is shown in Figure 4.25. The *Exchanger Details* page is shown in Figure 4.26. The actual exchanger area is calculated based on number of tubes, tube length, and tubes' OD.

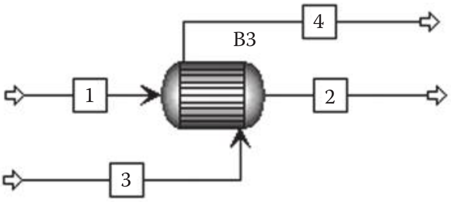
$$A_{\text{actual}} = \left(\pi D_{\text{o}} L\right) N_{\text{t}} = \left(\pi \times 0.75\ \text{in.} \frac{1\ \text{ft}}{12\ \text{in.}} \times 18\ \text{ft}\right) \times 440 = 1555.09\ \text{ft}^2$$

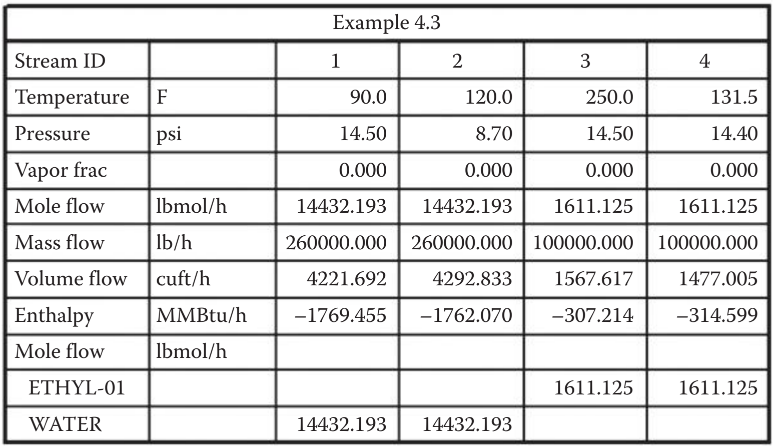
The required exchanger area calculated with Aspen is

$$A_{\text{required}} = \frac{Q_{\text{req}}}{U_{\text{o}} F \Delta T_{\text{LM}}} = \frac{7385318.5}{63.075 \times 68.55} = 1708.065\ \text{ft}^2$$

SuperPro Designer Simulation

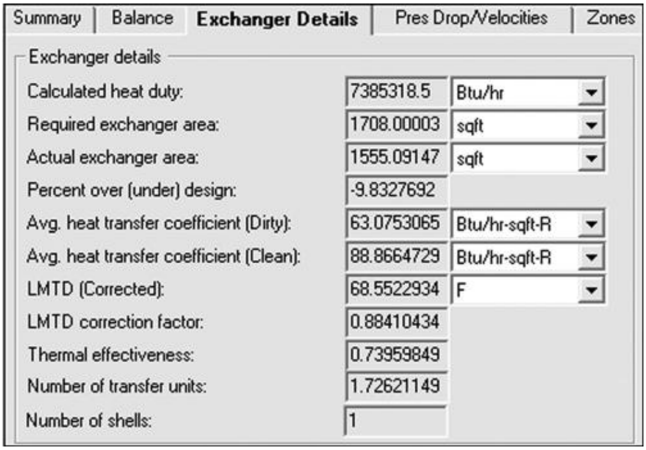
With SuperPro designer simple energy balance is performed as shown in Figure 4.27.





Example 4.3					
Stream ID		1	2	3	4
Temperature	F	90.0	120.0	250.0	131.5
Pressure	psi	14.50	8.70	14.50	14.40
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	lbmol/h	14432.193	14432.193	1611.125	1611.125
Mass flow	lb/h	260000.000	260000.000	100000.000	100000.000
Volume flow	cuft/h	4221.692	4292.833	1567.617	1477.005
Enthalpy	MMBtu/h	−1769.455	−1762.070	−307.214	−314.599
Mole flow	lbmol/h				
ETHYL-01				1611.125	1611.125
WATER		14432.193	14432.193		

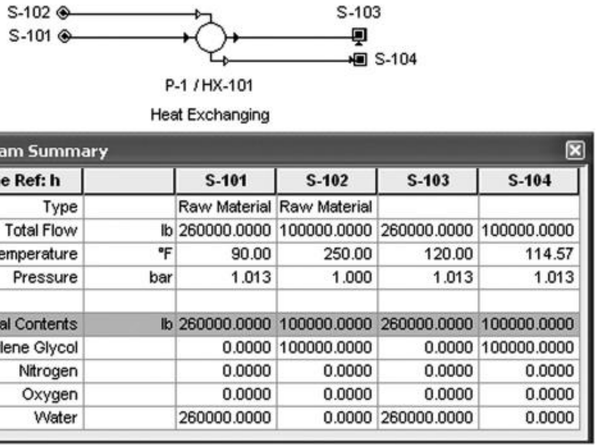
FIGURE 4.25
Process flow sheet and stream table property with Aspen.



Exchanger details

Calculated heat duty:	7385318.5	Btu/hr
Required exchanger area:	1708.00003	sqft
Actual exchanger area:	1555.09147	sqft
Percent over (under) design:	-9.8327692	
Avg. heat transfer coefficient (Dirty):	63.0753065	Btu/hr-sqft-R
Avg. heat transfer coefficient (Clean):	88.8664729	Btu/hr-sqft-R
LMTD (Corrected):	68.5522934	F
LMTD correction factor:	0.88410434	
Thermal effectiveness:	0.73959849	
Number of transfer units:	1.72621149	
Number of shells:	1	

FIGURE 4.26
Exchanger details design results.



Stream Summary

Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	lb	260000.0000	100000.0000	260000.0000	100000.0000
Temperature	°F	90.00	250.00	120.00	114.57
Pressure	bar	1.013	1.000	1.013	1.013
Total Contents	lb	260000.0000	100000.0000	260000.0000	100000.0000
Ethylene Glycol		0.0000	100000.0000	0.0000	100000.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		260000.0000	0.0000	260000.0000	0.0000

FIGURE 4.27
Process flow sheet and stream table properties simulated with SuperPro.

CONCLUSION

The Pro II simulation results were the closest to the hand calculations, Aspen results come in the second rank, followed by Hysys/Unisim.

Example 4.4 Demineralized Water-Raw Water Exchanger

Design a shell and tube heat exchanger to heat raw water at 75°F to 80°F using 150,000 lb/h of demineralized water enters the exchanger at 95°F and cooled to 85°F. Assume that the tube side fouling resistance is 0.001 (ft^2 h °F)/Btu.

TABLE 4.9

Physical Properties at Average Temperatures

	Shell Side	Tube Side
Parameters	Demineralized water (90°F)	Raw water (78°F)
ρ (lb/ft^3)	62.4	62.4
C_p (Btu/lb °F)	1.0	1.01
μ (cP)	0.81	0.92
K (Btu/h ft °F)	0.36	0.363

SOLUTION

HAND CALCULATIONS

The physical properties of the shell side and tube side fluid at average temperatures are shown in Table 4.9 and a schematic diagram of 1–2 shell and tube heat exchanger is shown in Figure 4.28.

The required heat duty, Q_{req}

$$Q_{\text{req}} = m_{\text{o}} C_{p_{\text{o}}} \Delta T_{\text{o}} = 150{,}000 \frac{\text{lb}}{\text{h}} \times 1.0 \frac{\text{Btu}}{\text{lb}\,°\text{F}} \left(95 - 85\right)°\text{F} = 1.5 \times 10^6 \frac{\text{Btu}}{\text{h}}$$

The tube side mass flow rate, $\dot{m}_{\text{i}}$

$$\dot{m}_{\text{i}} = \frac{Q_{\text{req}}}{C_{p_{\text{i}}} \Delta T_{\text{i}}} \frac{1.5 \times 10^6 (\text{Btu/h})}{1.01 (\text{Btu/lb}\,°\text{F}) \left(80 - 75\right)°\text{F}} = 3.0 \times 10^5 \frac{\text{lb}}{\text{h}}$$

The log mean temperature difference, ΔT_{LM}

$$\Delta T_{\text{LM}} = \frac{(95 - 80) - (85 - 75)}{\ln\left(95 - 80/85 - 75\right)} = 12.33°\text{F}$$

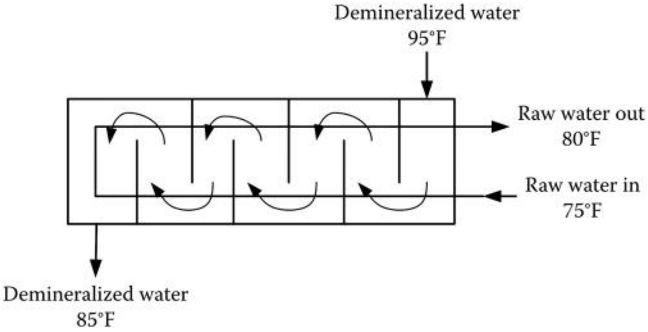


FIGURE 4.28
Schematic of 1–2 shell and tube heat exchanger.

Consider an exchanger configuration as 1 shell pass and 2 tube passes; 1–2 pass, the correction factor, F_{1-2}

$$F_{1-2} = \frac{\left[\sqrt{R^2+1}/(R-1)\right]\ln\left[(1-S)/(1-SR)\right]}{\ln\left[A+\sqrt{R^2+1}/A-\sqrt{R^2+1}\right]}$$

where,

$$A = \frac{2}{S} - 1 - R$$

Values of R, S, and A are calculated as follows:

$$R = \frac{95-85}{80-75} = 2.0$$

$$S = \frac{80-75}{95-75} = 0.25$$

$$A = \frac{2}{0.25} - 1 - 2 = 5.0$$

Substituting values of R, S, and A into the following equation to calculate F_{1-2},

$$F_{1-2} = \frac{\left[\sqrt{2^2+1}/2-1\right]\ln\left[1-0.25/1-0.25\times 4\right]}{\ln\left[5.0+\sqrt{2^2+1}/5.0-\sqrt{2^2+1}\right]} = 0.94$$

A typical heat transfer coefficient for the system demineralized water-raw water is within the range 300–500 Btu/ft^2 h °F. Assume the overall heat transfer coefficient is 400 Btu/ft^2 h °F

$$A_i = \frac{Q_{\text{req}}}{U_i F \Delta T_{\text{LM}}} = \frac{1.5\times 10^6(\text{Btu/h})}{400(\text{Btu/ft}^2\,\text{h}\,°\text{F})\times 0.94\times 12.33°\text{F}} = 324\ \text{ft}^2$$

The tubes' cross-sectional area/pass, A_{ci}

$$A_{ci} = \frac{F_i}{u_i} = \frac{m_i/\rho_i}{u_i} = \frac{300{,}000\,\frac{\text{lb}}{\text{h}}/62.4\,\frac{\text{lb}}{\text{ft}^3}}{5\,\frac{\text{ft}}{\text{s}}\times\frac{3600\ \text{s}}{\text{h}}} = 0.267\ \text{ft}^2/\text{pass}$$

Choosing a tube's OD, OD = $\frac{3}{4}$ in., 16 BWG tubing (ID = 0.62 in.) arranged on a 1-in. square pitch and tube length 10 ft. The data are required before estimating total number of tubes and number of tube passes.

The inside cross-sectional area/tube, A_{tc}

$$A_{tc} = \frac{\pi D_i^2}{4} = \frac{\pi \times \left(0.62\text{ in.}\right)^2}{4} = 0.302\text{ in.}^2\text{/tube}$$

The total number of tubes per pass, N_t

$$N_t = \frac{A_{ci}}{A_{tc}} = \frac{0.267\text{ ft}^2}{0.302\text{ in.}^2\text{/tube}}\frac{144\text{ in.}^2}{\text{ft}^2} = 127.3 \cong 128\text{ tube/pass}$$

A single-tube internal surface, A_t

$$A_t = \pi D_i L = \pi \times 0.62\frac{\text{in.}}{12\text{in./ft}} \times 10\text{ft} = 1.623\text{ft}^2$$

Number of tube passes, N_p

$$N_p = \frac{A_i}{A_t \times N_t}\frac{324\text{ ft}^2}{1.623(\text{ft}^2\text{/tube}) \times 128\text{ tubes/pass}} = 1.56\text{ passes}$$

The number of tube passes is approximated to 2; hence, $N_p = 2$, accordingly, the total heat transfer surface area (A_i) must be corrected,

$$A_i = N_p N_t \left(\pi D_i L\right) = 2 \times 128 \times \pi \times 0.62\text{ in.}\frac{1\text{ ft}}{12\text{ in.}} \times 10\text{ ft} = 416\text{ ft}^2$$

Because the required heat duty is fixed, the overall heat transfer coefficient should be corrected based on the new overall heat transfer area. The new overall heat transfer coefficient, U_i

$$U_i = \frac{Q_{req}}{A_i F \Delta T_{lm}} = \frac{1.5 \times 10^6(\text{Btu/h})}{416\text{ ft}^2 \times 0.94 \times 12.33°\text{F}} = 312\frac{\text{Btu}}{\text{ft}^2\text{ h°F}}$$

The new value of the overall all heat transfer coefficient is still within the design range (300–500 Btu/ft^2 h °F). The overall heat transfer coefficient of the designed exchanger should be calculated based on the tube side and shell side heat transfer coefficients.

The tube side film heat transfer coefficient, h_i [6]

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027 N_{\text{Re}i}^{0.8} N_{\text{Pr}i}^{1/3}\left(\frac{\mu}{\mu_w}\right)^{0.14}$$

where Reynolds number,

$$N_{\text{Re}i} = \frac{D_i \rho_i u_i}{\mu_i} = \frac{(0.62\text{ in./12 in./ft}) \times 62.4(\text{lb/ft}^3) \times 5(\text{ft/s})}{0.92\text{ cP} \times (1\text{lb/ft s/1488 cP})} = 26{,}072$$

Prandtl number,

$$N_{\mathrm{Pr\,i}} = \frac{C_{p\mathrm{i}}\mu_{\mathrm{i}}}{k_{\mathrm{i}}} = \frac{1\dfrac{\mathrm{Btu}}{\mathrm{lb\,°F}} \times 0.92\ \mathrm{cP} \times \dfrac{1\,\mathrm{lb/ft\,s}}{1488\ \mathrm{cP}} \times 3600\dfrac{\mathrm{s}}{\mathrm{h}}}{0.363\dfrac{\mathrm{Btu}}{\mathrm{ft\,h\,°F}}} = 6.13$$

Substituting values of Reynolds number and Prandtl number in tube side film heat transfer coefficient, h_{i}, [6]

$$\mathrm{Nu_i} = \frac{h_{\mathrm{i}}D_{\mathrm{i}}}{k_{\mathrm{i}}} = 0.027 N_{\mathrm{Re\,i}}^{0.8} N_{\mathrm{Pr\,i}}^{1/3}\left(\frac{\mu}{\mu_{\mathrm{w}}}\right)^{0.14} = 0.027\left(26072\right)^{0.8}\left(6.13\right)^{1/3} \times 1 = 168.57$$

$$h_{\mathrm{i}} = \frac{168.57 \times k_{\mathrm{i}}}{D_{\mathrm{i}}} = 168.57 \times \frac{0.363\dfrac{\mathrm{Btu}}{\mathrm{ft\,h\,°F}}}{\dfrac{0.62\ \mathrm{in.}}{12\ \mathrm{in./ft}}} = 1185\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

The shell side heat transfer coefficient, h_{o}, is calculated using the heat transfer equation from Kern [3]

$$\mathrm{Nu} = \frac{h_{\mathrm{o}}D_{\mathrm{e}}}{k_{\mathrm{o}}} = 0.36 N_{\mathrm{Reo}}^{0.55} N_{\mathrm{Pro}}^{1/3}\left(\frac{\mu_{\mathrm{o}}}{\mu_{\mathrm{w}}}\right)^{0.14}$$

where $N_{\mathrm{Reo}} = D_{\mathrm{e}}\, G_{\mathrm{o}}/\mu_{\mathrm{o}}$ and $N_{\mathrm{Pro}} = C_{po}\, \mu_{\mathrm{o}}/k_{\mathrm{o}}$.

The hydraulic effective diameter, D_{e}

$$D_{\mathrm{e}} = \frac{4\left(P_t^2 - (\pi D_{\mathrm{o}}^2/4)\right)}{\pi D_{\mathrm{o}}} = \frac{4 \times \left(1^2 - (\pi\left(0.75\right)^2/4)\right)}{\pi \times 0.75} = 0.948\ \mathrm{in.}$$

To calculate the mass velocity normal to tubes at the centerline of the exchanger, G_{o}, first the cross-sectional area between baffles and shell axis, A_{cf} is calculated. For 2 tube passes, 256 tubes, $\frac{3}{4}$ in. OD, 1 in. square pitch, the shell diameter can be found from tube sheet layouts (Table 4.3) or from Kern [3]. The closest value for 254 tubes is 270, the shell ID is 21 $\frac{1}{4}$ in., and assume the baffle spacing is 10 in.

$$A_{\mathrm{cf}} = \frac{D_{\mathrm{s}}}{P_{\mathrm{t}}} \times \mathrm{clearance} \times b$$

$$A_{\mathrm{cf}} = \frac{21.25\ \mathrm{in.}}{1\,\mathrm{in.}} \times \left(0.25\ \mathrm{in.}\frac{1\,\mathrm{ft}}{12\ \mathrm{in.}}\right) \times \left(10\ \mathrm{in.}\frac{\mathrm{ft}}{12\ \mathrm{in.}}\right) = 0.37\ \mathrm{ft^2}$$

The shell side mass velocity, G_{o}

$$G_{\mathrm{o}} = \frac{m_{\mathrm{o}}}{A_{\mathrm{cf}}} = \frac{150{,}000(\mathrm{lb/h})}{0.37\ \mathrm{ft^2}} = 405{,}405\frac{\mathrm{lb}}{\mathrm{ft^2\,h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{\mathrm{Reo}} = \frac{D_e G_o}{\mu_o} = \frac{0.948\ \mathrm{in.}(1\ \mathrm{ft}/12\ \mathrm{in.}) \times 405{,}405(\mathrm{lb}/\mathrm{ft}^2\ \mathrm{h})}{0.81\ \mathrm{cP} \times [1(\mathrm{lb}/\mathrm{ft\,s}) \times (3600\ \mathrm{s}/1\ \mathrm{h})]/(1488\ \mathrm{cP})} = 16{,}343$$

The shell side Prandtl number, $N_{\mathrm{Pr\,o}}$

$$N_{\mathrm{Pr\,o}} = \frac{C_{p_o}\mu_o}{k_o} = \frac{1.0(\mathrm{Btu/lb\,°F}) \times 0.81\mathrm{cP}(1(\mathrm{lb}/\mathrm{ft\,s})(3600\ \mathrm{s}/\mathrm{h}))/1488\ \mathrm{cP}}{0.36(\mathrm{Btu/ft^2\,h\,°F})} = 5.44$$

Substituting values of Reynolds number and Prandtl number in the heat transfer equations and neglecting the effect of change in viscosity,

$$\mathrm{Nu_o} = \frac{h_o D_e}{k_o} = 0.36\left(16343\right)^{0.55}\left(5.44\right)^{1/3}\left(1\right)^{0.14} = 131.5$$

The heat transfer coefficient, h_o

$$h_o = \mathrm{Nu_o}\frac{k_o}{D_e} = 131.5\frac{\left(0.36(\mathrm{Btu/ft\,h\,°F})\right)}{0.948\ \mathrm{in.} \times (1\ \mathrm{ft}/12\ \mathrm{in.})} = 599\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

The overall heat transfer coefficient, U_i

$$\frac{1}{U_i} = \frac{D_i}{D_o h_o} + \frac{D_i \Delta x}{D_{LM} k_w} + \frac{1}{h_i} + R_{fi}$$

Substituting looked-for values in the above equation,

$$\frac{1}{U_i} = \frac{0.62\ \mathrm{in.}}{0.75\ \mathrm{in.} \times 599(\mathrm{Btu/ft^2\,h\,°F})} + \frac{0.62\ \mathrm{in.} \times \left(0.065\ \mathrm{in./12\ in./ft}\right)}{0.683\ \mathrm{in.} \times 30(\mathrm{Btu/ft^2\,h\,°F})} + \frac{1}{1185(\mathrm{Btu/ft^2\,h\,°F})}$$

$$+\ 0.001\frac{\mathrm{ft^2\,h\,°F}}{\mathrm{Btu}} = 3.55 \times 10^{-3}\frac{\mathrm{ft^2\,h\,°F}}{\mathrm{Btu}}$$

Hence,

$$U_i = 295\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,ft}}$$

Based on the outside area, the overall heat transfer coefficient, U_o

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{A_o \Delta x}{A_{LM} k_w} + \left(\frac{A_o}{A_i}\right)\frac{1}{h_i} + \left(\frac{A_o}{A_i}\right)R_{fi}$$

where $A_i = 415$ ft² and $A_o = 502$ ft², the log mean area, A_{LM}

$$A_{LM} = \frac{A_o - A_i}{\ln(A_o/A_i)} = \frac{(502 - 415)}{\ln(502/415)} = 457 \text{ ft}^2$$

Hence,

$$\frac{1}{U_o} = \frac{1}{599} + \frac{502(0.065/12)}{(457)(30)} + \left(\frac{502}{415}\right)\frac{1}{1185} + \left(\frac{502}{415}\right)0.001$$

$$= 4.1 \times 10^{-3}\,\text{h ft}^2\,°\text{F/Btu}$$

Accordingly,

$$U_o = 244\,\text{Btu/h ft}^2\,°\text{F}$$

The calculated value based on exchanger design specifications is less than the assumed design value; consequently, the design is not successful and the heat exchanger is underspecified. The shell side film heat transfer coefficient should be increased so that the overall heat transfer coefficient is increased. Assuming baffle spacing, b is 7 in.

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times b$$

$$A_{cf} = \frac{21.25\,\text{in.}}{1\,\text{in.}} \times \left(0.25\,\text{in.}\frac{1\,\text{ft}}{12\,\text{in.}}\right) \times \left(7\,\text{in.}\frac{\text{ft}}{12\,\text{in.}}\right) = 0.259\,\text{ft}^2$$

The shell side mass velocity, G_o

$$G_o = \frac{m_o}{A_{cf}} = \frac{150{,}000(\text{lb/h})}{0.259\,\text{ft}^2} = 579150\frac{\text{lb}}{\text{ft}^2\,\text{h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{Reo} = \frac{D_e G_o}{\mu_o} = \frac{0.948\,\text{in.}(1\,\text{ft}/12\,\text{in.}) \times 579150(\text{lb/ft}^2\,\text{h})}{0.81\,\text{cP} \times (1(\text{lb/ft s}) \times (3600\,\text{s}/1\,\text{h}))/1488\,\text{cP}} = 23{,}347$$

Substituting values of Reynolds number and Prandtl number in the heat transfer equations and neglecting the effect of change in viscosity,

$$\text{Nu}_o = \frac{h_o D_e}{k_o} = 0.36(23{,}347)^{0.55}(5.44)^{1/3}(1)^{0.14} = 160$$

The heat transfer coefficient, h_o

$$h_o = \mathrm{Nu}\frac{k_o}{D_e} = 160\frac{\left(0.36(\mathrm{Btu/ft\,h\,°F})\right)}{0.948\text{ in.} \times (1\text{ ft}/12\text{ in.})} = 730\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

The new U-value

$$\frac{1}{U_i} = \frac{0.62\text{ in.}}{0.75\text{ in.} \times 730(\mathrm{Btu/ft^2h\,°F})} + \frac{0.62\text{ in.} \times \left(0.065\text{ in.}/12\text{ in./ft}\right)}{0.683\text{ in.} \times 30(\mathrm{Btu/ft^2\,h\,°F})}$$

$$+\frac{1}{1185(\mathrm{Btu/ft^2\,h\,°F})} + 0.001\frac{\mathrm{ft^2\,h\,°F}}{\mathrm{Btu}} = 3.14 \times 10^{-3}\frac{\mathrm{ft^2\,h\,°F}}{\mathrm{Btu}}$$

Hence,

$$U_i = 318.5\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,ft}}$$

PRESSURE DROP

The pressure drop for the flow of liquid without phase change through a circular tube is given by the following equations [6]:

$$-\Delta P_o = P_{in} - P_{out} = K_s\frac{2N_R f' G_o^2}{g_c \rho_c \phi}$$

$$N_{reversals} = \frac{L}{b} = \frac{10\text{ ft}}{7\text{ in.}}\frac{12\text{ in.}}{\text{ft}} = 17.14$$

The value of

$$K_s = 1.1 \times N_{reversals} = 1.1 \times 17.14 = 18.86$$

Number of tubes at the centerline

$$\cong \frac{D_s}{P_t} = \frac{21.25\text{ in.}}{1\text{ in.}} = 21.25$$

The number of tube rows across which the shell fluid flows, N_R, equals the total number of tubes at the center plane minus the number of tube rows that pass through the cut portions of the baffles. For 25% cut baffles, N_R may be taken as 50% of the number of the tubes at the center plane.

$$N_R = 0.5 \times 21.25 = 10.625 \cong 11$$

The modification friction factor, f'

$$f' = b_2\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15}$$

where b_2 for square pitch is

$$b_2 = 0.044 + \frac{0.08x_L}{(x_T - 1)^{0.43+1.13/x_L}}$$

where x_T is the ratio of the pitch transverse to flow to tube OD and x_L is the ratio of pitch parallel to tube OD. For square pitch $x_L = x_T$

$$x_L = x_T = \frac{P_t}{D_o} = \frac{1}{0.75} = 1.33$$

Hence,

$$b_2 = 0.044 + \frac{0.08 \times 1.333}{(1.333 - 1)^{0.43+1.13/1.333}} = 0.48$$

$$f' = b_2\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15} = 0.48\left(\frac{0.75\,\text{in./12 in./ft} \times 579{,}150\,\text{lb/ft}^2\,\text{h}}{0.81\,\text{cP} \times 2.42\,\text{lb/ft h/1 cP}}\right)^{-0.15} = 0.11$$

Substituting in the shell side pressure drop equation:

$$-\Delta P_o = K_s\frac{2N_R f' G_o^2}{g_c\rho_o\phi} = 18.86\frac{2 \times 11 \times 0.11\left(579{,}150\,\text{lb/ft}^2\,\text{h}\middle|\text{h/3600 s}\right)^2}{32.2(\text{ft lb/lb}_f\,\text{s}^2) \times 62.4\,\text{lb/ft}^3 \times 1} \times \frac{1\,\text{ft}^2}{144\,\text{in.}^2}$$

$$= 4.1\,\text{psi}$$

Estimating the pressure drop in the tube side is much easier than calculated pressure drop in the shell side. The pressure drop in the tube side is calculated using the following equations [6]:

$$-\Delta P_i = 1.2\frac{N_P f_D G_i^2 L}{2g_c\rho_i D_i\phi}$$

where

$$f_D = (1.82\log_{10} N_{Rei} - 1.64)^{-2}$$

$$f_D = (1.82\log_{10} 26{,}072 - 1.64)^{-2} = 0.0244$$

Tube side mass velocity

$$G_i = \rho_i u_i = 62.4\frac{\text{lb}}{\text{ft}^3} \times 5\frac{\text{ft}}{\text{s}} = 312\frac{\text{lb}}{\text{ft}^2\,\text{s}}$$

Substituting in pressure drop equation,

$$-\Delta P_i = 1.2\frac{N_P f_D G_i^2 L}{2g_c \rho_i D_i \phi}$$

$$= 1.2\frac{2\times 0.0244\times\left(312(\text{lb/ft}^2\,\text{s})\right)^2\times 10\ \text{ft}}{2\times 32.2(\text{ft lb/lb}_f\,\text{s}^2)\times 62.4(\text{lb/ft}^3)\times(0.62\ \text{in./12 in./ft})\times 1}\times\frac{1\,\text{ft}^2}{144\ \text{in.}}$$

$$= 1.91\,\text{psi}$$

The designed heat exchanger is summarized in Table 4.10.

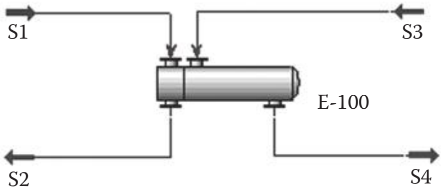
UNISIM/HYSYS SIMULATION

The heat exchanger model used is *Steady State Rating*. The exchanger is 1–2 number of shell–tube passes. However, on the *Rating/Sizing* page (Sizing Data) window, the shell and tube data are provided. Values obtained from hand calculations are used. The process flow sheet obtained using Unisim is shown in Figure 4.29. The fluid package used is NRTL-SRK.

TABLE 4.10

Design Specifications

	Shell Side	**Tube Side**
Components	Water (100%)	Water (100%)
Mass flow rate (lb/h)	150,000	300,000
Temperature (°F)	95/85	70/80°F
Pressure (bar)	1.0	1.0
Pass	1	2
Shell ID (in.)	$21\frac{1}{4}$	
Tubes: OD/ID/P_t (in.)		0.75/0.62/1
Tube configuration		Square
Length (ft)		10
Total number of tubes		256
Number of baffles		15
Baffle spacing (in.)	7	
Fouling factor (ft^2 °F h/Btu)	0.0	0.001
Pressure drop (psi)	4.1	1.91
LMTD (°F)	12.33	
F factor	0.94	
U_o (Btu/h.ft^2 °F)	232.72	
Duty (Btu/h)	1,500,000	



E-100		
Duty	1.506e+006	Btu/h
Tube side feed mass flow	3.000e+005	lb/h
Shell side feed mass flow	1.500e+005	lb/h
Tube inlet temperature	75.00	F
Tube outlet temperature	80.00	F
Shell inlet temperature	95.00	F
Shell outlet temperature	85.09	F
Control UA	1.292e+005	Btu/F-h
Ft factor	0.9427	
Uncorrected LMTD	12.36	F
Overall U	257.0	Btu/h-ft^2-F
Tube side pressure drop	3.743	psi
Shell side pressure drop	11.60	psi

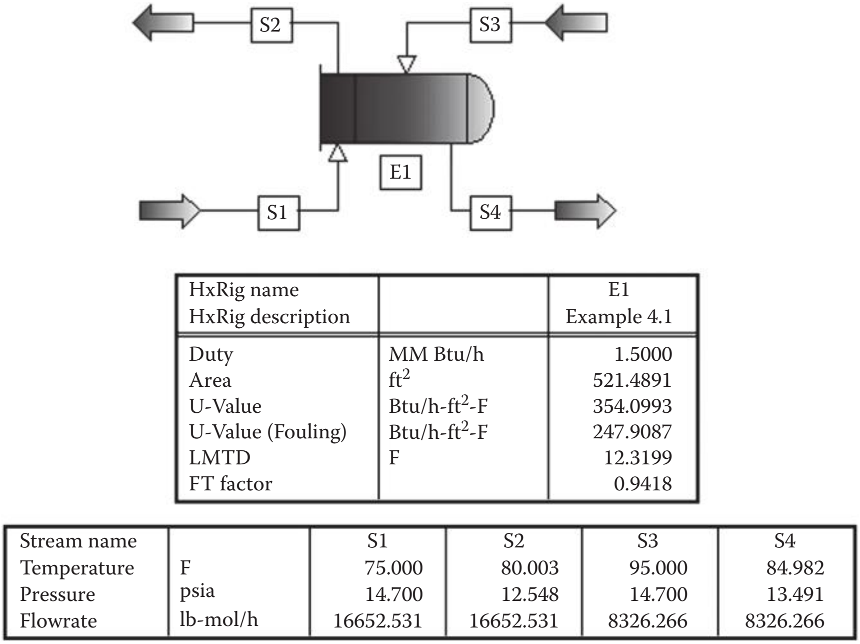
FIGURE 4.29
Process flow sheet of Example 4.4 by Unisim.

PRO/II SIMULATION

Using Pro II and selecting rigorous heat exchanger (*Rigorous HX*), NRTL fluid package is used. Shell side and tube side inlet streams need to be fully specified. *Fixed Duty* calculation type is used ($Q = 1.5 \times 10^6$ Btu/h). The process passes per shell is 2. On the *Film Coefficients Data* page, the overall *U*-value estimated is 300 Btu/h ft^2 °F as initial guess. Scale factors are left as default values. The tube flow sheet and stream table properties are shown in Figure 4.30. In the tubes pages, the tubes OD, ID, Pitch, and tube length must be provided, in the current example values are 0.75 in., 0.62 in., 1 in square-90 degrees and 10 ft, respectively. The number of tube side fouling resistance is 0.001 h ft^2 °F/Btu and zero for shell side. In the baffle geometry data, 0.25 for the fraction cut and 10 in. for center spacing. Nozzle can be left for Pro II default values. Filling all these data, the simulation is ready to run and the output data should look like that in Figure 4.30.

ASPEN SIMULATION

For this example *HeatX* heat exchanger from the model library is used; two inlet streams and two exit streams are connected with red arrows on the exchanger when in the connection mode. NRTL property estimation model is use. Feed streams temperature, pressure, flow rates, and compositions are provided same as the data given in the example, tube side fluid mass flow rate from hand calculation



HxRig name		E1
HxRig description		Example 4.1
Duty	MM Btu/h	1.5000
Area	ft^2	521.4891
U-Value	$Btu/h\text{-}ft^2\text{-}F$	354.0993
U-Value (Fouling)	$Btu/h\text{-}ft^2\text{-}F$	247.9087
LMTD	F	12.3199
FT factor		0.9418

Stream name		S1	S2	S3	S4
Temperature	F	75.000	80.003	95.000	84.982
Pressure	psia	14.700	12.548	14.700	13.491
Flowrate	lb-mol/h	16652.531	16652.531	8326.266	8326.266

FIGURE 4.30
Process flow sheet and stream table properties of Example 4.4.

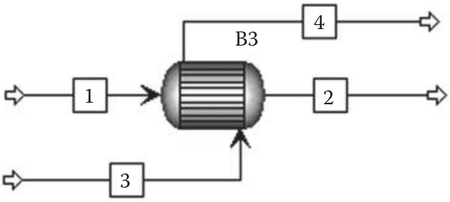
is used. While in the *Setup* page, and *Specifications* menu, *Detailed* and Rating are selected for the type of calculations. For *Exchanger specification, Exchanger duty is selected.* Film coefficient is selected for U-Methods. Film coefficient is set to be measured from exchanger geometry. The process flow sheet and stream table properties are shown in Figure 4.31. The results of the simulated detailed exchanger specifications are shown in Figure 4.32.

SuperPro Simulation

The simulated result of the shell and tube heat exchanger performed by SuperPro designer is shown in Figure 4.33.

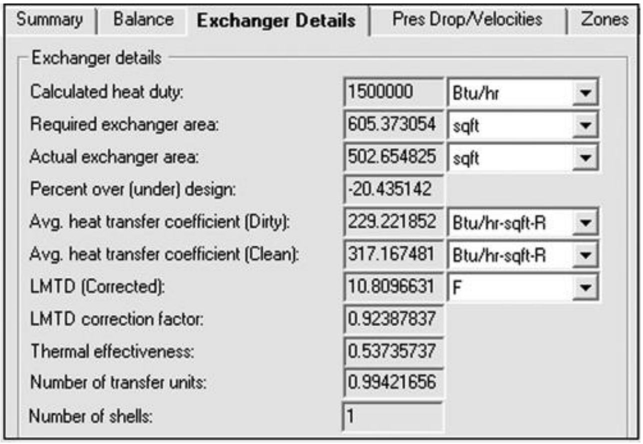
Example 4.5 Hot-Water–Cold-Water Exchanger

Hot water 100,000 lb/h at 250°F and 15 psi is used to heat a cold stream in a shell and tube heat exchanger. The inlet temperature and pressure of the cold stream are 125°F and 30 psi, respectively. The outlet temperature of the cold and hot streams is 150°F and 190°F, respectively. A hot-water stream is fed to the shell side of the heat exchanger and the cold-water stream called is fed into the tube side of the exchanger. Design a counter-current shell and tube heat exchange. Achieve the required heat duty. The assumed fouling factor for the tube side and shell side is 0.002 ft^2 h °F/Btu.



Example 4.4					
Stream ID		1	2	3	4
Temperature	F	75.0	80.4	95.0	84.2
Pressure	psi	14.50	11.58	14.50	13.71
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	lbmol/h	16652.531	16652.531	8326.265	8326.265
Mass flow	lb/h	300000.000	300000.000	150000.000	150000.000
Volume flow	cuft/h	4831.702	4845.918	2442.284	2427.959
Enthalpy	MMBtu/h	−2045.851	−2044.351	−1020.148	−1021.648
Mole flow	lbmol/h				
WATER		16652.531	16652.531	8326.265	8326.265

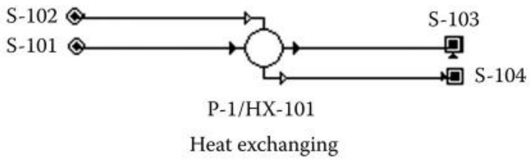
FIGURE 4.31
Process flow sheet and stream table with Aspen.

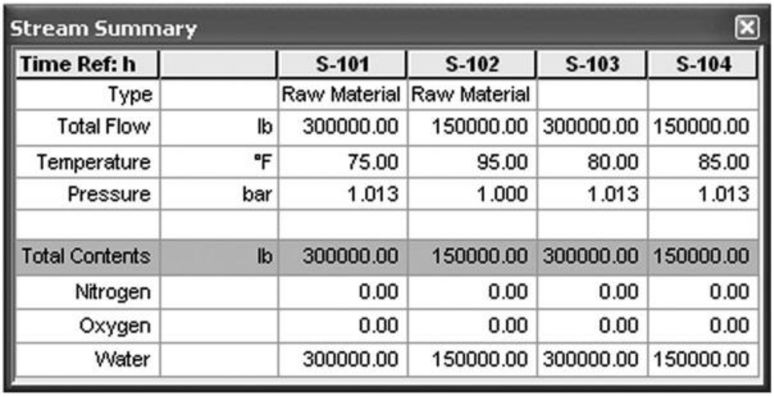


Exchanger details

Calculated heat duty: 1500000 Btu/hr
Required exchanger area: 605.373054 sqft
Actual exchanger area: 502.654825 sqft
Percent over (under) design: -20.435142
Avg. heat transfer coefficient (Dirty): 229.221852 Btu/hr-sqft-R
Avg. heat transfer coefficient (Clean): 317.167481 Btu/hr-sqft-R
LMTD (Corrected): 10.8096631 F
LMTD correction factor: 0.92387837
Thermal effectiveness: 0.53735737
Number of transfer units: 0.99421656
Number of shells: 1

FIGURE 4.32
Exchanger detailed design results.





Stream Summary

Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	lb	300000.00	150000.00	300000.00	150000.00
Temperature	°F	75.00	95.00	80.00	85.00
Pressure	bar	1.013	1.000	1.013	1.013
Total Contents	lb	300000.00	150000.00	300000.00	150000.00
Nitrogen		0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00
Water		300000.00	150000.00	300000.00	150000.00

FIGURE 4.33
Processes' flow sheet and stream table properties.

SOLUTION

HAND CALCULATIONS

Schematic diagram of 1–2 shell and tube heat exchanger for the hot-water–cold-water system is shown in Figure 4.34.

The physical properties data for the shell side and tube side fluids at average temperatures are shown in Table 4.11.

The required heat duty, *Q*

$$Q_{\text{req}} = m_o C_{p_o} \Delta T_o = 100{,}000 \frac{\text{lb}}{\text{h}} \times 1.0 \frac{\text{Btu}}{\text{lb}\,^\circ\text{F}} \left(250 - 190\right)^\circ\text{F} = 6.0 \times 10^6 \frac{\text{Btu}}{\text{h}}$$

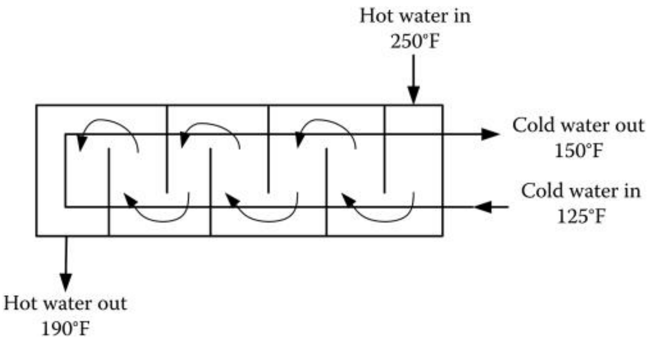


FIGURE 4.34
Schematic diagram of the hot-water–cold-water exchanger.

TABLE 4.11

Physical Properties at Average Temperatures

	Shell Side	Tube Side
Parameters	Hot water (220°F)	Cold water (138°F)
ρ (lb/ft^3)	60	61.4
C_p (Btu/lb °F)	1.0	1.01
μ (cP)	0.27	0.47
k (Btu/h ft °F)	0.39	0.38

The tube side cooling water mass flow rate, $\dot{m}_\text{i}$

$$\dot{m}_\text{i} = \frac{Q_\text{req}}{C_{p_\text{i}}\Delta T_\text{i}} \frac{6.0 \times 10^6(\text{Btu/h})}{1.01(\text{Btu/lb °F})(150 - 125)\text{°F}} = 2.4 \times 10^5 \frac{\text{lb}}{\text{h}}$$

The log means temperature difference, ΔT_LM.

$$\Delta T_\text{LM} = \frac{(250 - 150) - (190 - 125)}{\ln(250 - 150/190 - 125)} = \frac{35}{\ln(100/65)} = 81.25\text{°F}$$

The correction factor, F for 1–2 shell/tube passes or multiple of 2 tube passes is calculated from the following equation:

$$F_{1-2} = \frac{\left[\sqrt{R^2 + 1}/R - 1\right]\ln\left[1 - S/1 - SR\right]}{\ln\left[A + \sqrt{R^2 + 1}/A - \sqrt{R^2 + 1}\right]}$$

where

$$A = \frac{2}{S} - 1 - R$$

Hence,

$$R = \frac{250 - 190}{150 - 125} = 2.4$$

$$S = \frac{150 - 125}{250 - 125} = 0.2$$

$$A = \frac{2}{0.2} - 1 - 2.4 = 6.6$$

Substituting values of R, S, and A to calculate the temperature correction factor, F_{1-2}

$$F_{1-2} = \frac{\left[\sqrt{2.4^2+1}/2.4-1\right]\ln\left[1-0.2/1-0.2\times 2.4\right]}{\ln\left[6.6+\sqrt{2.4^2+1}/6.6-\sqrt{2.4^2+1}\right]} = 0.96$$

A typical overall heat transfer coefficient for the water–water exchanger is within the range 140–260 Btu/ft^2 h °F. Assume over all heat transfer coefficient as 200 Btu/ft^2 h °F

$$A_i = \frac{Q_{req}}{U_i F \Delta T_{LM}} = \frac{6.0\times 10^6 (\text{Btu/h})}{200(\text{Btu/ft}^2\,\text{h}°\text{F})\times 0.96\times 81.25°\text{F}} = 385\ \text{ft}^2$$

The tubes cross-sectional area/pass, A_{ci}

$$A_{ci} = \frac{F_i}{u_i} = \frac{m_i/\rho_i}{u_i} = \frac{2.4\times 10^5(\text{lb/h})/61.4(\text{lb/ft}^3)}{5(\text{ft/s})\times(3600\,\text{s/h})} = 0.217\ \text{ft}^2/\text{pass}$$

Utilizing $\frac{3}{4}$ in. tube OD, 16 BWG tubing (ID = 0.62 in.) arranged on a 1 in. square pitch and 12 ft tube length. The cross-sectional area/tube, A_{tc}

$$A_{tc} = \frac{\pi D_i^2}{4} = \frac{\pi\times(0.62\,\text{in.})^2}{4} = 0.302\,\text{in.}^2/\text{tube}$$

The total number of tubes per pass, N_t

$$N_t = \frac{A_{ci}}{A_{tc}} = \frac{0.217\ \text{ft}^2}{0.302\ \text{in.}^2/\text{tube}}\frac{144\ \text{in.}^2}{\text{ft}^2} = 104\ \text{tube/pass}$$

A single tube inside surface area, A_t

$$A_t = \pi D_i L = \pi\times 0.62\frac{\text{in.}}{12\ \text{in./ft}}\times 12\ \text{ft} = 1.95\ \text{ft}^2$$

The number of tube passes, N_p

$$N_p = \frac{A_i}{A_t\times N_t}\frac{385\ \text{ft}^2}{1.95(\text{ft}^2/\text{tube})\times 104\ \text{tubes/pass}} = 1.9 \cong 2\,\text{passes}$$

The number of tube passes is approximated to 2 ($N_p = 2$), accordingly, the corrected total tubes inside surface heat transfer area, A_i:

$$A_i = N_p N_t(\pi D_i L) = 2\times 104\times\pi\times 0.62\,\text{in.}\frac{1\,\text{ft}}{12\,\text{in.}}\times 12\ \text{ft} = 405\ \text{ft}^2$$

The tube outside surface area, A_o

$$A_o = N_p N_t \left(\pi D_o L\right) = 2 \times 104 \times \pi \times 0.75\,\text{in.}\frac{1\,\text{ft}}{12\,\text{in.}} \times 12\,\text{ft} = 490\,\text{ft}^2$$

The corrected overall heat transfer coefficient, U_i

$$U_i = \frac{Q}{A_i F \Delta T_{lm}} = \frac{6 \times 10^6 (\text{Btu/h})}{405\,\text{ft}^2 \times 0.96 \times 81.25°\text{F}} = 190\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

The corrected overall heat transfer coefficient is within the design range (140–260 Btu/ft^2 h °F). The assumed value should match U-value estimated from the heat exchanger design specifications that depends on the film heat transfer coefficient of tube side and shell side, fouling factor, and metal resistance.

$$\frac{1}{U_i} = \frac{A_i}{A_o h_o} + \frac{A_i \Delta x}{A_{LM} k_w} + \frac{1}{h_i} + R_{fi} + R_{fo}\frac{A_i}{A_o}$$

The tube side film heat transfer coefficient, h_i

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027 N_{\text{Rei}}^{0.8} N_{\text{Pri}}^{1/3}\left(\frac{\mu}{\mu_w}\right)^{0.14}$$

The Reynolds number of the tube side, N_{Rei}

$$N_{\text{Rei}} = \frac{D_i \rho_i u_i}{\mu_i} = \frac{0.62\,\text{in.} / 12\,\text{in./ft} \times 61.4(\text{lb/ft}^3) \times 5(\text{ft/s})}{0.47\,\text{cP} \times (1\,\text{lb/ft}\,\text{s}/1488\,\text{cP})} = 50{,}218$$

The Prandtl number of the tube side, N_{Pri}

$$N_{\text{Pri}} = \frac{C_{p_i} \mu_i}{k_i} = \frac{1.01(\text{Btu/lb}\,°\text{F}) \times 0.47\,\text{cP} \times (1\,\text{lb/ft}\,\text{s}/1488\,\text{cP}) \times 3600(\text{s/h})}{0.38(\text{Btu/ft}\,\text{h}\,°\text{F})} = 3.02$$

The tube side heat transfer coefficient, h_i, [6]

$$\text{Nu}_i = \frac{h_i D_i}{k_i} = 0.027 N_{\text{Rei}}^{0.8} N_{\text{Pri}}^{1/3}\left(\frac{\mu}{\mu_w}\right)^{0.14} = 0.027\left(50218\right)^{0.8}\left(3.02\right)^{1/3} \times 1 = 225$$

Hence, the tube side film heat transfer coefficient h_i,

$$h_i = \frac{225 \times k_i}{D_i} = 225 \times \frac{0.38(\text{Btu/ft}\,\text{h}\,°\text{F})}{0.62\,\text{in./12\,in./ft}} = 1654\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

The shell side heat transfer coefficient, h_o, is calculated using the heat transfer equation from Kern [3]:

$$\text{Nu}_o = \frac{h_o D_e}{k_o} = 0.36 N_{\text{Reo}}^{0.55} N_{\text{Pro}}^{1/3} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

where the Reynolds number and the Prandtl number are

$$N_{\text{Reo}} = \frac{D_e G_o}{\mu_o}$$

$$N_{\text{Pro}} = \frac{C_{p_o} \mu_o}{k_o}$$

The hydraulic effective diameter, D_e

$$D_e = \frac{4\left(P_t^2 - (\pi D_o^2/4)\right)}{\pi D_o} = \frac{4 \times \left(1^2 - \left(\pi(0.75)^2/4\right)\right)}{\pi \times 0.75} = 0.948 \text{ in.}$$

The shell side mass velocity normal to tubes at the centerline of the exchanger, G_o, requires estimation of the cross-sectional area between baffles and shell axis, A_{cf}. For 2 tube passes, 104 tubes (Total = 208 tubes), $\frac{3}{4}$ in. OD, 1 in. square pitch, the shell diameter can be found from tube sheet layouts [3]. The closest available value for the number of tubes that got Ds value for 208 tubes is 220, belongs to shell ID is $19\frac{1}{4}$ in., and assume baffle spacing 10 in.

$$A_{cf} = \frac{D_s}{P_t} \times \text{clearance} \times \text{b}$$

$$A_{cf} = \frac{19.25 \text{ in.}}{1 \text{ in.}} \times \left(0.25 \text{ in.} \frac{1 \text{ ft}}{12 \text{ in.}}\right) \times \left(10 \text{ in.} \frac{\text{ft}}{12 \text{ in.}}\right) = 0.335 \text{ ft}^2$$

The shell side mass velocity, G_o

$$G_o = \frac{m_o}{A_{cf}} = \frac{100{,}000(\text{lb}/h)}{0.335 \text{ ft}^2} = 298{,}700 \frac{\text{lb}}{\text{ft}^2 \text{ h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{\text{Reo}} = \frac{D_e G_o}{\mu_o} = \frac{0.948 \text{ in.}(1 \text{ ft}/12 \text{ in.}) \times 298{,}700(\text{lb}/\text{ft}^2 \text{ h})}{0.27 \text{ cP} \times [1(\text{lb}/\text{ft s}) \times (3600 \text{ s}/1 \text{ h})]/(1488 \text{ cP})} = 36{,}125$$

The shell side Prandtl number, N_{Pro}

$$N_{\text{Pro}} = \frac{C_{p_o} \mu_o}{k_o} = \frac{1.0(\text{Btu}/\text{lb}\,°\text{F}) \times 0.27 \text{ cP}[1(\text{lb}/\text{ft s})(3600 \text{ s}/\text{h})]/(1488 \text{ cP})}{0.39(\text{Btu}/\text{ft}^2 \text{ h}\,°\text{F})} = 1.675$$

Substituting values of Reynolds number and Prandtl number in the shell side film heat transfer equations and neglecting the effect of change in viscosity,

$$\mathrm{Nu_o} = \frac{h_o D_e}{k} = 0.36(36{,}125)^{0.55}(1.675)^{1/3}(1)^{0.14} = 137$$

The shell side heat transfer coefficient, h_o

$$h_o = \mathrm{Nu}\frac{k_o}{D_e} = 137\frac{\left(0.39(\mathrm{Btu/ft^2\,h\,°F})\right)}{0.948\text{ in.} \times (1\text{ ft}/12\text{ in.})} = 678\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,°F}}$$

Substituting estimated values of shell side and tube side film heat transfer coefficients in the following equation:

$$\frac{1}{U_i} = \frac{A_i}{A_o h_o} + \frac{A_i \Delta x}{A_{LM} k_w} + \frac{1}{h_i} + R_{fi} + R_{fo}\frac{A_i}{A_o}$$

where

$$A_i = \pi D_i L = \pi \times 0.62\text{ in.}\frac{1\text{ ft}}{12\text{ in.}} \times 12\text{ ft} = 1.95\text{ ft}^2,$$

$$A_o = \pi D_o L = \pi \times 0.75\text{ in.}\frac{1\text{ ft}}{12\text{ in.}} \times 12\text{ ft} = 2.356\text{ ft}^2$$

$k_w = 30$ Btu/ft h° F.

The tube wall thickness, Δx

$$\Delta x = \frac{0.75 - 0.62}{2} = 0.0.065\text{ in.}$$

The log means area, A_{LM}

$$A_{LM} = \frac{A_o - A_i}{\ln(A_o/A_i)} = \frac{2.356 - 1.95}{\ln(2.356/1.95)} = 2.147\text{ ft}^2$$

Substituting values:

$$\frac{1}{U_i} = \left(\frac{1.95}{2.356}\right)\frac{1}{678} + \frac{(1.95)(0.065/12)}{2.147(30)} + \frac{1}{1654} + 0.002 + 0.002\left(\frac{1.95}{2.356}\right)$$

$$= 5.645 \times 10^{-3}$$

The overall heat transfer coefficient based on inside area is

$$U_i = 177\frac{\mathrm{Btu}}{\mathrm{ft^2\,h\,ft}}$$

The overall designed heat exchanger is less than the assumed value; consequently, the designed heat exchanger is not successful. Shell side heat transfer coefficient could be increased by decreasing the baffle spacing; the value should not be less than fifth of the shell ID and not exceeding shell side diameter. Assuming baffle spacing equal to 5 in.:

$$A_{\text{cf}} = \frac{D_{\text{s}}}{P_{\text{t}}} \times \text{clearance} \times b$$

$$A_{\text{cf}} = \frac{19.25\text{ in.}}{1\text{ in.}} \times \left(0.25\text{ in.}\frac{1\text{ ft}}{12\text{ in.}}\right) \times \left(5\text{ in.}\frac{\text{ft}}{12\text{ in.}}\right) = 0.167\text{ ft}^2$$

The shell side mass velocity, G_{o}

$$G_{\text{o}} = \frac{m_{\text{o}}}{A_{\text{cf}}} = \frac{100{,}000(\text{lb}/h)}{0.167\text{ ft}^2} = 598{,}802\frac{\text{lb}}{\text{ft}^2\,\text{h}}$$

The shell side Reynolds number, N_{Reo}

$$N_{\text{Reo}} = \frac{D_{\text{e}}G_{\text{o}}}{\mu_{\text{o}}} = \frac{0.948\text{ in.}(1\text{ ft}/12\text{ in.}) \times 598{,}802(\text{lb}/\text{ft}^2\,\text{h})}{0.27\text{ cP} \times [1(\text{lb}/\text{ft s}) \times (3600\text{ s}/1\text{ h})]/(1488\text{ cP})} = 72{,}202$$

Shell side Prandtl number, N_{Pro}

$$N_{\text{Pro}} = \frac{C_{p_{\text{o}}}\mu_{\text{o}}}{k_{\text{o}}} = \frac{1.0(\text{Btu}/\text{lb}\,°\text{F}) \times 0.27\text{ cP}[2.42(\text{lb}/\text{ft}\,\text{h})]/(1\text{ cP})}{0.39(\text{Btu}/\text{ft}^2\,\text{h}\,°\text{F})} = 1.675$$

Substituting values of shell side Reynolds number and Prandtl number in the heat transfer equations and neglecting the effect of change in viscosity,

$$\text{Nu} = \frac{h_{\text{o}}D_{\text{e}}}{k} = 0.36(72{,}202)^{0.55}(1.675)^{1/3}(1)^{0.14} = 201$$

The heat transfer coefficient, h_{o}

$$h_{\text{o}} = \text{Nu}\frac{k_{\text{o}}}{D_{\text{e}}} = 201\frac{0.39(\text{Btu}/\text{ft}^2\,\text{h}\,°\text{F})}{0.948\text{ in.} \times (1\text{ ft}/12\text{ in.})} = 992\frac{\text{Btu}}{\text{ft}^2\,\text{h}\,°\text{F}}$$

The overall heat transfer coefficient, U_{i}

$$\frac{1}{U_{\text{i}}} = \frac{D_{\text{i}}}{D_{\text{o}}h_{\text{o}}} + \frac{D_{\text{i}}\Delta x}{D_{\text{LM}}k_{\text{w}}} + \frac{1}{h_{\text{i}}} + R_{f\text{i}} + R_{f\text{o}}\left(\frac{D_{\text{i}}}{D_{\text{o}}}\right)$$

Substituting estimated values (h_{o}, h_{i}, k_{w}, $R_{f\text{i}}$, $R_{f\text{o}}$) as follows:

$$\frac{1}{U_{\text{i}}} = \frac{0.62}{0.75 \times 992} + \frac{(0.62)(0.065/12)}{0.683(30)} + \frac{1}{1654} + 0.002 + 0.002\left(\frac{0.62}{0.75}\right)$$

$$= 0.00526.$$

The calculated over all heat transfer coefficient:

$$U_i = 190.26 \frac{\text{Btu}}{\text{ft}^2\,\text{h}\,\text{ft}}$$

The value is very close to the corrected overall heat transfer coefficient (190 Btu/ft^2 h °F); as a result, the designed exchanger is successful.

Based on outside area, U_o

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{A_o \Delta x}{A_{LM} k_w} + \left(\frac{A_o}{A_i}\right)\frac{1}{h_i} + \left(\frac{A_o}{A_i}\right) R_{fi} + R_{fo}$$

Substituting values:

$$\frac{1}{U_o} = \frac{1}{992} + \frac{2.356 \times 0.065/12}{2.147 \times 30} + \left(\frac{2.356}{1.95}\right)\frac{1}{1654} + \left(\frac{2.356}{1.95}\right)(0.002) + 0.002$$

$$= 6.346 \times 10^{-3}$$

The overall heat transfer coefficient based on outside tube surface area.

$$U_o = 157.57 \frac{\text{Btu}}{\text{h}\,\text{ft}^2\,°\text{F}}$$

PRESSURE DROP

The pressure drop for the flow of liquid without phase change through a circular tube is given by the following equations [6]:

$$-\Delta P_o = P_{in} - P_{out} = K_s \frac{2 N_R f' G_o^2}{g_c \rho_c \phi}$$

$$N_{\text{reversals}} = \frac{L}{b} = \frac{12\,\text{ft}}{5\,\text{in.}} \frac{12\,\text{in.}}{\text{ft}} = 28.8$$

The value of

$$K_s = 1.1 \times N_{\text{reversals}} = 1.1 \times 28.8 = 31.68$$

Number of tubes at the centerline

$$\cong \frac{D_s}{P_t} = \frac{19.25\,\text{in.}}{1\,\text{in.}} = 19.25$$

The number of tube rows across which the shell fluid flows, N_R, equals the total number of tubes at the center plane minus the number of tube rows that pass through the cut portions of the baffles. For 25% cut baffles, N_R may be taken as 50% of the number of the tubes at the center plane.

$$N_R = 0.5 \times 19.25 = 9.625 \cong 10$$

The modification friction factor, f'

$$f' = b_2\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15}$$

where b_2 for square pitch is

$$b_2 = 0.044 + \frac{0.08x_L}{\left(x_T - 1\right)^{0.43+1.13/x_L}}$$

where x_T is the ratio of the pitch transverse to flow to tube OD and x_L is the ratio of pitch parallel to tube OD, for square pitch; $x_T = x_L$.

$$x_L = x_T = \frac{P_t}{D_o} = \frac{1}{0.75} = 1.33$$

Hence,

$$b_2 = 0.044 + \frac{0.08 \times 1.333}{\left(1.333 - 1\right)^{0.43+1.13/1.333}} = 0.48$$

$$f' = b_2\left(\frac{D_oG_o}{\mu_o}\right)^{-0.15} = 0.48\left(\frac{(0.75\text{ in.}/12\text{ in.}/\text{ft}) \times (598{,}441\,\text{lb}/\text{ft}^2\,\text{h})}{0.27\text{ cP} \times (2.42\,\text{lb}/\text{ft}\,\text{h}/1\text{cP})}\right)^{-0.15}$$

$$= 0.093$$

Substituting in the shell side pressure drop equation:

$$-\Delta P_o = K_s\frac{2N_Rf'G_o^2}{g_c\rho_o\phi} = 31.68\frac{2 \times 10 \times 0.093\left((598{,}441\,\text{lb}/\text{ft}^2\,\text{h})|(\text{h}/3600\,\text{s})\right)^2}{32.2(\text{ft}\,\text{lb}/\text{lb}_f\,\text{s}^2) \times 60(\text{lb}/\text{ft}^3) \times 1} \times \frac{1\,\text{ft}^2}{144\,\text{in.}^2}$$

$$= 5.82\,\text{psi}$$

The pressure drop in the tube side is calculated using the following equations [6]:

$$-\Delta P_i = 1.2\frac{N_Pf_DG_i^2L}{2g_c\rho_iD_i\phi}$$

where

$$f_D = \left(1.82\log_{10} N_{Rei} - 1.64\right)^{-2}$$

$$f_D = \left(1.82\log_{10} 50{,}218 - 1.64\right)^{-2} = 0.021$$

Tube side mass velocity

$$G_i = \rho_i u_i = 61.4\frac{\text{lb}}{\text{ft}^3} \times 5\frac{\text{ft}}{\text{s}} = 307\frac{\text{lb}}{\text{ft}^2\,\text{s}}$$

Substituting in pressure drop equation,

$$-\Delta P_i = 1.2\frac{N_P f_D G_i^2 L}{2g_c\rho_i D_i\phi}$$

$$= 1.2\frac{2 \times 0.021 \times \left(307(\text{lb/ft}^2\,\text{s})\right)^2 \times 10\ \text{ft}}{2 \times 32.2(\text{ft lb/lb}_f\,\text{s}^2) \times 61.4(\text{lb/ft}^3) \times 0.62\ \text{in./12 in./ft} \times 1} \times \frac{1\ \text{ft}^2}{144\ \text{in.}}$$

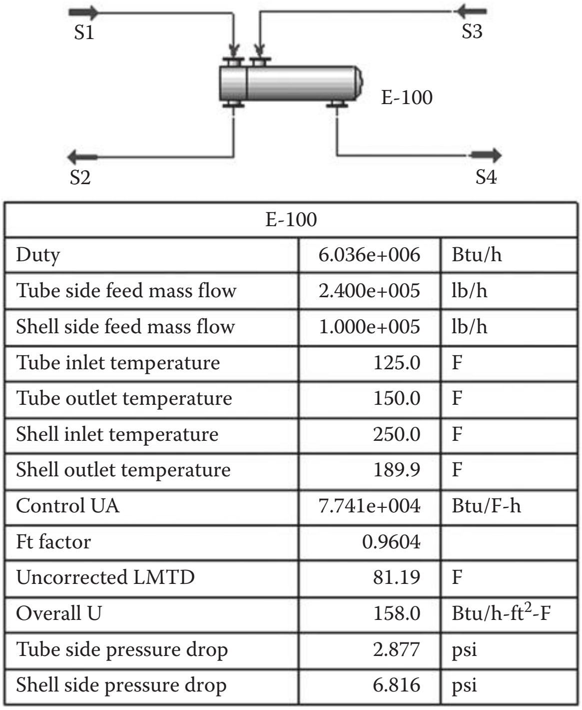
$$= 1.615\ \text{psi}$$

A summary of the heat exchange design specification is shown in Table 4.12.

TABLE 4.12

Design Specifications

	Shell Side	**Tube Side**
Components	Hot water	Cold water
Mass flow rate (lb/h)	100,000	240,000
Temperature (°F)	250/190	125/150°F
Pressure (bar)	1.0	1.0
Pass	1	2
Shell ID (in.)	$19\frac{1}{4}$	
Tubes: OD/ID/P_t (in.)		0.75/0.62/1
Tube configuration		Square pitch
Length (ft)		12
Total number of tubes		208
Number of baffles		28
Baffle spacing (in.)	5	
Fouling factor (ft^2 °F h/Btu)	0.002	0.002
Pressure drop (psi)	5.82	1.615
LMTD (°F)	81.25	
F factor	0.96	
U_o(Btu/h ft^2 °F)	157.57	
Duty (Btu/h)	6,000,000	



E-100		
Duty	6.036e+006	Btu/h
Tube side feed mass flow	2.400e+005	lb/h
Shell side feed mass flow	1.000e+005	lb/h
Tube inlet temperature	125.0	F
Tube outlet temperature	150.0	F
Shell inlet temperature	250.0	F
Shell outlet temperature	189.9	F
Control UA	7.741e+004	Btu/F-h
Ft factor	0.9604	
Uncorrected LMTD	81.19	F
Overall U	158.0	Btu/h-ft^2-F
Tube side pressure drop	2.877	psi
Shell side pressure drop	6.816	psi

FIGURE 4.35
Simulation results by Unisim.

HYSYS/UNISIM SIMULATION

The process flow sheet shown in Figure 4.35 is obtained by Unisim, results are close to the hand calculations with some deviation in the shell side exit temperature and duty, and this is due to mass heat capacity values difference between hand calculations and Hysys value.

PRO/II SIMULATION

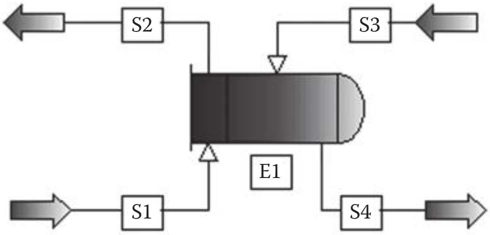
The process flow sheet the stream table properties obtained using Pro II software is shown in Figure 4.36. Based on the outside area, U_o is 155 Btu/h ft^2 °F.

ASPEN SIMULATION

The shell and tube heat exchange design using Aspen Plus is done as that in Example 4.4. The process flow sheet and stream table properties are shown in Figure 4.37. The Exchanger details are shown in Figure 4.38.

SUPERPRO SIMULATION

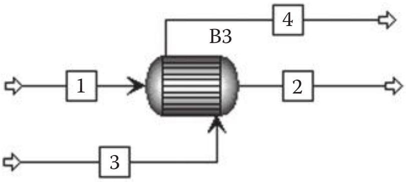
The stream summary results performed by SuperPro Designer are shown in Figure 4.39.



HxRig name HxRig description		E1 Example 4.5
Duty	MM Btu/h	6.0000
Area	ft^2	493.2561
U-Value	Btu/h-ft^2-F	493.8533
U-Value (Fouling)	Btu/h-ft^2-F	155.1772
LMTD	F	81.5563
FT factor		0.9612

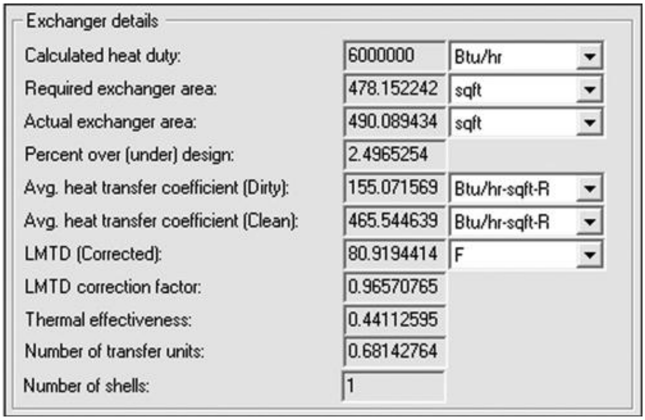
Stream name		S1	S2	S3	S4
Temperature	F	125.000	150.041	250.000	190.564
Pressure	psia	15.000	12.795	30.000	28.428
Flowrate	lb-mol/h	13322.024	13322.024	5550.843	5550.843

FIGURE 4.36
Process flow sheet and stream table properties.



Example 4.5					
Stream ID		1	2	3	4
Temperature	F	125.0	150.5	250.0	194.8
Pressure	psi	15.00	11.72	30.00	28.22
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	lbmol/h	13322.024	13322.024	5550.844	5550.844
Mass flow	lb/h	240000.000	240000.000	100000.000	100000.000
Volume flow	cuft/h	3973.902	4033.096	1789.413	1726.280
Enthalpy	MMBtu/h	−1625.369	−1619.369	−664.211	−670.211
Mole flow	lbmol/h				
Water		13322.024	13322.024	5550.844	5550.844

FIGURE 4.37
Process flow sheet and stream table property with Aspen.



Exchanger details

Calculated heat duty: 6000000 Btu/hr

Required exchanger area: 478.152242 sqft

Actual exchanger area: 490.089434 sqft

Percent over (under) design: 2.4965254

Avg. heat transfer coefficient (Dirty): 155.071569 Btu/hr-sqft-R

Avg. heat transfer coefficient (Clean): 465.544639 Btu/hr-sqft-R

LMTD (Corrected): 80.9194414 F

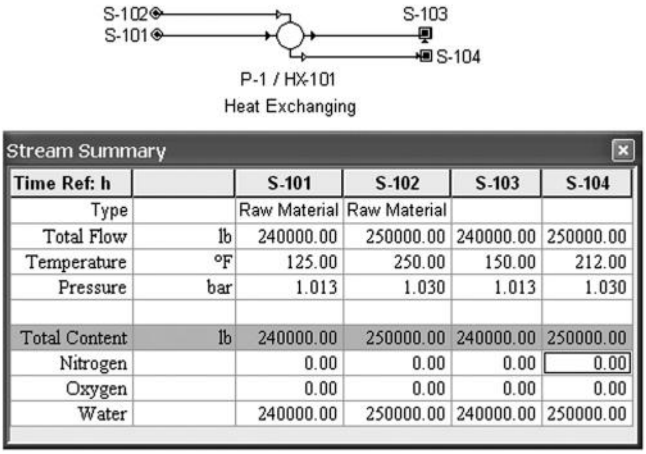
LMTD correction factor: 0.96570765

Thermal effectiveness: 0.44112595

Number of transfer units: 0.68142764

Number of shells: 1

FIGURE 4.38
Exchanger detailed design data.



Stream Summary

Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	lb	240000.00	250000.00	240000.00	250000.00
Temperature	°F	125.00	250.00	150.00	212.00
Pressure	bar	1.013	1.030	1.013	1.030
Total Content	lb	240000.00	250000.00	240000.00	250000.00
Nitrogen		0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00
Water		240000.00	250000.00	240000.00	250000.00

FIGURE 4.39
Process flow sheet and stream table properties with SuperPro.

PROBLEMS

4.1 Hot-Water–Cold-Water Heat Exchanger

Design a shell and tube heat exchanger for hot water at 100,000 lb/h and 160°F is cooled with 200,000 lb/h of cold water at 90°F, which is heated to 120°F in a counter current shell and tube heat exchanger. Assume that the exchanger has 20 ft steel tubes (Thermal conductivity of steel is 26 Btu/(ft h °F), 0.75 in. OD, and 0.62 in. ID.) The tubes are on 1 in. square pitch.

4.2 Heating of Natural Gas with Hot Water

Hot water at 240°F is used to heat 115,000 lb/h of natural gas (60% methane, 25% ethane, 15% propane) at 500 psia from 80°F to 95°F. The heating water is available at 250°F and 90 psia with a flow rate of 30,000 lb/h. Hot water is flowing on the shell side. Assuming that the fouling factor for water is 0.002 (h ft °F)/Btu. Design a shell and tube heat exchanger for this purpose.

4.3 Cooling Diethanolamine Solution in Sweetening Plant

Design a shell and tube heat exchanger to cool 50,000 lb/h of diethanolamine (DEA) solution (0.2 mass fractions DEA/0.8 water) from 144°F to 113°F by using water at 77°F heated to 100°F. Assume that the tube inside fouling resistance is 0.002 ft^2 h °F/Btu, and shell side fouling resistance is 0.002 ft^2 h °F/Btu. Compare design results with Example 4.1.

4.4 Cooling Ethylene Glycol in the Dehydration Process

Design a shell and tube heat exchanger for 100,000 lb/h of ethylene glycol (EG) at 250°F cooled to 130°F using cooling water heated from 90°F to 120°F. The shell side fouling resistance is 0.004 (h ft^2 °F)/Btu and tube side fouling resistance is also 0.004 (h ft^2 °F)/Btu. Compare results with Example 4.2.

4.5 Rich Glycol: Lean Glycol Heat Exchanger

Rich glycol (TEG) from the absorber at 14,900 kg/h and 65°F is exchanging heat with 14,500 kg/h lean glycol from air cooler at 140°F and leaving at 83°F. Design a shell and tube heat exchanger for this purpose.

4.6 Shell Side Heat Transfer Coefficient (McCabe p. 441)

A shell and tube heat exchanger is used to heat 100,000 lb/h of benzene is heated from 40°F to 80°F in the shell side heat exchanger using 100,000 lb/h hot water at 180°F. The exchanger contains 828 tubes, $\frac{3}{4}$ in. OD, 12 ft long on 1 in. square pitch. The baffles are 25% cut and baffle spacing is 12 in. the shell side is 35 in. Calculate the shell side heat transfer coefficient using Donohue equation (4.18) and compare with Equation 4.14.

4.7 Heat Exchanger for Ethylbenzene and Styrene

Design a shell-and-tube heat exchanger to preheat a stream of 66,150 lb/h containing ethylbenzene and styrene from 50°F to 207°F. Heat supply is medium saturated steam at 240°F. Additional data:

Density = 856 kg m^3
Viscosity = 0.4765 cP
Specific heat = 0.428 kcal/kg °C
Thermal conductivity = 0.133 kcal/h m °C

References

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5

Reactor Design

At the end of this chapter you should be able to

1. Develop the ability to analyze the performance of reactors in which single and multiple reactions are occurring.
2. Find the volume of CSTR and PFR to achieve a specific conversion.
3. Obtain the ability to analyze reactors with catalytic reactions and to employ the results of such analyses in designing simple reactors.
4. Design isothermal and nonisothermal reactors involving single/multiple reactions.

5.1 Introduction

Chemical reactors are vessels designed to contain chemical reactions. Chemical engineers design reactors to ensure that the reaction proceeds with the highest efficiency toward the desired output product, producing the highest yield of product while requiring the least amount of money to purchase and operate. Normal operating expenses include energy input, energy removal, and raw material costs. Energy changes can come in the form of heating or cooling. The three major types of reactors that will be covered in this chapter are CSTR, PFR, and packed-bed reactors (PBR). Conversion reactors are simply used to solve material and energy balance of single or multiple reactions. In a CSTR, one or more fluid reagents are introduced into a tank reactor equipped with an impeller while the reactor effluent is removed. The impeller stirs the reagents to ensure proper mixing. Simply dividing the volume of the tank by the average volumetric flow rate through the tank gives the residence time, or the average amount of time a discrete quantity of reagent spends inside the tank. Using chemical kinetics, the reaction's expected percent completion can be calculated. At steady state, the mass flow rate in must equal the mass flow rate out, otherwise the tank will overflow or go empty (transient state). In a PFR, one or more fluid reagents are pumped through a pipe or tube. The chemical reaction proceeds as the reagents travel through the PFR. In this type of reactor, the changing reaction rate creates a gradient with respect to the distance traversed; at the inlet to the PFR the rate is very high, but as the concentrations of the reagents decrease and the concentration of the product(s) increases the reaction rate slows down. PBRs are tubular and are filled with solid catalyst particles, most often used to catalyze gas reactions. The chemical reaction takes place on the surface of the catalyst. The advantage of using a PBR is the higher conversion per weight of the catalyst than other catalytic reactors. The reaction rate is based on the amount of the solid catalyst rather than the volume of the reactor [1,2].

5.2 Plug Flow Reactor

The PFR generally consists of a bank of tubes. The reactants are continually consumed while flowing through the reactor; consequently, there will be an axial variation in concentration. By contrast, considering plug flow, there is no change in the mass or energy in the radial direction and axial mixing is negligible. Consider the gas-phase reaction taking place in PFR (Figure 5.1). In the simplest case of a PFR model, several assumptions must be made in order to simplify the problem, that is, plug flow, steady state, constant density (reasonable for some liquids but a 20% error for polymerizations; valid for gases only if there is no pressure drop, no net change in the number of moles, nor any large temperature change), and constant tube diameter. The PFR model can be used to model multiple reactions as well as reactions involving changing temperatures, pressures, and densities of the flow. Although these complications are ignored in what follows; they are often relevant to industrial processes [3].

$$A \rightarrow B + C$$

Molar flow rate of component A,

$$\frac{dF_A}{dV} = r_A, \quad \text{where } r_A = -kC_A \tag{5.1}$$

Molar flow rate of component B,

$$\frac{dF_B}{dV} = r_B \tag{5.2}$$

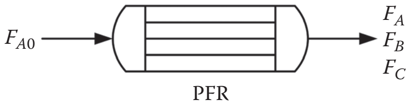


FIGURE 5.1
Process flow sheet of a PFR.

Molar flow rate of component *C*,

$$\frac{\mathrm{d}F_C}{\mathrm{d}V} = r_C, \quad \text{where } r_A = -r_B = -r_C \tag{5.3}$$

As a function of change in conversion,

$$F_A = F_{A0}(1 - X) \tag{5.4}$$

Differentiating both sides of Equation 5.4,

$$\mathrm{d}F_A = -F_{A0}\,\mathrm{d}X \tag{5.5}$$

Substituting into Equation 5.1

$$\frac{\mathrm{d}X}{\mathrm{d}V} = \frac{-r_A}{F_{A0}} \tag{5.6}$$

Rate of reaction, for first order with respect to *A*

$$r_A = -kC_A \tag{5.7}$$

Concentration as a function of conversion, x

$$C_A = \frac{F_A}{v_A} \tag{5.8}$$

Gas volumetric flow rate

$$v = v_0(1 + \varepsilon X)\frac{T}{T_0}\frac{P_0}{P} \tag{5.9}$$

$$\varepsilon = y_A 0 * \delta$$

Change in stoichiometric coefficient

$$\delta = \sum v_i, \quad \delta = \sum v_i = 1 + 1 - 1 = 1$$

Hence, the concentration of component *A*,

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - X)}{v_0(1 + X)(T/T_0)(P_0/P)} \tag{5.10}$$

Substituting Equation 5.10 into Equation 5.7 at constant pressure

$$-r_A = \frac{kC_{A0}(1-X)}{(1+X)}\frac{T_0}{T} \tag{5.11}$$

Change in reaction temperature as a function of the reactor volume

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{(-r_A)(-\Delta H_{\mathrm{rxn}})}{F_{A0}\left(\sum \theta_i C_{\mathrm{p}i} + X\Delta C_{\mathrm{p}}\right)} \tag{5.12}$$

Heat of reaction at temperatures other than reference temperature (25°C)

$$\Delta H_{\mathrm{rxn}} = \Delta H^{o}_{\mathrm{rxn}} + \Delta a(T - T_{\mathrm{r}}) + \frac{\Delta b}{2}(T^2 - T_{\mathrm{r}}^2) + \frac{\Delta c}{3}(T^2 - T_{\mathrm{r}}^2) \tag{5.13}$$

Second method, the second form of the energy balance is

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{(-r_A)(-\Delta H_{\mathrm{rxn}})}{F_A C_{\mathrm{p}A} + F_B C_{\mathrm{p}B} + F_C C_{\mathrm{p}C}} \tag{5.14}$$

5.3 Packed-Bed Reactors

As previously mentioned, in PBRs the reaction rate is based on the amount of the solid catalyst rather than the volume of the reactor. The schematic diagram of a PBR is shown in Figure 5.2. The steady-state design equation

$$\frac{\mathrm{d}F_A}{\mathrm{d}W} = r'_A \tag{5.15}$$

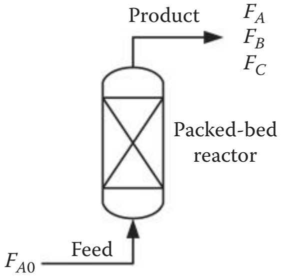


FIGURE 5.2
Schematic of a PBR.

The Ergun equation can be used to predict the pressure drop along the length of a packed bed given the fluid velocity, the packing size, the viscosity, and density of the fluid [2].

$$\frac{dP}{dz} = \frac{G}{\rho D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)}{D_p} + 1.75G\right] \tag{5.16}$$

where G is the superficial mass velocity, kg/(m^2 s), ρ is the fluid density, μ is the fluid viscosity, ϕ is the void fraction, and D_P is the particle diameter.

5.4 Continuous Stirred Tank Reactor

CSTRs (Figure 5.3) are usually used to handle liquid-phase reactions. The behavior of a CSTR is often modeled as an ideal perfectly mixed reactor. The CSTR model is often used to simplify engineering calculations. In practice, it can only be approached in industrial size reactors.

Assume perfect or ideal mixing, the steady-state material balance for the CSTR reactor

$$F_{A0}\,X + r_A V = 0 \tag{5.17}$$

The concentration of component A in the exit stream,

$$C_A = C_{A0}(1 - X) \tag{5.18}$$

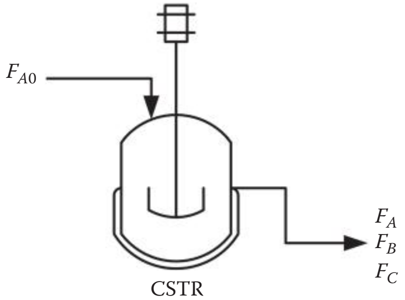


FIGURE 5.3
CSTR process flow sheet.

The second-order reaction rate with respect to component *A*,

$$r_A = -kCA^2 \tag{5.19}$$

The CSTR reactor volume a function of fractional conversion,

$$V_{\text{CSTR}} = \frac{F_{A0}X}{kC_{A0}^2(1-X)^2} \tag{5.20}$$

Example 5.1: CSTR Reactor Volume

Find the reactor volume that achieves 94% conversion of ethanol, for the following liquid-phase reaction in an isothermal CSTR. The inlet molar flow rate is 50 kgmol/h ethanol, 50 kmol/h diethylamine, and 100 kgmol/h water. The reaction is in second order with respect to ethanol

$$\mathrm{A + B \rightarrow C + D}$$

where A = ethanol, B = diethylamine, C = water, and D = triethylamine.

$$r_A = -kCA^2$$

$$k = Ae^{-E/RT}$$

E = activation energy = 1×10^4 J/mol, T = 50°C; A = Pre-exponential factor = 4775 L/mol h; R = 8.314 J/mol K; P = 3.5 atm; Molar density of ethanol is 16.6 mol/L; Molar density of diethylamine is 9.178 mol/L; Molar density of water is 54.86 mol/L.

SOLUTION

Hand Calculations

The feed average molar density, ρ

$$\frac{1}{\rho} = \sum \frac{x_i}{\rho_i} = \frac{0.25}{16.6} + \frac{0.25}{9.178} + \frac{0.5}{54.86} = \frac{0.0514}{1}$$

$$\rho = 19.45 \text{ mol/L}$$

The steady-state material balance on the CSTR reactor

$$F_{A0}\,X + (-r_A)(V) = 0$$

Concentration as a function of conversion, C_A

$$C_A = C_{A0}\,(1 - X)$$

The rate of consumption of reactant, r_A

$$r_A = -kCA^2$$

The design equation for the CSTR reactor volume as a function of conversion

$$V_{\text{CSTR}} = \frac{F_{A0}X}{kC_{A0}^2(1-X)^2}$$

The initial feed concentration, C_{A0}

$$C_{A0} = \frac{50\ \text{kmol/h}}{9.901\,\text{m}^3/\text{h}} = \frac{50\ \text{kmol}}{\text{m}^3} = \frac{5.05\ \text{mol}}{\text{L}}$$

The volume of the CSTR necessary to achieve 94% of the limiting reactant, V_{CSTR}

$$V_{\text{CSTR}} = \frac{F_{A0}X}{kC_{A0}^2(1-X)^2} = \frac{50{,}000\ \text{mol/h}(0.94)}{115.28\ \text{L/mol h}(5.05\ \text{mol/L})^2(1-0.94)^2} = 4440.8\ \text{L}$$

Using polymath software (Table 5.1), results are shown in Figure 5.4.

HYSYS SIMULATION

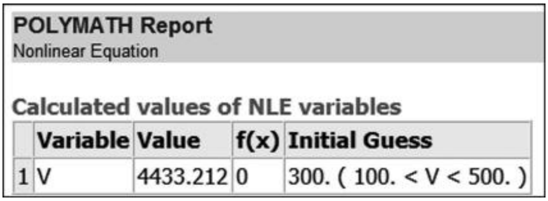
The CSTR reactor in the Hysys object palette can be used for this purpose as follows:

1. Open a new case in Hysys.
2. Add components, click on *Add Pure*, and select the components: ethanol, diethylamine, triethylamine, and water. Close the selected components window.

TABLE 5.1

Polymath Program for Example 5.1

```
#Example 5.1 CSTR
Fain = 50,000 #mol/h
x = 0.94
CA0 = 5.05 #mol/L
A = 4775 #L/mol h
Ea = 10,000 #J/mol
R = 8.314
T = 50 + 273.15 #K
CA = CA0*(1 − x)
k = A*exp(−Ea/(R*T))
ra = k*CA ^2
f(V) = V − (Fain*x/ra)
V(min) = 100 # liter
V(max) = 500 # liter
```



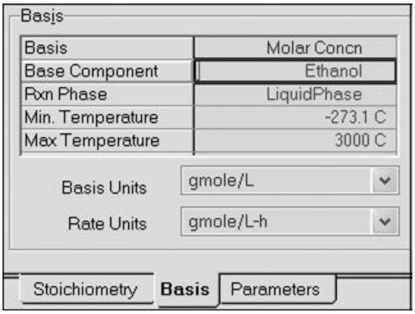
POLYMATH Report
Nonlinear Equation

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	V	4433.212	0	300. (100. < V < 500.)

FIGURE 5.4
Polymath results for Example 5.1.

3. Select a suitable fluid package by clicking on *Fluid Pkgs* tab; in this case, the Non-Random Two-Liquid, NRTL is the most suitable fluid package. Close the fluid package window.
4. Under *Flowsheet* in toolbar menu, the Reactions Package is to be selected. The *Kinetic* reaction rate type is selected.
5. Add the components ethanol, diethylamine, triethylamine, and water to the reaction. Make the stoichiometric coefficients –1 for ethanol and diethlyamine (because they are being consumed) and 1 for both triethylamine and water (because they are being produced with a stoichiometry of 1). The forward order is automatically defaulted to the stoichiometric number 1; for this case, it is different than how we defined our reaction data. Assume no reverse reactions. Change the reaction order to 2 with respect to ethanol and 0 with respect to diethylamine for the forward reaction order. Since the reaction is irreversible, under *Rev Order*, type zero for all components.
6. On the *Basis* page. Ethanol is the basis component and the basis unit is gmol/L. The units of the reaction rate are gmol/L h. The reaction is taking place in the liquid phase (Figure 5.5).
7. On the *Parameters* page. Enter in the values of $A = 4775$ L/mol h, $E = 10{,}000$ J/mol (Figure 5.6).
8. Click on *Add Set* to bring the set under Current Reaction Sets. Close the window and click on *Enter Simulation Environment*.
9. Select the graphic that is a CSTR from the object palette and add it to PFD workspace. Add energy stream, feed, and product streams.

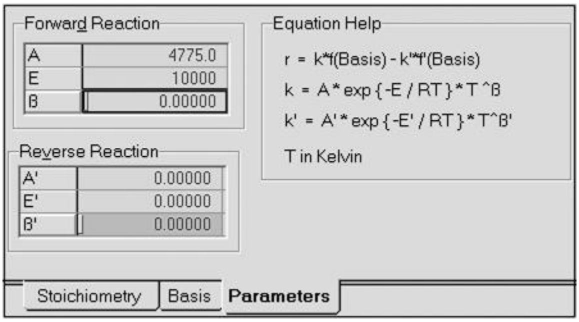


Basis

Basis	Molar Concn
Base Component	Ethanol
Rxn Phase	LiquidPhase
Min. Temperature	-273.1 C
Max Temperature	3000 C

Basis Units: gmole/L
Rate Units: gmole/L-h

FIGURE 5.5
Reaction phase and units of base components.



Forward Reaction

A	4775.0
E	10000
β	0.00000

Reverse Reaction

A'	0.00000
E'	0.00000
β'	0.00000

Equation Help

r = k*f(Basis) - k'*f'(Basis)
k = A * exp{-E / RT} * T ^β
k' = A' * exp{-E' / RT} * T^β'
T in Kelvin

FIGURE 5.6
Forward reaction rate constant in Hysys.

10. Energy stream must be added since the reactor is assumed to operate isothermally; consequently, heat must be added or removed to keep the temperature constant.
11. Click on the *Rating* tab and set the volume to 4433 L (the same value obtained with polymath calculations for comparison).
12. Click on composition and set 1 for water and 0.5 for ethanol and diethylamine.
13. Click on the feed stream and set the pressure to 354.5 kPa and $T = 50°C$. Feed molar flow rate is 200 kgmol/h. Click on *Composition* and then edit, enter 0.25 for ethanol, 0.25 for diethylamine, and 0.5 for water.
14. Double click on the reactor again and click on the *Reaction* tab. Add the *global rxn set* to the available reactions (if the default name was not changed). The reaction set status fields should change to green when fully specified.
15. Click on *Reactions* and then on *Results*; the percent conversion is 93.85%. The reaction is in the liquid phase, and so most of the product will be in stream number 3. Right click on streams 1 and 3 and then on show table. Double click on tables and modify content to the form shown in Figure 5.7.

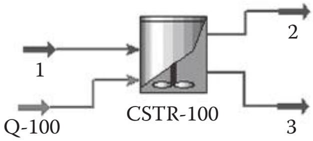
    The fractional conversion

$$x = \frac{50 - 3.07}{50} = 0.9386(93.86\%)$$

PRO/II Simulation

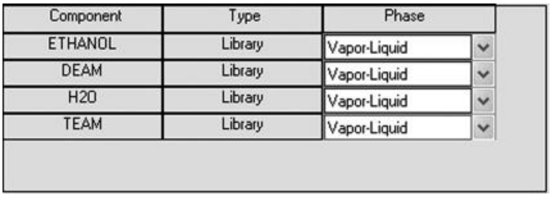
The CSTR in PRO/II can only work for liquids and vapor pahses; one must declare all components for just the vapour and liquid phase, otherwise a warning message will pop up when running the system. After selecting component click on *Components Phases*, and change the component phases as shown in Figure 5.8.

The kinetic data are shown in Figure 5.9. The process flow sheet and stream property table are shown in Figure 5.10.



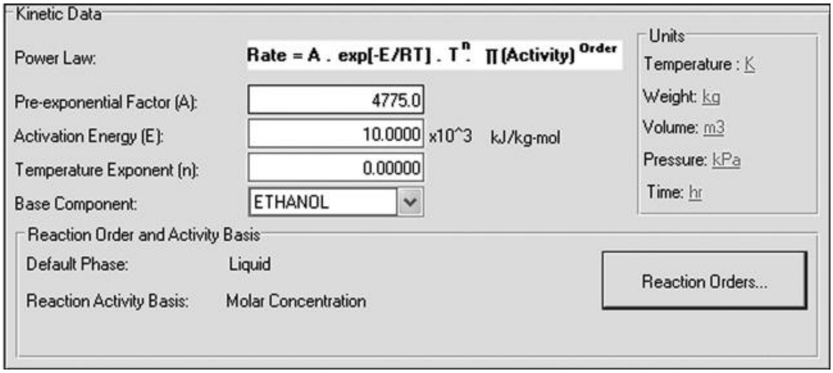
Streams				
		1	2	3
Temperature	C	50.00	50.00	50.00
Pressure	kPa	354.6	354.6	354.6
Molar flow	kgmol/h	200.0	0.0000	200.0
Comp molar flow (ethanol)	kgmol/h	50.00	0.00	3.07
Comp molar flow (diethylamine)	kgmol/h	50.00	0.00	3.07
Comp molar flow (triethylamine)	kgmol/h	0.00	0.00	46.93
Comp molar flow (H_2O)	kgmol/h	100.00	0.00	146.93

FIGURE 5.7
Process flow sheet and product stream molar flow rate.



Component	Type	Phase
ETHANOL	Library	Vapor-Liquid
DEAM	Library	Vapor-Liquid
H2O	Library	Vapor-Liquid
TEAM	Library	Vapor-Liquid

FIGURE 5.8
CSTR reactors are desgined for liquid and vapor only.



Kinetic Data

Power Law: $\text{Rate} = A \cdot \exp[-E/RT] \cdot T^n \cdot \prod(\text{Activity})^{\text{Order}}$

Pre-exponential Factor (A): 4775.0

Activation Energy (E): 10.0000 x10^3 kJ/kg-mol

Temperature Exponent (n): 0.00000

Base Component: ETHANOL

Reaction Order and Activity Basis

Default Phase: Liquid

Reaction Activity Basis: Molar Concentration

Units

Temperature : K

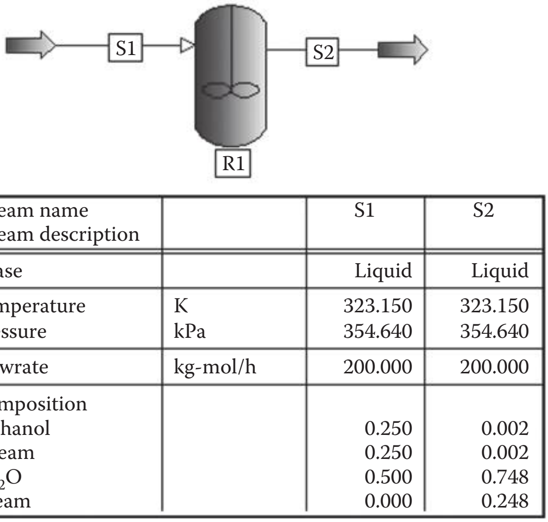
Weight: kg

Volume: m3

Pressure: kPa

Time: hr

FIGURE 5.9
Kinetic data.



Stream name Stream description		S1	S2
Phase		Liquid	Liquid
Temperature	K	323.150	323.150
Pressure	kPa	354.640	354.640
Flowrate	kg-mol/h	200.000	200.000
Composition			
Ethanol		0.250	0.002
Deam		0.250	0.002
H_2O		0.500	0.748
Team		0.000	0.248

FIGURE 5.10
Process flow sheet and stream summary table generated by PRO/II.

The fraction converison

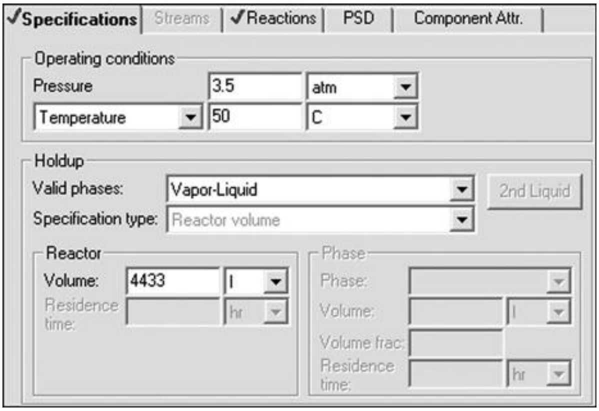
$$x = \frac{50 - 3.0438}{50} = 0.939$$

Aspen Simulation

Using CSTR in Aspen Plus, the following procedure can be followed:

Open a new case by choosing a blank simulation. SI units should be used for all reactors with kinetics. Choose the *Components* option in the data browser window to start adding chemical components. Insert the chemicals for a reactor: Ethanol, diethylamine, triethylamine, and water. Use *Find* to find the components ID and then add it.

Under *Properties*, *Specifications*, select the base property method. Since these components are liquids, NRTL thermodynamic package is the most convenient fluid package. Install CSTR reactor under *Reactors* in the model library, and connect inlet and exit streams. Specify the feed stream conditions and composition. Input the reactor specifications; double click on the reactor block. The reactor *Data Browser* opens. Specify an adiabatic reactor and the reactor volume to 4433 liters; the value obtained from hand calculations (Figure 5.11). Add the reactions to complete the specifications of the CSTR. Choose the *Reactions* block in the browser window and then click on *Reactions*. Click *New* on the window that appears. A new dialog box opens; enter a reaction ID and specify the reaction as *Power Law*. Then click on *Ok*. The kinetic data are very important to make Aspen converge. Mainly specifying accurate units for pre-exponential factor; A, is very important (see the *k* value in Figure 5.12). The value MUST be in SI units.



Pressure: 3.5 atm

Temperature: 50 C

Valid phases: Vapor-Liquid

Specification type: Reactor volume

Volume: 4433 l

Residence time: hr

Phase:

Volume: l

Volume frac:

Residence time: hr

FIGURE 5.11
Reactor specifications menu in Aspen Plus.

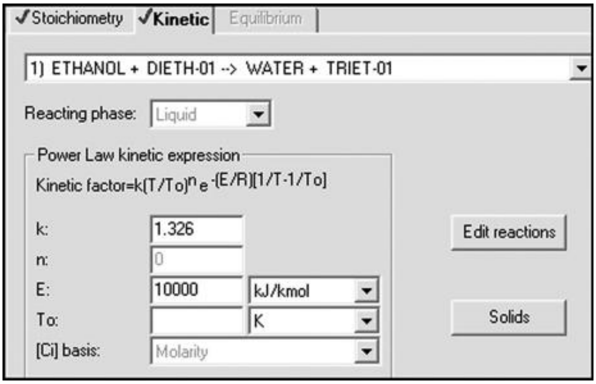
$$A = 4775\frac{\text{L}}{\text{mol.h}}\left(\frac{1000\,\text{mol}}{1\,\text{kmol}}\right)\left(\frac{\text{h}}{3600\,\text{s}}\right)\left(\frac{\text{m}^3}{1000\,\text{L}}\right) = 1.326\frac{\text{m}^3}{\text{kmols}}$$

The result of stream summary is shown in Figure 5.13.
The fractional conversion achieved using Aspen is

$$x = \frac{50 - 2.887}{50} = 0.942$$

SUPERPRO DESIGNER SIMULATION

Register the components involved in the reaction, ethylalcohol, diethylamine, water, and triethylamine. Select the CSTR reactor from the *Unit Procedure* menu,



1) ETHANOL + DIETH-01 --> WATER + TRIET-01

Reacting phase: Liquid

Kinetic factor=k(T/To)^n e$^{-(E/R)[1/T-1/To]}$

k: 1.326

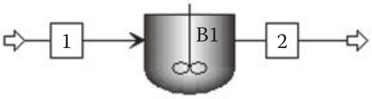
n: 0

E: 10000 kJ/kmol

To: K

[Ci] basis: Molarity

FIGURE 5.12
Kinetic data values required by Aspen Plus.



Example 5.1			
Stream ID		1	2
Temperature	K	323.1	323.1
Pressure	atm	3.50	3.50
Vapor frac		0.000	0.000
Mole flow	kmol/h	200.000	200.000
Mass flow	kg/h	7761.884	7761.884
Volume flow	L/min	169.063	158.614
Enthalpy	MMBtu/h	−44.694	−46.525
Mole flow	kmol/h		
Ethanol		50.000	2.887
Dieth-01		50.000	2.887
Water		100.000	147.113
Triet-01			47.113

FIGURE 5.13
Process flow sheet and stream table generated by Aspen Plus.

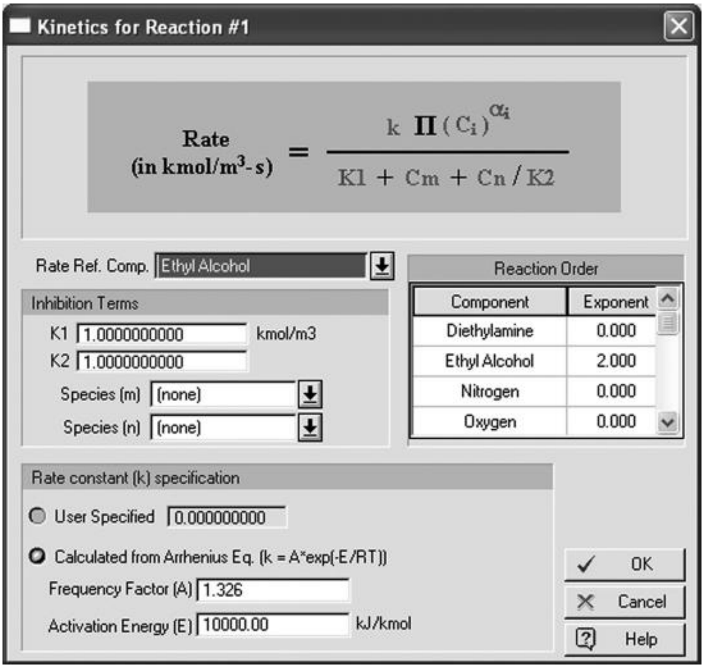
select *Continuous reaction*, *Kinetic*, and then *in CSTR*. Connect feed and product streams. Double click on the feed stream and specify feed components mass flow rate and feed stream conditions (50°C, 3.5 atm). Double click on the reactor, and in the reaction page (click on *Reaction* tab) define the reaction stoichiometry (double click on *Reaction#1*). The kinetic parameters have to be defined; to do that, double click on the symbol *R* (*view/Edit kinetic Rate*) and fill in the kinetic parameters as shown in Figure 5.14. On the operating conditions page, the exit temperature should be set to 50°C (isothermal operation mode). The volume of the reactor can be set by right clicking on the reactor and then selecting *Equipment Data*. If the ratio of work volume to vessel volume is set to 90%, then the vessel volume must be divided by 0.9 to achieve the actual working volume of 4433 L (Figure 5.15). Solving for mass and energy balances should lead to the result shown in Figure 5.16.

The fractional conversion achieved using SuperPro is

$$x = \frac{50 - 3.10}{50} = 0.938$$

Conclusions

The results obtained by hand calculations and the available software packages, Hysys, PRO/II, Aspen Plus, and SuperPro Designer, are almost the same.



$$\text{Rate (in kmol/m}^3\text{-s)} = \frac{k \, \Pi (C_i)^{\alpha_i}}{K1 + Cm + Cn / K2}$$

Rate Ref. Comp. Ethyl Alcohol

Inhibition Terms

K1 1.0000000000 kmol/m3

K2 1.0000000000

Species (m) (none)

Species (n) (none)

Reaction Order

Component	Exponent
Diethylamine	0.000
Ethyl Alcohol	2.000
Nitrogen	0.000
Oxygen	0.000

Rate constant (k) specification

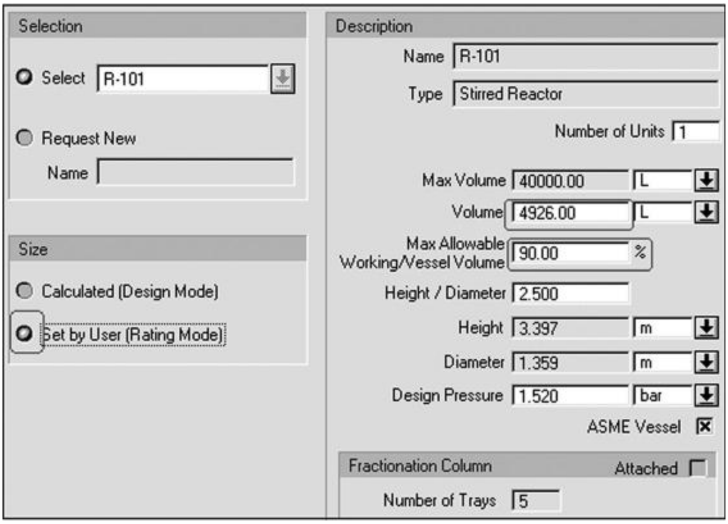
○ User Specified 0.000000000

● Calculated from Arrhenius Eq. (k = A*exp(-E/RT))

Frequency Factor (A) 1.326

Activation Energy (E) 10000.00 kJ/kmol

FIGURE 5.14
Kinetic parameters of reaction rate required by SuperPro.



Selection

● Select R-101

○ Request New

Name

Size

○ Calculated (Design Mode)

● Set by User (Rating Mode)

Description

Name R-101

Type Stirred Reactor

Number of Units 1

Max Volume 40000.00 L

Volume 4926.00 L

Max Allowable Working/Vessel Volume 90.00 %

Height / Diameter 2.500

Height 3.397 m

Diameter 1.359 m

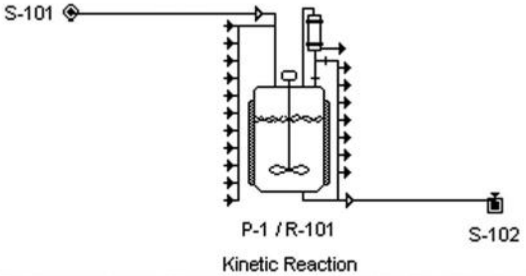
Design Pressure 1.520 bar

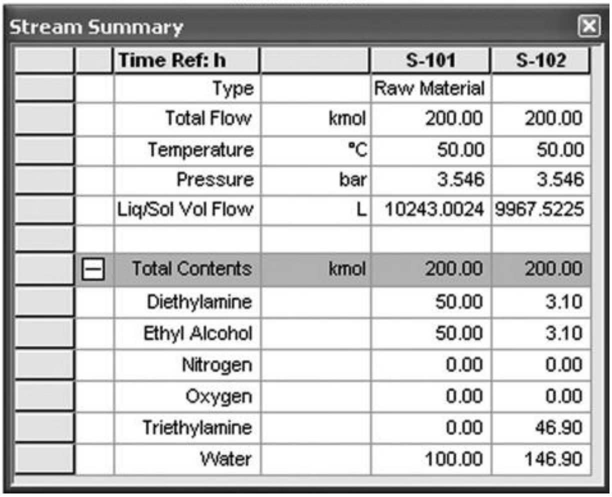
ASME Vessel ☒

Fractionation Column Attached ☐

Number of Trays 5

FIGURE 5.15
Equipment data menu in SuperPro.





Stream Summary

	Time Ref: h		S-101	S-102
	Type		Raw Material	
	Total Flow	kmol	200.00	200.00
	Temperature	°C	50.00	50.00
	Pressure	bar	3.546	3.546
	Liq/Sol Vol Flow	L	10243.0024	9967.5225
⊟	Total Contents	kmol	200.00	200.00
	Diethylamine		50.00	3.10
	Ethyl Alcohol		50.00	3.10
	Nitrogen		0.00	0.00
	Oxygen		0.00	0.00
	Triethylamine		0.00	46.90
	Water		100.00	146.90

FIGURE 5.16
CSTR process flow sheet and stream table properties generated by SuperPro.

Example 5.2: Production of Acetic Anhydride in PFR

Pure acetone is fed into an adiabatic PFR at a mass flow rate of 7.85 kg/h. The inlet temperature and pressure of the feed stream is 760°C and 162 kPa (1.6 atm), respectively. In a vapor-phase reaction, acetone (CH_3COCH_3) is cracked to ketene (CH_2CO) and methane (CH_4). The following reaction takes place:

$$CH_3COCH_3(A) \rightarrow CH_2CO(B) + CH_4(C)$$

The reaction is in first-order with respect to acetone and the specific reaction rate constant can be expressed by

$$k(\mathrm{s}^{-1}) = 8.2 \times 10^{14} \exp\left[\frac{-2.845 \times 10^{5}(\mathrm{kJ/kmol})}{RT}\right]$$

Calculate the conversion achieved using a reactor volume of 5 m^3.

SOLUTION

HAND CALCULATIONS

The steady-state material balance for the PFR
Molar flow rate of ethanol

$$\frac{dF_A}{dV} = r_A$$

Molar flow rate of ketene

$$\frac{dF_B}{dV} = r_B$$

Molar flow rate of methane

$$\frac{dF_C}{dV} = r_C$$

The change in conversion with reactor volume

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

The rate of reaction (first order with respect to acetone)

$$r_A = -kC_A \quad \text{and} \quad r_A = -r_B = -r_C$$

Gas volumetric flow rate, v

$$v = v_0(1 + \varepsilon X)\frac{T}{T_0}\frac{P_0}{P}$$

$$\varepsilon = y_{A0} * \delta$$

Changes in stoichiometric coefficients

$$\delta = \sum v_i$$

$$\delta = \sum v_i = 1 + 1 - 1$$

Since we have pure acetone; $y_{A0} = 1$
Concentration as a function of conversion, X

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - X)}{v_0(1 + X)(T/T_0)(P_0/P)}$$

Substituting above equations in the reaction rate and rearranging,

$$-r_A = \frac{k\,C_{A0}(1 - X)}{(1 + X)}\frac{T_0}{T}$$

The change in temperature as a function of reactor volume (adiabatic operation)

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{(-r_A)\left(-\Delta H_{\text{rxn}}\right)}{F_{A0}\left(\sum \theta_i C_{\text{p}i} + X\Delta C_{\text{p}}\right)}$$

Heat of reaction at temperatures other than reference temperature (25°C),

$$\Delta H_{\text{rxn}} = \Delta H_{\text{rxn}}^{0} + \Delta a(T - T_{\text{r}}) + \frac{\Delta b}{2}(T^2 - T_{\text{r}}^2) + \frac{\Delta c}{3}(T^2 - T_{\text{r}}^2)$$

$$\Delta a = 6.8$$

$$\frac{\Delta b}{2} = -5.75 \times 10^{-3}$$

$$\frac{\Delta c}{3} = -1.27 \times 10^{-6}$$

The standard heat of reaction, $\square H_{\text{rxn}}^{0}$

$$\Delta H_{\text{rxn}}^{0} = 80770\ (\text{J/mol})$$

The change in the specific heat, ΔC_{p}

$$\Delta C_p = 6.8 - 11.5 \times 10^{-3}\,T - 3.81 \times 10^{-6}\,T^2\ (\text{J/mol K})$$

The heat capacity of ethanol, Cp_A

$$Cp_i = Cp_A = 26.63 + 0.183\ T - 45.86 \times 10^{-6}\,T^2\ (\text{J/mol K})$$

The set of the equations are solved using the polymath program shown in Table 5.2.

The second method for the change in reaction temperature with reactor volume (adiabatic operation)

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{(-r_A)(-\Delta H_{\text{rxn}})}{F_A C_{\text{p}A} + F_B C_{\text{p}B} + F_C C_{\text{p}C}}$$

The components' specific heat capacities (J/mol K):

$$Cp_A = 26.63 + 0.183\ T - 45.86 \times 10^{-6}\,T^2$$

TABLE 5.2

Polymath Code for Example 5.2 (Method 1)

Polymath Program	Initial Conditions
`d(X)/d(V) =-ra/FA0`	0
`d(T)/d(V) =-ra*(-DHrxn)/(FA0*(Cpi + X*Dcp))`	1035
`ra =-k*CA0*(1 - X)*(T0/T)/(1 + X)`	
`DHrxn = DHrxn0 + Da*(T - Tr) + (Db/2)*(T^2 - Tr^2) + (Dc/3)*(T^3 - Tr^3)`	
`FA = FA0*(1 - X)`	
`FB = FA0*X`	
`FC = FA0*X`	
`DHrxn0 = 80770 # J/mol`	
`Cpi = 26.63 + 0.183*T - 45.86E - 6*T^2`	
`Dcp = 6.8 - 11.5E - 3*T - 3.81E - 6*T^2`	
`k = 8.2E14*exp(-34222/T)`	
`CA0 = 18.85 # mol/m^3`	
`Da = 6.8`	
`Db = -(5.75E - 3)*2`	
`Dc = -(1.27E - 6)*3`	
`FA0 = 0.03754`	
`T0 = 1035 # K`	
`Tr = 298`	
`V(0) = 0, V(f) = 5 # m^3`	

$$Cp_B = 20.04 + 0.0945\ T - 30.95 \times 10^{-6}\, T^2$$

$$Cp_C = 13.39 + 0.077\ T - 18.71 \times 10^{-6}\, T^2$$

The initial concentration, C_{A0},

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{162\ \text{kPa}}{8.314\ \text{kPa.m}^3/\text{kmol.K}(760 + 273.15\ \text{K})(1\ \text{kmol}/1000\ \text{mol})}$$

$$= 18.87\ \text{mol/m}^3$$

The ethanol initial molar flow rate, F_{A0},

$$F_{A0} = \left(\frac{7.850\ \text{kg/h}}{58\ \text{kg/kmol}}\right)\frac{1000\ \text{mol}}{1\ \text{kmol}}\,\frac{1\ \text{h}}{3600\ \text{s}} = 0.0376\ \frac{\text{mol}}{\text{s}}$$

The set of equations used in method are solved using the Polymath program shown in Table 5.3.

The Polymath program for methods 1 and 2 is shown in Tables 5.2 and 5.3, respectively. Previous results show that both methods give the same results. A reactor volume of 5 m^3 is required to achieve a percent conversion of 52%.

TABLE 5.3

Polymath Program for Example 5.2 (Method 2)

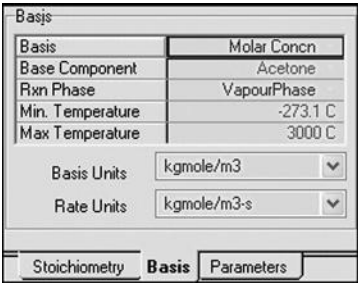
Polymath Program	Initial Conditions
`d(X)/d(V)= -ra/FA0`	0
`d(T)/d(V)= -ra*(-DHrxn)/(FA*CpA+FB*CpB+FC*CpC)`	1035
`ra=-k*CA0*(1-X)*(T0/T)/(1+X)`	
`DHrxn=DHrxn0+Da*(T-Tr) + (Db/2)*(T^2-Tr^2) + (Dc/3)*(T^3-Tr^3)`	
`FA=FA0*(1-X)`	
`FB=FA0*X`	
`FC=FA0*X`	
`DHrxn0=80770 # J/mol`	
`CpA=26.63+0.183*T-45.86E-6*T^2`	
`CpB=20.04+0.0945*T-30.95E-6*T^2`	
`CpC=13.39+0.077*T-18.71E-6*T^2`	
`k=8.2E14*exp(-34222/T)`	
`CA0=18.85 # mol/m3`	
`Da=6.8`	
`Db=-(5.75E-3)*2`	
`Dc=-(1.27E-6)*3`	
`FA0=0.03754`	
`T0=1035`	
`Tr=298`	
`V(0)=0, V(f)=5`	

HYSYS SIMULATION

Perform Hysys process flow sheet (PFD) using the PFR from the object palette, and identify feed stream conditions, temperature 760°C, pressure 162 kPa, and mass flow rate 7.850 kg/h. For the fluid package BWRS is a suitable property package. Under *Flowsheet* select *Reaction package*, when adding the reaction selects the kinetic type of reactions. The reaction stoichiometric coefficients are shown in Figure 5.17. The base component is acetone; the reaction takes place in vapor phase (Figure 5.18). The kinetic parameters are shown in Figure 5.19. When the *Ready* message appears, the results are generated and after adding tables for each stream and rearranging should appear as that in Figure 5.20.

Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
Acetone	58.080	-1.000	1.00	0.00
Ketene	42.038	1.000	0.00	0.00
Methane	16.043	1.000	0.00	0.00
Add Comp				

FIGURE 5.17
Reaction stoichiometry used by Hysys.

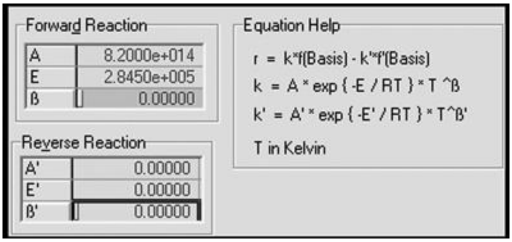


Basis	Molar Concn
Base Component	Acetone
Rxn Phase	VapourPhase
Min. Temperature	-273.1 C
Max Temperature	3000 C

Basis Units: kgmole/m3

Rate Units: kgmole/m3-s

FIGURE 5.18
Reaction basis in Hysys reaction menu.



Forward Reaction

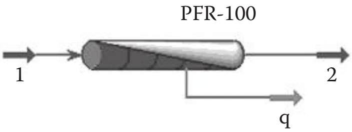
A	8.2000e+014
E	2.8450e+005
ß	0.00000

Reverse Reaction

A'	0.00000
E'	0.00000
ß'	0.00000

Equation Help

r = k*f(Basis) - k'*f'(Basis)
k = A * exp { -E / RT } * T ^ß
k' = A' * exp { -E' / RT } * T^ß'
T in Kelvin



Streams			
		1	2
Temperature	C	760.0	491.4
Pressure	kPa	162.0	162.0
Molar flow	kgmol/h	0.1352	0.2023
Comp molar flow (acetone)	kgmol/h	0.1352	0.0680
Comp molar flow (ketene)	kgmol/h	0.0000	0.0671
Comp molar flow (methane)	kgmol/h	0.0000	0.0671

FIGURE 5.20
Process flow sheet and streams molar flow rates generated by Hysys.

The fractional conversion

$$x = \frac{0.135 - 0.068}{0.135} = 0.496$$

PRO/II SIMULATION

PFR and CSTR in PRO/II can work for liquid and vapor phases only; consequently, it must be declared that all components involved in the reaction are vapor and liquid phases (solid should be excluded). After selecting component click on *Components Phases*, and change the components phase to liquid and vapor only. From the *Thermodynamic Data* select BWRS which is the most suitable thermodynamic fluid package for such components. Build the PFR process flow sheet and specify inlet stream conditions (760°C, 162 kPa). The inlet mass flow rate of acetone is 7.85 kg/h. Under the Input menu, select *Reaction Data*, use the power law, and enter stoichiometric coefficients. Double click on the reactor in the PFD area and select the reaction set name. Click on *Unit Reaction Definitions* and specify the kinetic data as shown in Figure 5.21. Press Reactor Data, indicate 6.366 m for length and 1 m for the diameter (total volume of 5 m^3). The process flow sheet and stream table properties are exposed in Figure 5.22.

The fractional conversion:

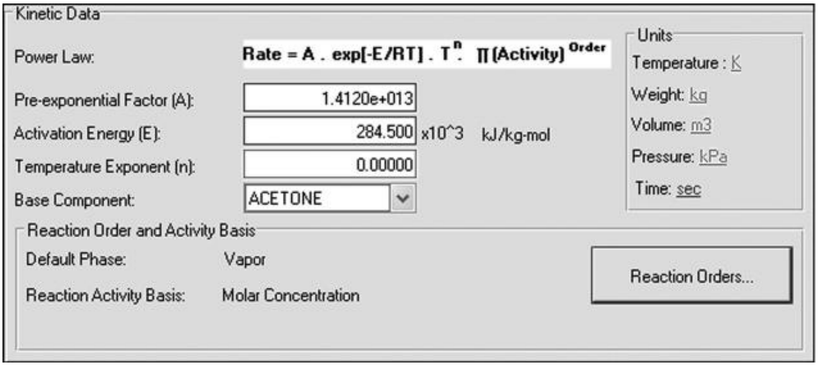
$$x = \frac{0.135 - 0.067}{0.135} = 0.504$$

ASPEN PLUS SIMULATION

The following procedures are followed in building the PFR with Aspen Plus:

A new case is opened by choosing a blank simulation. SI units should be used for all reactors with kinetics. Build the process flow sheet for the PFR.

Choose *Data* from the main menu and click on *Setup*. The title and brief description can be entered by choosing the *Description* tab.



Kinetic Data

Power Law: $\text{Rate} = A \,.\, \exp[-E/RT] \,.\, T^{n} .\ \Pi\,(\text{Activity})^{\text{Order}}$

Pre-exponential Factor (A): 1.4120e+013

Activation Energy (E): 284.500 x10^3 kJ/kg-mol

Temperature Exponent (n): 0.00000

Base Component: ACETONE

Reaction Order and Activity Basis

Default Phase: Vapor

Reaction Activity Basis: Molar Concentration

Units

Temperature : K

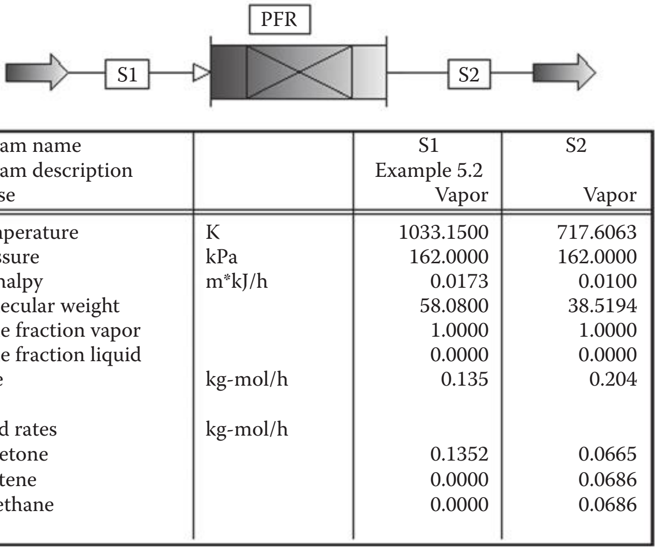
Weight: kg

Volume: m3

Pressure: kPa

Time: sec

FIGURE 5.21
Kinetic parameters required in PRO/II.



Stream name		S1	S2
Stream description		Example 5.2	
Phase		Vapor	Vapor
Temperature	K	1033.1500	717.6063
Pressure	kPa	162.0000	162.0000
Enthalpy	m*kJ/h	0.0173	0.0100
Molecular weight		58.0800	38.5194
Mole fraction vapor		1.0000	1.0000
Mole fraction liquid		0.0000	0.0000
Rate	kg-mol/h	0.135	0.204
Fluid rates	kg-mol/h		
Acetone		0.1352	0.0665
Ketene		0.0000	0.0686
Methane		0.0000	0.0686

FIGURE 5.22
Process flow sheet and stream table of Example 5.2 using PRO/II.

Select SI units for input on the Global tab.

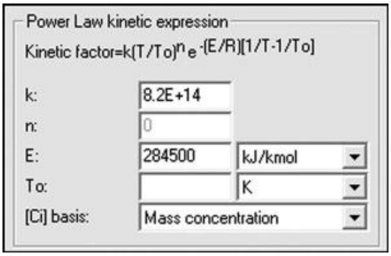
Under the Report Options, Stream tab, specify Mole both for the Flow Basis and the Fraction Basis.

Choose the *Components* option in the data browser window to start adding chemical components. Install the chemicals for a reactor: acetone, ketene, and methane. Use the *Find* option to find the components ID and then add it. Next, under *Properties*, *Specifications*, select your base Property method. Since these components are liquids, use the BWRS thermodynamic package (Peng Robinson did not work for this example). Install the PFR reactor and add inlet and exit streams. Specify the feed stream. Input the reactor specifications; double click on the reactor block. The reactor *Data Browser* opens. Specify an adiabatic reactor and the reactor volume to 5 m^3 (1 m diameter and 6.366 m length), the value obtained from hand calculations.

Specify the reactions to complete the specifications of the PFR. Choose the *Reactions* block in the browser window. Then click on *Reactions*. Click on *New* on the window that appears. In the new dialog box opened window, enter a reaction ID and specify the reaction as *Power Law*. Then click on *Ok*. The kinetic data are very important to make Aspen converge. Mainly specifying accurate units for the pre-exponential factor, the parameters *A* and *k* are very important. The value MUST be in SI unit (Figure 5.23). *PFR* flow sheet and stream table results are shown in Figure 5.24.

The fractional conversion using Aspen is

$$x = \frac{0.135 - 0.062}{0.135} = 0.54$$



Power Law kinetic expression

Kinetic factor=k(T/To)^n e$^{-(E/R)[1/T-1/To]}$

k: 8.2E+14

n: 0

E: 284500 kJ/kmol

To: K

[Ci] basis: Mass concentration

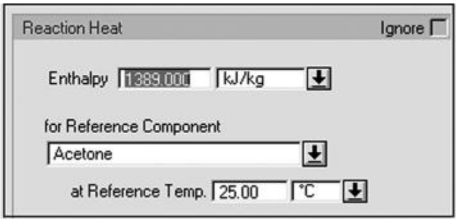
FIGURE 5.23
Power low kinetic reactions used for Example 5.2.

SuperPro Designer Simulation

In the current version of SuperPro 7.5, there should exist liquid /solid in the feed line even for a PFR. When selecting the pure component, iron component should be added and given a small value in the feed such as 0.001 kg/h; this is not included in the reaction just to overcome the error generated if no solid/liquid exists in the feed stream. The process is adiabatic. The heat of reaction (1389 kJ/g) should be entered as shown in Figure 5.25. The reaction rate constants are as shown in Figure 5.26. The *size* of the reactor on the *Equipment Data* page is specified by user (Rating Mode) as 5000 L. Number of units can be set as 100 to overcome errors. Results should appear as those in Figure 5.27.

Example 5.2			
Stream ID		1	2
Temperature	K	1033.2	693.5
Pressure	atm	1.60	1.60
Vapor frac		1.000	1.000
Mole flow	kmol/h	0.135	0.208
Mole flow	kg/h	7.850	7.850
Volume flow	L/min	119.392	123.340
Enthalpy	MMBtu/h	–0.016	–0.016
Mass flow	kmol/h		
Acetone		0.135	0.062
Ketene			0.073
Methane			0.073

FIGURE 5.24
Process flow sheet and stream summary table generated by Aspen.



Reaction Heat

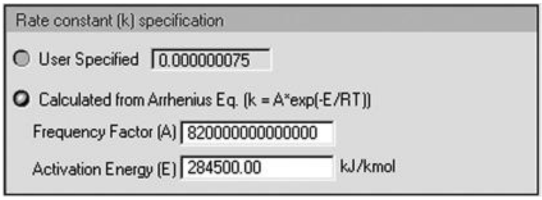
Ignore ☐

Enthalpy 1389.000 kJ/kg

for Reference Component Acetone

at Reference Temp. 25.00 °C

FIGURE 5.25
Standard heat of reaction required by SuperPro.



Rate constant (k) specification

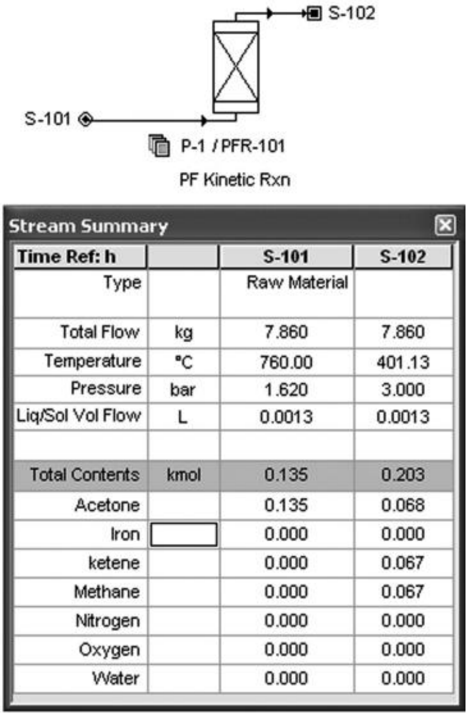
○ User Specified 0.000000075

● Calculated from Arrhenius Eq. (k = A*exp(-E/RT))

Frequency Factor (A) 820000000000000

Activation Energy (E) 284500.00 kJ/kmol

FIGURE 5.26
Frequency factor and activation energy required by SuperPro.



Stream Summary

Time Ref: h		S-101	S-102
Type		Raw Material	
Total Flow	kg	7.860	7.860
Temperature	°C	760.00	401.13
Pressure	bar	1.620	3.000
Liq/Sol Vol Flow	L	0.0013	0.0013
Total Contents	kmol	0.135	0.203
Acetone		0.135	0.068
Iron		0.000	0.000
ketene		0.000	0.067
Methane		0.000	0.067
Nitrogen		0.000	0.000
Oxygen		0.000	0.000
Water		0.000	0.000

FIGURE 5.27
PFR process flow sheet and stream table properties generated by SuperPro.

The single-pass conversion:

$$x = \frac{0.135 - 0.068}{0.135} = 0.496$$

Conclusions

On drawing a comparison between hand calculations, Hysys, and Aspen, it became clear that Aspen results are closer than those obtained by Hysys and SuperPro Designer.

Example 5.3: Packed-Bed Reactors

Styrene is made from the dehydrogenation of ethylbenzene in a PBR,

$$C_6H_5 - C_2H_5 \rightarrow C_6H_5 - CH = CH_2 + H_2$$

The feed consists of 217.5 mol/s ethylbenzene, 2610 mol/s of inert steam, the reaction is isothermal, $T = 880$ K, and 1.378 bar. The reaction rate is in first order with respect to ethylbenzene. The volume of the reactor is 160 m^3, 3 m length, and a void fraction of 0.445. The catalyst particle diameter is 0.0047 m, and particle density is 2146.3 kg/m^3. Rate of reaction

$$r = -kP_{EB}$$

Specific reaction rate constant:

$$k\left(\frac{\text{mol}}{g_{\text{cat}}\,\text{s}\,kP_a}\right) = 7.491 \times 10^{-2} \exp\left[\frac{-21874\,\text{cal/mol}}{(1.987\,\text{cal/molK})T}\right]$$

SOLUTION

Hand Calculations

The steady-state material balances can be performed as follows:

Ethylbenzene material balance,

$$\frac{dF_{EB}}{dw} = r'_{EB}$$

Styrene material balance,

$$\frac{dF_S}{dw} = +r_S = -r'_{EB}$$

Hydrogen material balance,

$$\frac{dF_H}{dw} = r_H = -r'_{EB}$$

The pressure drop is calculated by using the Ergun equation,

$$\frac{dP}{dz} = \frac{G}{\rho D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)}{D_p} + 1.75G\right]$$

where G is the superficial mass velocity, kg/(m^2 s), ρ is the fluid density, μ is the fluid viscosity, ϕ is the void fraction, and D_P is the particle diameter.

$$G = \frac{F_{EB0}MW_{EB} + F_W MW_W}{\pi D^2/4} = \frac{217.5 \times 106.17 + 2610 \times 18}{\pi\left(9.73\,\text{m}\right)^2/4} = 0.941\,\text{kg/m}^2\,\text{s}$$

ρ is the fluid density, the mass flow rate

$$m = \rho v = m_0 = \rho_0 v_0 \Rightarrow v = v_0\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)\left(\frac{F_T}{F_{T0}}\right)$$

Fluid density as a function of temperature and pressure, ρ,

$$\rho = \rho_0\left(\frac{v_0}{v}\right) = \rho_0\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)\left(\frac{F_{T0}}{F_T}\right)$$

The initial fluid density, ρ_0,

$$\rho_0 = \frac{P\bar{M}W}{RT} = \frac{1.378 \times 10^5\,\text{Pa}}{8.314\,\text{Pa}\,\text{m}^3/\text{molK}\left(880\,\text{K}\right)} \times \left[106.17\left(\frac{217.7}{217.5 + 2610}\right)\right.$$
$$\left. + 18\left(\frac{2610}{217.5 + 2610}\right)\frac{\text{g}}{\text{mol}}\right]$$

$$\rho = 466.89\ \text{g/m}^3 = 0.467\ \text{kg/m}^3$$

$$\beta_0 = \frac{G(1-\phi)}{\rho_0 D_P \phi^3}\left[\frac{150(1-\phi)}{D_p}\mu + 1.75G\right]$$

Substituting values:

$$\beta_0 = \frac{0.941\,\text{kg/m}^2\,\text{s}(1-0.445)}{(0.467\ \text{kg/m}^3)(0.0047\,\text{m})(0.445)^3}\left[\frac{150(1-0.445)}{0.0047\,\text{m}}3 \times 10^{-5} + 1.75\left(0.941\right)\right]$$

$$= 5881.29\frac{\text{kg}}{\text{m}^2\,\text{s}^2}$$

$$\beta = \frac{\beta_0}{A_c(1-\phi)\rho_c}$$

Substituting values:

$$\beta = \frac{5881.29\,\text{kg/m}^2\,\text{s}^2}{(\pi(9.43)^2/4)\,\text{m}^2(1-0.445)\times 2146.3\,\text{kg/m}^3} = 0.0664\frac{\text{Pa}}{\text{kg}}$$

The pressure drop as a function of weight of the catalyst:

$$\frac{\text{d}P}{\text{d}w} = -\beta * \left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)\left(\frac{F_T}{F_{T_0}}\right)$$

The total molar flow rate,

$$F_T = F_{w_O} + F_{\text{EB}} + F_{\text{S}} + F_{\text{H}}$$

The initial partial pressure of ethylbenzene,

$$P_{\text{EB0}} = \frac{F_{\text{EB}}}{F_{\text{T}}} \times P = \left(\frac{217.5}{2827.5}\right)1.378\times 10^5\,P_{\text{a}}\frac{1\,\text{kPa}}{1000\,\text{Pa}} = 10.6\,\text{kPa}$$

$$P_0 = 1.378\times 10^5\,\text{Pa} = 137.8\,\text{kPa}$$

At steady state and adiabatic operation, no shaft works. The change in temperature with variable catalyst weight,

$$\frac{\text{d}T}{\text{d}w} = \frac{(-r_A)\left(-\Delta H_{\text{rxn}}\right)}{F_A C_{\text{p}A} + F_B C_{\text{p}B} + F_C C_{\text{p}C}}$$

Expected catalyst weight obtained from HYSYS simulation ($V = 163\ \text{m}^3$)

$$W = 163\,m_R^3\,\frac{(1-0.445)m_{\text{C}}^3}{m_{\text{R}}^3}\,\frac{2146\,k\,g_{\text{Cat}}}{m_{\text{Cat}}^3} = 194{,}138\,\text{kg} = 1.948\times 10^8\,g_{\text{cat}}$$

ISOTHERMAL OPERATION USING POLYMATH

The above equations can be easily solved using the polymath program for isothermal operation (Table 5.4). The results are shown in Table 5.5, and the adiabatic operation (Table 5.6), where the results are shown in Table 5.7.

ADIABATIC OPERATION WITH POLYMATH SOLUTION

Polymath program shown in Table 5.3 is used to solve the adiabatic operation.

TABLE 5.4

Packed-Bed Reactor Polymath Program (Isothermal Operation)

Equations	Initial Values
d(FEB)/d(W) = −rEB	217.5
d(FS)/d(W) = rEB	0
d(FH)/d(W) = rEB	0
d(P)/d(W) = −B*P0/P*FT/FT0	1.378E + 05
FW = 2610	
T = 880 # K	
rho_cat = 2146	
phi = 0.445 # void fraction	
k = 7.491e − 2*exp(−21874/1.987/T)	
FT = FEB + FS + FH + FW	
P0 = 1.378e5	
pEB = FEB/FT*P/1000	
rEB = k*pEB	
FEB0 = 217.5 # mol/s	
MWEB = 106.17	
FW0 = 2610 # mol/s	
MWw = 18	
FT0 = FEB0 + FW0	
D = 9.73 # m	
pi = 3.14	
Ac = (pi*D^2/4)	
G = (FEB0*MWEB + FW0*MWw)/(Ac*1000) # kg/s	
rh0 = 0.467 # kg/m^3 average density	
Dp = 4.7E − 3 # m	
mu = 3E − 5 # kg/m s	
B01 = (G*(1 − phi)/(rh0*Dp*phi^3))	
B0 = B01*((150*(1 − phi)*mu/Dp) + 1.75*G)	
B = B0/(Ac*rho_cat*(1 − phi))/1000	
X = (217.5 − FEB)/217.5	
W(0) = 0, W(f) = 1.948e8	

TABLE 5.5

Polymath Results (Isothermal)

Variable	Final Value
F_{EB} (mol/s)	20.16
F_S (mol/s)	197.34
F_H (mol/s)	197.34
P (Pa)	1.23E + 05
X	0.91

TABLE 5.6

Polymath Program (Adiabatic Operation)

Equations	Initial Values
`d(FEB)/d(W) = -rEB`	`217.5`
`d(FS)/d(W) = rEB`	`0`
`d(FH)/d(W) = rEB`	`0`
`d(P)/d(W) = -B*P0/P*FT/FT0`	`1.378E+05`
`d(T)/d(W) = rEB*(-DHrxn)/(FEB*CpEB + FS*CpS + FH*CpH + FW0*CpW)`	`880`
`DHrxn = DHrxn0 + CpH + CpS - CpEB`	
`DHrxn0 = 1.2E5 # J/mol`	
`CpEB = -43.006 + 0.7067*T - 4.81E-4*T^2 + 1.3E-7*T^3`	
`CpS = -36.91 + 0.665*T - 4.85E-4*T ^ 2 + 1.408E-7*T^3`	
`CpH = 28.84 + 0.00765E-2*(T-273) + 0.3288E-5*(T-273)^2 # C`	
`Tr = 298 # K`	
`CpW = 33.46 + (0.688E-2)*(T-273) + 0.7604e-5*(T-273)^2 # K`	
`Da = 28.84 - 36.91 + 43.006`	
`Db = (0.00765E-2 + 0.665 - 0.7067)`	
`Dc = 0.3288E-5 - 4.85E-4 + 4.81E-4`	
`FW = 2610`	
`rho_cat = 2146`	
`phi = 0.445 # void fraction`	
`k = 7.491e-2*exp(-21874/1.987/T)`	
`FT = FEB + FS + FH + FW`	
`P0 = 1.378e5`	
`pEB = FEB/FT*P/1000`	
`rEB = k*pEB`	
`FEB0 = 217.5 # mol/s`	
`MWEB = 106.17`	
`FW0 = 2610 # mol/s`	
`MWw = 18`	
`FT0 = FEB0 + FW0`	
`D = 9.73 # m`	
`pi = 3.14`	
`Ac = (pi*D ^ 2/4)`	
`G = (FEB0*MWEB + FW0*MWw)/(Ac*1000) # kg/s`	
`rh0 = 0.467 # kg/m3 average density`	
`Dp = 4.7E-3 # m`	
`mu = 3E-5 # kg/m s`	
`B01 = (G*(1-phi)/(rh0*Dp*phi^3))`	
`B0 = B01*((150*(1-phi)*mu/Dp) + 1.75*G)`	
`B = B0/(Ac*rho_cat*(1-phi))/1000`	
`X = (217.5 - FEB)/217.5`	
`W(0) = 0, W(f) = 1.948e8`	

TABLE 5.7

Results of Example 5.3 (Adiabatic)

Variable	Final Value
W	1.95×10^8
F_{EB}	84.76
F_S	132.74
F_H	132.74
P	1.24×10^5
T	784.20
X	0.6103121

HYSYS SIMULATION (ISOTHERMAL OPERATION)

The units of reaction rates in Hysys are in "mol/volume. s". The conversions from gram catalyst (g_{cat}) given in the reaction rate of Example 5.5 to Hysys units are

$$A\left(\frac{\text{mol}}{L\,\text{s}\,\text{kPa}}\right) = \left(\frac{\text{mol}}{g_{cat}\,\text{s}\,\text{kPa}}\right)(\rho_{cat})\left(\frac{1-\varepsilon}{\varepsilon}\right)$$

where ρ_{cat} is the catalyst density, ε is the void fraction

$$A = 7.491 \times 10^{-2}\left(\frac{\text{mol}}{g_{cat}\,\text{s}\,\text{kPa}}\right)\left(\frac{2146\,g_{cat}}{L}\right)\left(\frac{1-0.445}{0.445}\right)\frac{\text{m}^3\,\text{cat}}{\text{m}^3\,\text{gas}} = 200.49\frac{\text{mol}}{L\,\text{s}\,\text{kPa}}$$

The rate of reaction in mol/L s kPa is shown below

$$r_{EB}\left(\frac{\text{mol}}{L_{gas}\,\text{s}\,\text{kPa}}\right) = -200.49\exp\left[-21874\frac{\text{cal}}{\text{mol}}/RT\right]$$

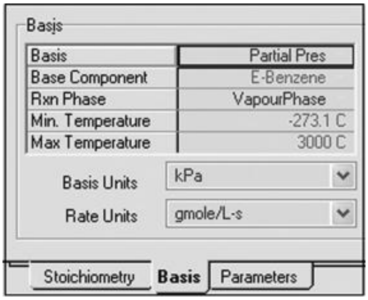
The gas constant, R,

$$R = 1.987\frac{\text{cal}}{\text{molK}}$$

HYSYS SIMULATION (ISOTHERMAL OPERATION)

Select a new case in Hysys, add the components involved, and then select PRSV as a fluid package. Enter the simulation environment, select material stream, and specify feed conditions, that is, temperature, pressure, and flow rates. In the composition page specify the mole fraction of feed components or specify feed components molar flow rates by clicking on *Basis* (Figure 5.28). Specify the reaction stoichiometric coefficients after selecting the kinetic reaction type. In the reaction basis, specify reaction basis unit, rate units, and reaction phase.

Enter reaction parameters, pre-exponential factor (A) and activation energy (E_a), as shown in Figure 5.29.



Basis	Partial Pres
Base Component	E-Benzene
Rxn Phase	VapourPhase
Min. Temperature	-273.1 C
Max Temperature	3000 C

Basis Units: kPa

Rate Units: gmole/L-s

FIGURE 5.28
Reaction phase and basis units.

The number of segments affects the results accuracy, and as the number of segment increases the results become more accurate. The default value in Hysys is 20 (Figure 5.30).

For isothermal operation, the inlet temperature and exit temperature are the same but heat duty is to be calculated. *Set operator* in Hysys can be used to set the exit temperature same as the inlet temperature (Figure 5.31).

The fractional conversion of ethylbenzene

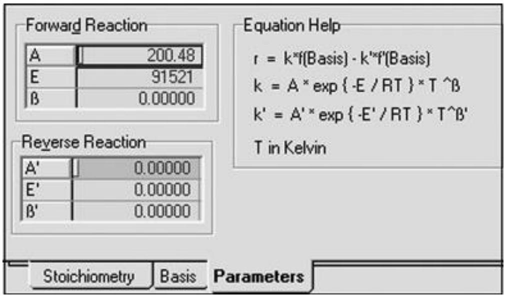
$$x = \frac{783 - 50.79}{783} = 0.935(93.5\%)$$

Hysys Simulation (Adiabatic Operation)

In Hysys, isothermal operation changes into the adiabatic mode. For adiabatic operation, delete the temperature from the exit stream and click on the energy stream and set the duty to zero (Figure 5.32).

The fraction conversion of the adiabatic mode is less than that in isothermal because the reaction is endothermic and needs heat for the conversion to proceed further.

$$x = \frac{783 - 310.55}{783} = 0.60(60\%)$$



A	200.48
E	91521
ß	0.00000

A'	0.00000
E'	0.00000
ß'	0.00000

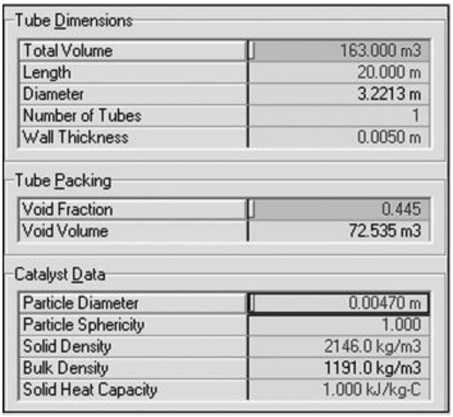
r = k*f(Basis) - k'*f'(Basis)

k = A * exp { -E / RT } * T ^ß

k' = A' * exp { -E' / RT } * T^ß'

T in Kelvin

FIGURE 5.29
Kinetic parameters menu in Hysys.



Tube Dimensions

Total Volume	163.000 m3
Length	20.000 m
Diameter	3.2213 m
Number of Tubes	1
Wall Thickness	0.0050 m

Tube Packing

Void Fraction	0.445
Void Volume	72.535 m3

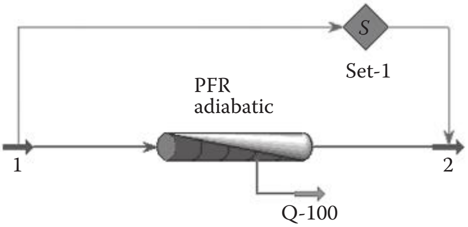
Catalyst Data

Particle Diameter	0.00470 m
Particle Sphericity	1.000
Solid Density	2146.0 kg/m3
Bulk Density	1191.0 kg/m3
Solid Heat Capacity	1.000 kJ/kg-C

FIGURE 5.30
PBR data.

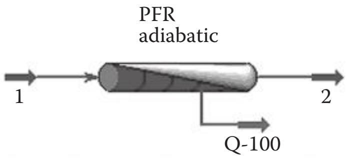
PRO II SIMULATION (ISOTHERMAL OPERATION MODE)

PFRs and CSTRs in PRO/II, can only work for liquids and vapor phases; consequently, it must be declared that all components involved in the reaction are vapor and liquid Phases (solid should be excluded). After selecting components, click on *Components Phases*, and change the component phases to liquid and vapor only. From the *Thermodynamic Data* select Peng–Robinson, the most commonly used thermodynamic fluid package for hydrocarbons. Build the PFR process flow



Streams			
		1	2
Temperature	C	606.9	606.9
Pressure	kPa	137.8	137.8
Molar flow	kgmol/h	8559	9291
Comp molar flow (E-benzene)	kgmol/h	783	51
Comp molar flow (styrene)	kgmol/h	0	732
Comp molar flow (hydrogen)	kgmol/h	0	732
Comp molar flow (H_2O)	kgmol/h	7776	7776

FIGURE 5.31
Isothermal operation.



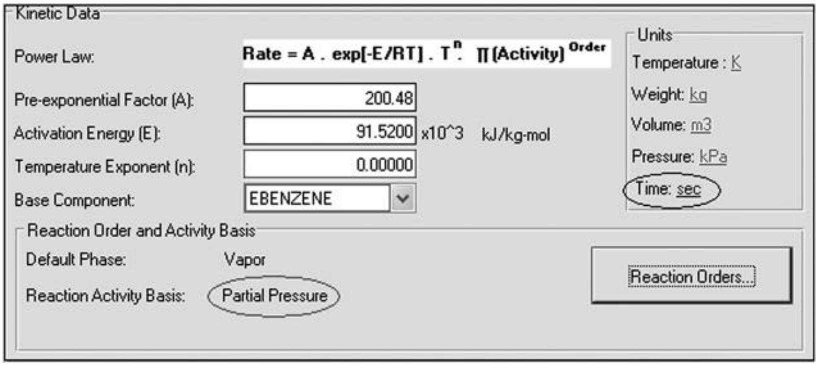
Streams			
		1	2
Temperature	C	606.9	497.2
Pressure	kPa	137.8	137.8
Molar flow	kgmol/h	8559	9031
Comp molar flow (E-benzene)	kgmol/h	783	311
Comp molar flow (styrene)	kgmol/h	0	472
Comp molar flow (hydrogen)	kgmol/h	0	472
Comp molar flow (H_2O)	kgmol/h	7776	7776

FIGURE 5.32
Adiabatic operation modes.

sheet and specify inlet stream conditions (880 K, 137.8 kPa). Under Input menu, select *Reaction Data*, use the power law, and enter stoichiometric coefficients. Double click on the reactor in the PFD area and select the reaction set name. Click on *Unit Reaction Definitions* and specify the kinetic data and order of reaction (Figure 5.33). Click on *Reaction Data* and specify the reactor length and diameter (10 m, 3.039 m, and a volume of 72.535 m^3). The temperature is fixed at 880 K (isothermal operation). Neglect pressure drop. The final process flow sheet and stream table properties are shown in Figure 5.34.

The fractional conversion for the isothermal operation:

$$x = \frac{783 - 64.28}{783} = 0.918(91.8\%)$$


Kinetic Data

Power Law: $\text{Rate} = A \,.\, \exp[-E/RT] \,.\, T^n \,.\, \Pi(\text{Activity})^{\text{Order}}$

Pre-exponential Factor (A): 200.48

Activation Energy (E): 91.5200 x10^3 kJ/kg-mol

Temperature Exponent (n): 0.00000

Base Component: EBENZENE

Units

Temperature : K

Weight: kg

Volume: m3

Pressure: kPa

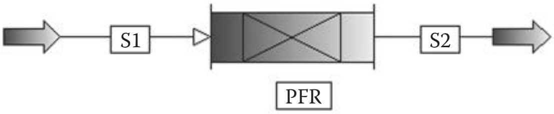
Time: sec

Reaction Order and Activity Basis

Default Phase: Vapor

Reaction Activity Basis: Partial Pressure

FIGURE 5.33
Kinetic data of Example 5.3.



Stream name Stream description Phase		S1 Example 5.3-1 Vapor	S2 Vapor
Temperature	K	880.0000	880.0000
Pressure	kPa	137.8000	137.8000
Enthalpy	m*kJ/h	767.6738	775.1890
Moleculara weight		24.7962	23.1609
Mole fraction vapor		1.0000	1.0000
Mole fraction liquid		0.0000	0.0000
Rate	kg-mol/h	10179.000	10897.721
Fluid rates	kg-mol/h		
Ebenzene		783.0001	64.2795
Styrene		0.0000	718.7206
Hydrogen		0.0000	718.7206
Water		9396.0000	9396.0000

FIGURE 5.34
Process flow sheet and stream table (isothermal operation).

PRO/II SIMULATION (ADIABATIC OPERATION MODE)

For adiabatic operation mode in Pro II, the Fixed Duty radio button will be selected and set to zero (adiabatic operation mode) as shown in Figure 5.35. The process flow sheet and stream table property of the adiabatic operation are shown in Figure 5.36. Note that the product temperature decreases because the reaction is endothermic.

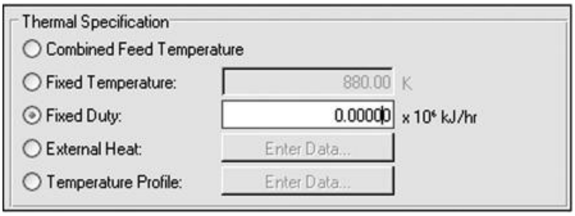
The fractional conversion of the adiabatic operation mode obtained by Pro II is

$$x = \frac{783 - 298.57}{783} = 0.619(61.9\%)$$

ASPEN SIMULATION (ISOTHERMAL OPERATION MODE)

The volume of the reactor is 72.535 m^3. Assuming that the PFR length is 10 m, consequently the reactor diameter is 3.039 m. The pre-exponential factor is

$$k = 0.20048 \frac{\text{kmol}}{\text{m}^3\,\text{s}\,\text{Pa}}$$



Thermal Specification

○ Combined Feed Temperature

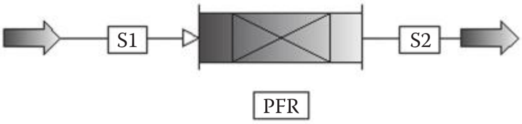
○ Fixed Temperature: 880.00 K

● Fixed Duty: 0.0000 $\times 10^6$ kJ/hr

○ External Heat: Enter Data...

○ Temperature Profile: Enter Data...

FIGURE 5.35
Adiabatic operation.



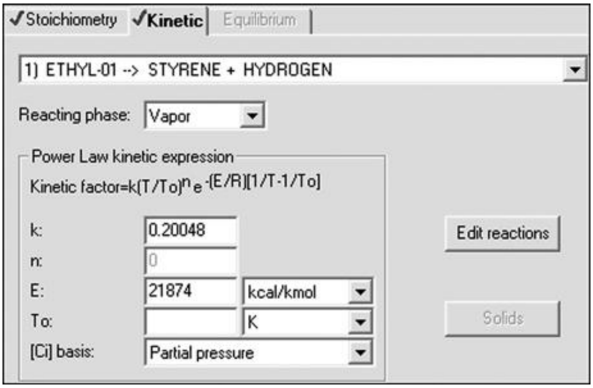
Stream name		S1	S2
Stream description		Example 5.3-2	
Phase		Vapor	Vapor
Temperature	K	880.0000	779.0169
Pressure	kPa	137.8000	137.8000
Enthalpy	m*kJ/h	767.6738	712.9523
Molecular weight		24.7962	23.6700
Mole fraction vapor		1.0000	1.0000
Mole fraction liquid		0.0000	0.0000
Rate	kg-mol/h	10179.000	10663.295
Fluid rates	kg-mol/h		
Ebenzene		783.0001	298.7052
Styrene		0.0000	484.2948
H_2		0.0000	484.2948
H_2O		9396.0000	9396.0000

FIGURE 5.36
Adiabatic operation.

The kinetic data are shown in Figure 5.37 and the process flow sheet and stream table for isothermal operation are shown in Figure 5.38.

The fractional conversion for the isothermal operation method is

$$x = \frac{783 - 65.794}{783} = 0.916(91.6\%)$$



1) ETHYL-01 --> STYRENE + HYDROGEN

Reacting phase: Vapor

Power Law kinetic expression

Kinetic factor=k(T/To)^n e$^{-(E/R)[1/T-1/To]}$

k: 0.20048

n: 0

E: 21874 kcal/kmol

To: K

[Ci] basis: Partial pressure

FIGURE 5.37
Kinetic parameters page.

Example 5.3			
Stream ID		1	2
Temperature	K	880.0	880.0
Pressure	atm	1.36	1.36
Vapor frac		1.000	1.000
Mole flow	kmol/h	10179.000	10896.206
Mass flow	kg/h	252400.643	252400.643
Volume flow	L/min	8.99961E+6	9.63642E+6
Enthalpy	MMbtu/h	−1845.865	−1761.258
Mole flow	kmol/h		
Ethyl-01		783.000	65.794
Styrene			717.206
Hydrogen			717.206
Water		9396.000	9396.000

FIGURE 5.38
Isothermal operation.

ASPEN SIMULATION (ADIABATIC OPERATION MODE)

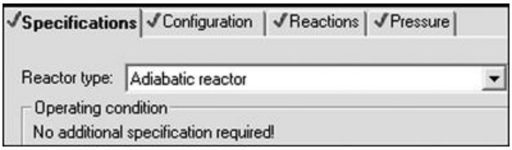
For adiabatic operation (Figure 5.39), the process flow sheet and stream table are shown in Figure 5.40. Since the reaction is endothermic, the fractional conversion of adiabatic operation is less than that of isothermal operation.

The fractional conversion for the adiabatic operation method is

$$x = \frac{783 - 306.925}{783} = 0.608\,(60.8\%)$$

SUPERPRO DESIGNER SIMULATION (ISOTHERMAL)

The PFR of the current version (version 7.5 build 10) required solid/liquid material to be present in feed stream (this problem will be settled in future versions). To

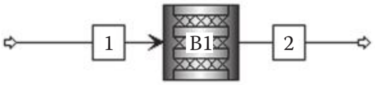


Reactor type: Adiabatic reactor

Operating condition

No additional specification required!

FIGURE 5.39
Adiabatic operation.



Example 5.3-adiabatic			
Stream ID		1	2
Temperature	K	880.0	780.3
Pressure	atm	1.36	1.36
Vapor frac		1.000	1.000
Mole flow	kmol/h	10179.000	10655.075
Mass flow	kg/h	252400.643	252400.643
Volume flow	L/min	8.99961E+6	8.35164E+6
Enthalpy	MMBtu/h	−1845.865	−1845.865
Mole flow	kmol/h		
Ethyl-01		783.000	306.925
Styrene			476.075
Hydrogen			476.075
Water		9396.000	9396.000

FIGURE 5.40
Adiabatic operation.

overcome this problem in the following example, a negligible amount of iron is added in the feed stream. The heat of reaction should be given in the units of kJ/kg. The residence time was set to 1.09 h (Volume of reactor 163 m^3). Design mode of operation was used in the simulation (Figure 5.41).

The fractional conversion of the isothermal operational mode

$$x = \frac{783 - 50.46}{783} = 0.936(93.6\%)$$

SuperPro Designer Simulation (Adiabatic)

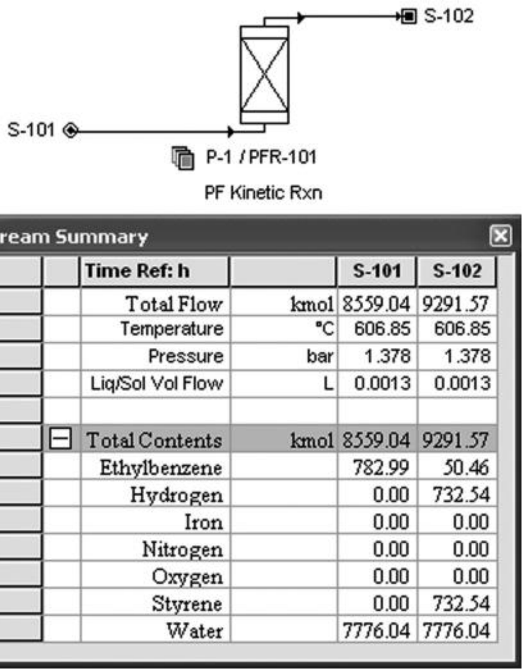
Everything was kept constant as isothermal operation, except for the mode of operation, was changed to adiabatic (the heat of reaction must be supplied). The results are shown in Figure 5.42.

The fractional conversion of the adiabatic operation mode

$$x = \frac{783 - 383.42}{783} = 0.51(51\%)$$

Conclusions

Results of simulations and hand calculations are close to each other, except that of SuperPro Designer where external data had been added such as heat of reaction.



Time Ref: h		S-101	S-102
Total Flow	kmol	8559.04	9291.57
Temperature	°C	606.85	606.85
Pressure	bar	1.378	1.378
Liq/Sol Vol Flow	L	0.0013	0.0013
⊟ Total Contents	kmol	8559.04	9291.57
Ethylbenzene		782.99	50.46
Hydrogen		0.00	732.54
Iron		0.00	0.00
Nitrogen		0.00	0.00
Oxygen		0.00	0.00
Styrene		0.00	732.54
Water		7776.04	7776.04

FIGURE 5.41
Isothermal operation method.

Example 5.4: Ethane Cracking Process

Ethylene is widely produced using thermal cracking of light hydrocarbons such as ethane. Ethylene is formed in large volume among the important base petrochemicals that forms the building blocks of the petrochemical industry. Thus, any improvement in the process of ethylene production may enhance the industrial economic output. An industrial plant uses 4587 kgmol/h of ethane as a feed to the steam cracking process to produce ethylene. The following reactions along with reaction rate constant are shown in Table 5.8.

SOLUTION

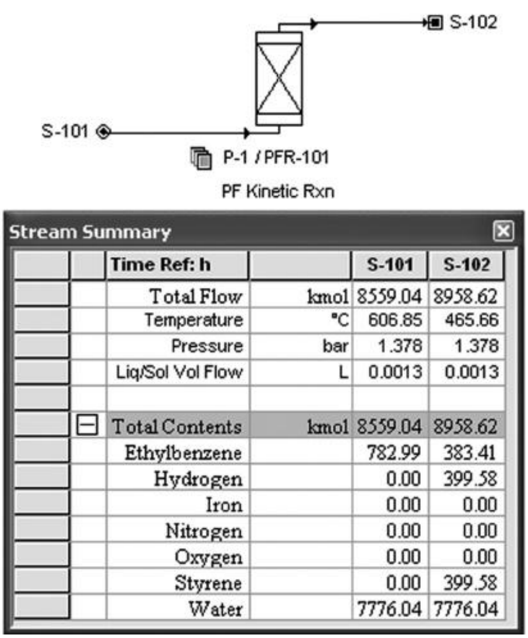
HAND CALCULATIONS

The change in the molar flow rate of component *j* as a function of reactor length,

$$\frac{dF_j}{dV} = \sum \alpha_{ij} r_i$$

where F_j the molar flow is rate of component *j*, and α_{ij} is the stoichiometric coefficient of component *j* in the reaction *i*. The rate of reaction *i*,

$$r_i = k_i \prod_j C_i$$



		Time Ref: h		S-101	S-102
		Total Flow	kmol	8559.04	8958.62
		Temperature	°C	606.85	465.66
		Pressure	bar	1.378	1.378
		Liq/Sol Vol Flow	L	0.0013	0.0013
	⊟	Total Contents	kmol	8559.04	8958.62
		Ethylbenzene		782.99	383.41
		Hydrogen		0.00	399.58
		Iron		0.00	0.00
		Nitrogen		0.00	0.00
		Oxygen		0.00	0.00
		Styrene		0.00	399.58
		Water		7776.04	7776.04

FIGURE 5.42
Adiabatic operation method.

Reaction rate constants,

$$k_i = A_i \exp \frac{-E_i}{RT}$$

Component molar concentrations of component j,

$$C_j = \left(\frac{F_j}{F_T}\right)\left(\frac{P}{RT}\right)$$

TABLE 5.8
Reaction Scheme of Ethane Steam Cracking Process

Reaction	Reaction Rate (mol/L s)	Rate Constant
$C_2H_6 \xrightarrow{K_1} C_2H_4 + H_2$	$r_1 = k_1 C_{C_2H_6}$	$k_1 = 4.65 \times 10^{13} e^{-65210/RT}$
$2C_2H_6 \xrightarrow{K_2} C_3H_8 + CH_4$	$r_2 = k_2 C^2_{C_2H_6}$	$k_2 = 3.85 \times 10^{11} e^{-65250/RT}$
$C_3H_6 \xrightarrow{K_3} C_2H_2 + CH_4$	$r_3 = k_3 C_{C_3H_6}$	$k_3 = 9.81 \times 10^{8} e^{-36920/RT}$
$C_2H_2 + C_2H_4 \xrightarrow{K_4} C_4H_6$	$r_4 = k_4 C_{C_2H_2} C_{C_2H_4}$	$k_4 = 1.03 \times 10^{12} e^{-41260/RT}$
$C_2H_4 + C_2H_6 \xrightarrow{K_5} C_3H_6 + CH_4$	$r_5 = k_5 C_{C_2H_4} C_{C_2H_6}$	$k_5 = 7.08 \times 10^{13} e^{-60430/RT}$

Source: Data from Levenspiel, O. 1998. *Chemical Reaction Engineering*, 3rd edn, John Wiley, New York, NY; Sundaram, K. M. and G. F. Froment 1977. *Chemical Engineering Science*, 32, 601; Froment, G. F. et al. *Industrial and Engineering Chemistry, Process Design and Development*, 1, 495.

where F_T is the total molar flow rate, P is the reactor pressure, T is the absolute temperature, and R is the gas constant. Total molar flow rate,

$$F_T = F_{\text{steam}} + \sum_i F_j$$

The above set of equations are easily solved using the Polymath program shown in Table 5.9 and the results are shown in Table 5.10.

TABLE 5.9

Polymath Program for Example 5.4

Program Code	Initial Conditions (mol/s)
`d(FC2H6)/d(V)= -k1*C2H6 - 2*k2*C2H6 ^2 - k5*C2H6*C2H4`	1330
`d(FC4H6)/d(V)=k4*C2H2*C2H4`	0
`d(FC3H8)/d(V)=k2*C2H6^2`	0
`d(FC3H6)/d(V)= -k3*C3H6 + k5*C2H4*C2H6`	0
`d(FC2H2)/d(V)=k3*C3H6 - k4*C2H2*C2H4`	0
`d(FC2H4)/d(V)=k1*C2H6 - k4*C2H4*C2H2 - k5*C2H4*C2H6`	0
`d(FH2)/d(V)=k1*C2H6`	0
`d(FCH4)/d(V)=k2*C2H6^2 + k3*C3H6 + k5*C2H6*C2H4`	
`FC2H60 = 1330`	
`Fsteam = 0.4*FC2H60`	
`k1 = 4.65*10^13*exp(-65210/(R*T))`	
`k2 = 3.85*10^11*exp(-65250/(R*T))`	
`k3 = 9.81*10^8*exp(-36920/(R*T))`	
`k4 = 1.03*10^12*exp(-41260/(R*T))`	
`k5 = 7.08*10^13*exp(-60430/(R*T))`	
`P = 3 # atm`	
`R = 1.987`	
`T = 1073.15 # K`	
`FT = FC2H6 + FC4H6 + FC3H8 + FC3H6 + FC2H2 + FC2H4 + FCH4 + FH2 + Fsteam`	
`CT = P/(0.08314*T)`	
`C2H6 = FC2H6*CT/FT`	
`C3H6 = FC3H6*CT/FT`	
`C3H8 = FC3H8*CT/FT`	
`C4H6 = FC4H6*CT/FT`	
`C2H2 = FC2H2*CT/FT`	
`C2H4 = FC2H4*CT/FT`	
`CH4 = FCH4*CT/FT`	
`H2 = FH2*CT/FT`	
`x = (FC2H60 - FC2H6)/FC2H60`	
`V(0) = 0, V(f) = 20000 # in liters`	

TABLE 5.10

Streams Molar Flow Rate (Volume = 20,000 L)

Molar Flow Rate	Feed (mol/s)	Product (mol/s)
$F_{C_2H_6}$	1330.0	609.15
$F_{C_4H_6}$	0.0	32.82
$F_{C_3H_8}$	0.0	0.08
$F_{C_3H_6}$	0.0	5.86
$F_{C_2H_2}$	0.0	5.77
$F_{C_2H_4}$	0.0	599.02
F_{H_2}	0.0	676.30
F_{CH_4}	0.0	83.14

The fractional conversion of ethane in a 20 m^3 reactor

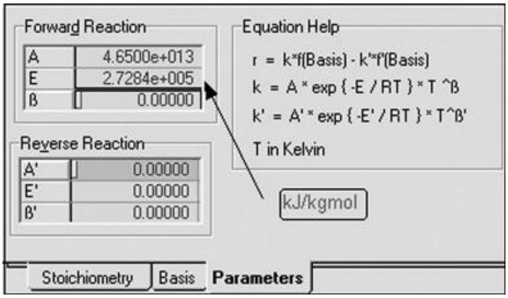
$$x = \frac{1330 - 609.15}{1330} = 0.54$$

HYSYS SIMULATION

Perform Hysys process flow sheet, and select *Reaction Packages* under *Flowsheet*. Enter the five reactions involved, all as vapor phase. All the reactions are assumed to be irreversible elementary reactions. Peng–Robinson is used as the fluid package. The volume of reactor is assumed as 20 m^3 (the value used in the hand calculations). On the kinetic reaction and the *Basis* page, Basis *Units* is set as gmol/L and *Rate Units* as gmol/L s. On the parameters page the values given in the data can be set as is for the pre-exponential factor, *A*, and units should be taken into account for the activation energy *E* (Figure 5.43). Results are shown in Figure 5.44.

The fractional conversion of ethane:

$$x = \frac{4788 - 2206.5}{4788} = 0.539(53.9\%)$$



Forward Reaction

A 4.6500e+013

E 2.7284e+005

ß 0.00000

Reverse Reaction

A' 0.00000

E' 0.00000

ß' 0.00000

Equation Help

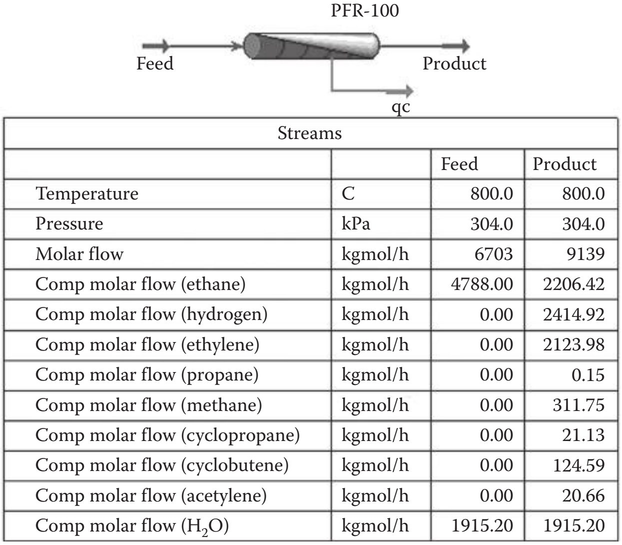
r = k*f(Basis) - k'*f'(Basis)

k = A * exp { -E / RT } * T ^ß

k' = A' * exp { -E' / RT } * T^ß'

T in Kelvin

FIGURE 5.43
Kinetic parameters of the first reaction entered in Hysys reaction menu.



Streams			
		Feed	Product
Temperature	C	800.0	800.0
Pressure	kPa	304.0	304.0
Molar flow	kgmol/h	6703	9139
Comp molar flow (ethane)	kgmol/h	4788.00	2206.42
Comp molar flow (hydrogen)	kgmol/h	0.00	2414.92
Comp molar flow (ethylene)	kgmol/h	0.00	2123.98
Comp molar flow (propane)	kgmol/h	0.00	0.15
Comp molar flow (methane)	kgmol/h	0.00	311.75
Comp molar flow (cyclopropane)	kgmol/h	0.00	21.13
Comp molar flow (cyclobutene)	kgmol/h	0.00	124.59
Comp molar flow (acetylene)	kgmol/h	0.00	20.66
Comp molar flow (H_2O)	kgmol/h	1915.20	1915.20

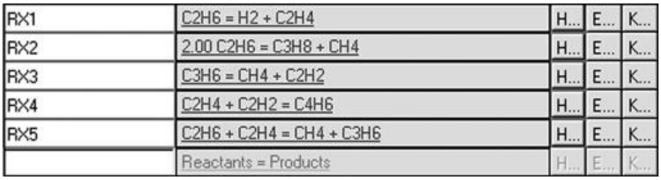
FIGURE 5.44
Process flow sheet and stream table properties generated by Hysys.

PRO/II SIMULATION

Build in the process flow sheet for the PFR as in previous examples. Select the all components involved in the process (nine components). Peng–Robinson is being selected as the thermodynamic fluid package. The volume of the PFR is 20 m^3. Form the *Reaction Data* under *Input* builds in the five involved reactions (Figure 5.45). Double click on the reactor and then click on *Unit Reaction Definitions* and fill in the reaction rate constants as shown in Figure 5.46 for the first reaction. Click on Reaction Order and set the order as 1 for ethane and 0 for others. The time should be changed to *sec*. After all given data are specified, the system is ready to run. Running the system suppose to give the results that appear as those in Figure 5.47.

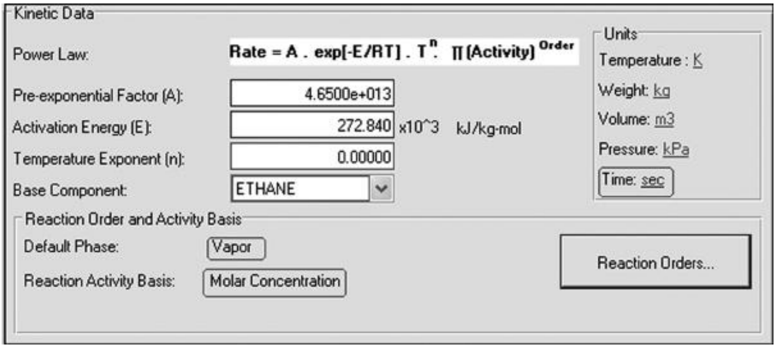
The fractional conversion is,

$$x = \frac{4788 - 2166.17}{4788} = 0.548(54.8\%)$$



RX1	C2H6 = H2 + C2H4	H...	E...	K...
RX2	2.00 C2H6 = C3H8 + CH4	H...	E...	K...
RX3	C3H6 = CH4 + C2H2	H...	E...	K...
RX4	C2H4 + C2H2 = C4H6	H...	E...	K...
RX5	C2H6 + C2H4 = CH4 + C3H6	H...	E...	K...
	Reactants = Products	H...	E...	K...

FIGURE 5.45
Reactions involved in the process entered in PRO/II reaction menu for Example 5.4.



Kinetic Data

Power Law: Rate = A . exp[-E/RT] . T^n . ∏ (Activity) ^{Order}

Pre-exponential Factor (A): 4.6500e+013

Activation Energy (E): 272.840 x10^3 kJ/kg-mol

Temperature Exponent (n): 0.00000

Base Component: ETHANE

Reaction Order and Activity Basis

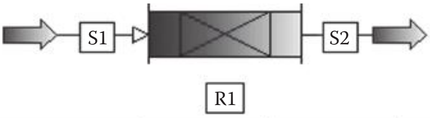
Default Phase: Vapor

Reaction Activity Basis: Molar Concentration

FIGURE 5.46
Kinetic parameters of the first reaction required by PRO/II.

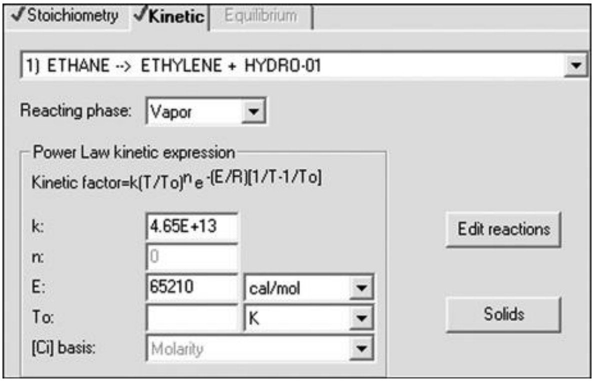
ASPEN SIMULATION

The process flow sheet for a PFR in Aspen Plus is constructed in the same way as previous examples. In the data browser, specify the feed stream properties. Specify inlet reactions stoichiometry and parameters as shown in Figure 5.48 for the first reaction. For the thermodynamic data, Peng–Robinson is selected. The reactor is considered isothermal. The process flow sheet and stream property table are both shown in Figure 5.49.



Stream name Stream description Phase		S1 Vapor	S2 Vapor
Temperature	K	1073.1500	1073.1500
Pressure	kPa	304.0000	304.0000
Enthalpy	m*kJ/h	554.8422	568.0806
Molecular weight		26.6255	19.4407
Mole fraction vapor		1.0000	1.0000
Mole fraction liquid		0.0000	0.0000
Rate	kgmol/h	6703.200	9180.527
Fluid rates	kgmol/h		
Ethane		4788.0000	2166.1741
H_2		0.0000	2169.6387
Ethylene		0.0000	0.3079
Propane		0.0000	20.5911
Methane		0.0000	21.2576
CYPR		0.0000	122.6247
12BD		0.0000	307.9970
Acetyln		0.0000	2456.7371
H_2O		1915.1998	1915.2001

FIGURE 5.47
Process flow sheet and stream table property generated by PRO/II.



1) ETHANE --> ETHYLENE + HYDRO-01

Reacting phase: Vapor

Power Law kinetic expression

Kinetic factor=$k(T/To)^n e^{-(E/R)[1/T-1/To]}$

k: 4.65E+13

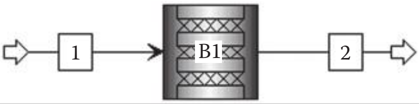
n: 0

E: 65210 cal/mol

To: K

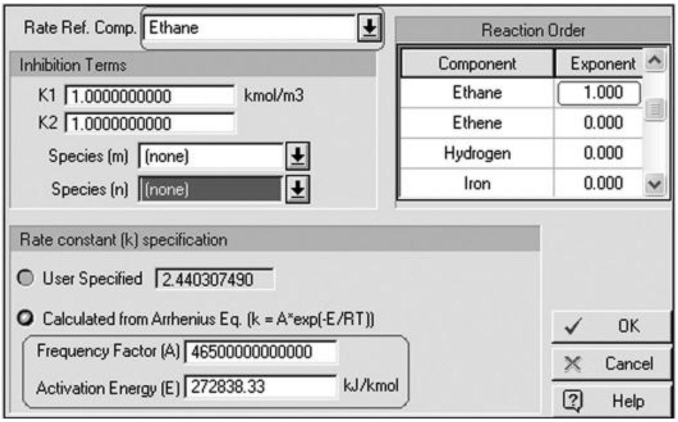
[Ci] basis: Molarity

FIGURE 5.48
Kinetic parameters of the first reaction entered in Aspen reaction's menu.



Example 5.4			
Stream ID		1	2
Temperature	K	1073.2	1073.2
Pressure	atm	3.00	3.00
Vapor frac			1.000
Mole flow	kmol/h	6703.200	9150.545
Mass flow	kg/h	178476.299	178476.299
Volume flow	L/min		4.48039E+6
Enthalpy	MMBtu/h		−100.137
Mole flow	kmol/h		
Ethane		4788.000	2199.620
Ethylene			2146.263
Propane			0.306
Acety-01			20.724
Cyclo-01			21.214
1-Butyne			119.210
Metha-01			301.388
Hydro-01			2426.621
Water		1915.200	1915.200

FIGURE 5.49
Process flow sheet and stream table property generated by Aspen Plus.



Rate Ref. Comp. Ethane

Inhibition Terms

K1 1.0000000000 kmol/m3

K2 1.0000000000

Species (m) (none)

Species (n) (none)

Reaction Order

Component	Exponent
Ethane	1.000
Ethene	0.000
Hydrogen	0.000
Iron	0.000

Rate constant (k) specification

○ User Specified 2.440307490

● Calculated from Arrhenius Eq. (k = A*exp(-E/RT))

Frequency Factor (A) 46500000000000

Activation Energy (E) 272838.33 kJ/kmol

FIGURE 5.50
Kinetic parameters of the first reaction entered in SuperPro reaction's menu.

The fractional conversion of ethane,

$$x = \frac{4788 - 2199.62}{4788} = 0.541(54.1\%)$$

SuperPro Designer Simulation

The PFR in SuperPro is selected; a similar procedure is followed as previous examples. The kinetic parameters of first reaction are shown in Figure 5.50. Results are shown in Figure 5.51.

The fractional conversion

$$x = \frac{4788 - 2184.724}{4788} = 0.544(54.4\%)$$

PROBLEMS

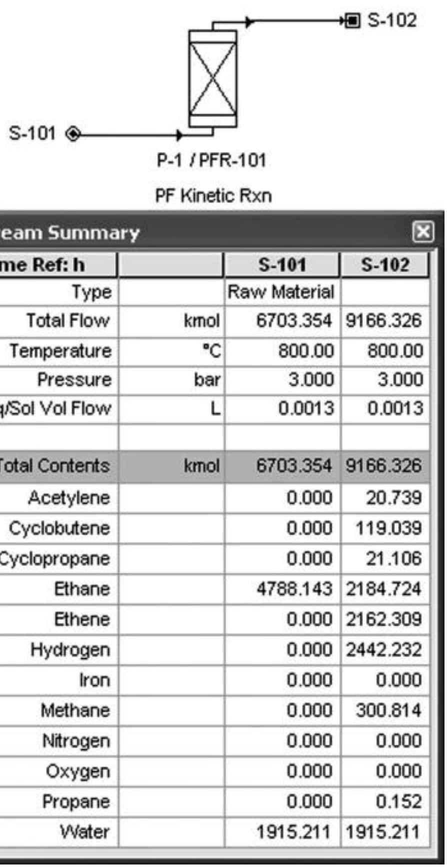
5.1 Volume of CSTR Reactor

The inlet molar feed rate to the CSTR reactor is of 50 kgmol/h ethanol, 50 kmol/h diethylamine, and 100 kgmol/h water. The reaction is in second order with respect to ethanol, and the rate constant, *k*,

$$A(\text{ethanol}) + B(\text{diethylamine}) \xrightarrow{k} C(\text{triethylamine} + D(\text{water})$$

where,

$$k = \left(4775\frac{\text{m}^3}{\text{kmol.h}}\right)\text{e}^{-\left(10{,}000\frac{\text{kJ}}{\text{kmol}}\right)/RT}$$



Time Ref: h		S-101	S-102
Type		Raw Material	
Total Flow	kmol	6703.354	9166.326
Temperature	°C	800.00	800.00
Pressure	bar	3.000	3.000
Liq/Sol Vol Flow	L	0.0013	0.0013
Total Contents	kmol	6703.354	9166.326
Acetylene		0.000	20.739
Cyclobutene		0.000	119.039
Cyclopropane		0.000	21.106
Ethane		4788.143	2184.724
Ethene		0.000	2162.309
Hydrogen		0.000	2442.232
Iron		0.000	0.000
Methane		0.000	300.814
Nitrogen		0.000	0.000
Oxygen		0.000	0.000
Propane		0.000	0.152
Water		1915.211	1915.211

FIGURE 5.51
Process flow sheet and stream table properties generated by SuperPro.

Find the reactor volume that achieves 90% conversion of ethanol

a. If the reactor is isothermal.
b. If the reactor is adiabatic.
c. Compare the results in a and b.

5.2 Conversion in the PFR Reactor

A measure of 100 kgmol/h of acetone is fed into an isothermal PFR. The inlet temperature and pressure of the feed stream are 750°C and 1.5 atm, respectively. The reaction is taking place in vapor phase. Acetone (CH_3COCH_3) is cracked to ketene (CH_2CO) and methane (CH_4) according to the following reactions:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

The reaction is in first-order with respect to acetone and the specific reaction rate can be expressed by

$$k = 8.2 \times 10^{14}(s^{-1})e^{\frac{-2.845\times 10^{5}(\text{kJ/kmol})}{RT}}$$

Calculate the reactor volume required to achieve 45% of limiting components.

5.3 Styrene Production

Styrene is made from the dehydrogenation of ethylbenzene in a PFR,

$$C_8H_{10} \rightarrow C_8H_8 + H_2$$

The feed consists of 780 kmol/h ethylbenzene, the reaction is isothermal, and the inlet temperature and pressure are 600°C, and 1.5 atm, respectively. The reaction rate is in first order with respect to ethylbenzene. Calculate the percent conversion of ethylbenzene if the reaction takes place in a 150 m^3, 3 m-long PFR.

The reaction rate is: $r = -kP_{\text{EB}}$, where P_{EB} is the partial pressure of ethylbenzene.

The specific reaction rate constant,

$$k = 200\frac{\text{kmol}}{\text{m}^3\,\text{s}\,kP_a}\exp\left[-90{,}000\frac{\text{kJ}}{\text{kmol}}/RT\right]$$

5.4 Ethylene Production

Ethylene is produced by dehydrogenation of ethane in an isothermal PFR at 800°C and 3 atm. The reaction taking place is

$$C_2H_6 \xrightarrow{K_1} C_2H_4 + H_2$$

Reaction rate: $r_1 = k_1C_{C_2H_6}$

Specific reaction rate constant:

$$k = 4.65 \times 10^{13}(\text{s}^{-1})\exp\left(-2.7 \times 10^{5}\frac{\text{kJ}}{\text{kmol}}/RT\right)$$

Find the reactor volume that is required to achieve 65% conversion of ethane.

a. If the reaction takes place isothermally.
b. If the reaction takes place in an adiabatic reactor.
c. Discuss results in parts a and b.

TABLE 5.11

Reaction Rate Constant

ρ_b	1200 kg/m^3
A_1	5.517×10^6 mol/kg s atm
Ea_1	1.849×10^8 J/mol
R	8.314 J/mol/K
P	30.0 atm
K_a	4.053 atm^{-1}
A_2	4.95×10^8 mol/kg/s
Ea_2	1.163×10^5 J/mol
K_{eq2}	$e^{-4.946+4897/T}$ (T in K)

5.5 Catalytic Reaction

Consider the multiple reactions taking place in PFR; the reaction parameters are shown in Table 5.11.

$$CH_4 + H_2O \Leftrightarrow 3H_2 + CO$$

$$CO + H_2O \Leftrightarrow H_2 + CO_2$$

Reaction rate

$$r_1 = \frac{\rho_b * A_1 * e^{(-Ea_1/R*T)} P_{CH_4}}{(1 + K_a * P_{H_2})}$$

$$r_2 = \rho_b * A_2 * e^{-Ea_2/R*T} \left(y_{CH_4} * y_{H_2O} - \frac{y_{CO_2} * y_{H_2}}{K_{eq2}} \right)$$

where ρ_b is the bulk density, A_1, A_2 is the pre-exponential factor or Arrhenius constant of the first and second reactions, respectively. E_{a1} E_{a2}, are the activation energy of the first and second reaction, respectively. k_a is an absorption parameter. y_i is the mole fraction of component i.

Feed enters the reactor at 350°C, 30 atm and 2110 mol/s with feed mole fractions, that is, 0.098 CO, 0.307 H_2O, 0.04 CO_2, 0.305 hydrogen, 0.1 methane, and 0.15 nitrogen.

References

1. Schmidt, L. D., 1998. *The Engineering of Chemical Reactions*, Oxford University Press, New York, NY.
2. Fogler, H. S., 2006. *Elements of Chemical Reaction Engineering*, 4th edn, Prentice-Hall, NJ.

3. Levenspiel, O., 1998. *Chemical Reaction Engineering*, 3rd edn, John Wiley, New York, NY.
4. Sundaram, K. M. and G. F. Froment, 1977. Modeling of thermal cracking kinetics. 1. Thermal cracking of ethane, propane and their mixtures, *Chemical Engineering Science*, 32, 601.
5. Froment, G. F., B. O. Van de Steen, P. S. Van Damme, S. Narayanan, and A. G. Goossens, 1976. Thermal cracking of ethane and ethane-propane mixtures, *Industrial and Engineering Chemistry, Process Design and Development*, 1, 495.

6

Distillation Column

At the end of this chapter you should be able to

1. Understand the function of distillation column.
2. Determine the minimum reflux ratio.
3. Determine the minimum and actual number of stages and optimum feed stage.
4. Determine the tower diameter.
5. Verify hand calculations with simulation results obtained with Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer.

6.1 Introduction

Distillation is a separation technique based on differences in boiling point which results in a dissimilarity in vapor pressure. In the design of any distillation column it is important to know at least two factors: one is the minimum number of plates required for the separation if no product or practically no product is withdrawn for the column (the condition of total reflux). The second point is the minimum reflux that can be used to accomplish the design separation. The tools used in the design of the distillation column are

- Material balance
- Energy balance
- Thermodynamic equilibrium
- Summation of a bubble point and a dew point

Distillation columns consist of three main parts: condenser, column, and reboiler.

Condenser: The condenser temperature should be high enough so that cooling water can be used in the condenser. If this requires very high pressure, then a refrigerated condenser should be considered.

Column: The bottom pressure must be higher than the top pressure so that the vapors can move from the bottom to the top. Specify a condenser and a reboiler pressure drop as zero.

Reboiler: The reboiler temperature should not be too high so that the lowest possible steam pressure can be used in the reboiler. This is because the steam cost is directly proportional to steam pressure [1].

6.2 Separation of Binary Components

Binary component distillation is the simplest form of separation. Commonly, feed to distillation columns consist of more than two components [2–4]. The schematic diagram of a distillation column is shown in Figure 6.1.

6.2.1 Material Balance and Energy Balance around the Column

Total balance:

$$F = D + B \tag{6.1}$$

Component balance:

$$x_F F = x_D D + x_B B \tag{6.2}$$

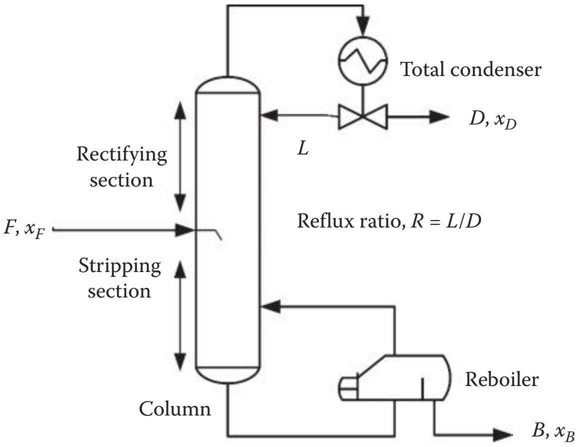


FIGURE 6.1
Schematic of distillation column.

Energy balance:

$$Fh_F + Q_{\text{reboiler}} = h_D D + h_B B + Q_{\text{condenser}} \tag{6.3}$$

The top section, bottom section, and feed stream material balance are shown in Figure 6.2. From these three material balances, column operating lines are derived.

6.2.2 Material Balance on the Top Section of the Column

Assuming constant molar overflow,

$$y_{n+1} V_{n+1} = L_n x_n + Dx_D \tag{6.4}$$

The reflux ratio

$$R = \frac{L}{D} \tag{6.5}$$

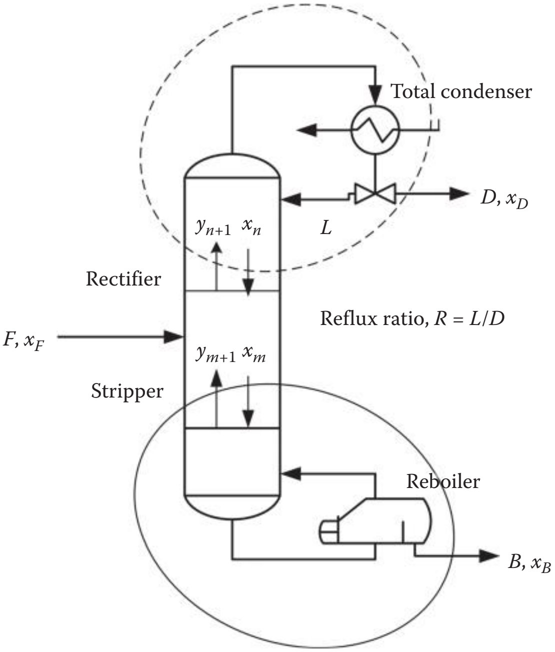


FIGURE 6.2
Distillation column rectifying and stripping sections.

The vapor leaving the top of the column equals recycled liquid and distillate:

$$V = L + D \tag{6.6}$$

Substituting L as a function of R,

$$V = (R + 1)D \tag{6.7}$$

The rectifying section operating line

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{1}{R+1} x_D \tag{6.8}$$

6.2.3 Material Balance on the Bottom Section of the Column

Assuming constant molar flow of vapor and liquid,

$$L_m x_m = y_{m+1} V_{m+1} + B x_B \tag{6.9}$$

The bottom section operating line

$$y_{m+1} = \frac{L}{V} x_m - \frac{B}{V} x_B \tag{6.10}$$

If $x_B = x_m$ and $V = L - B$, then $y_{m+1} = x_B$ and the operating line for the stripping section crosses the diagonal at point (x_B, x_B); this is always true no matter what type of reboiler is used, as long as there is only one bottom product. The lower operating line could then be constructed using the point (x_B, x_B) and the slope L/L – B which equals L/V.

6.2.4 Material Balances on the Feed Tray

Material balance around the feed tray (Figure 6.3):

$$yV + L'x = Lx + V'y + Fz_F \tag{6.11}$$

Rearranging,

$$y(V - V') = x(L - L') + Fz_F \tag{6.12}$$

q is the fraction of liquid in the feed stream:

$$q = \frac{L - L'}{F} = 1 + \frac{V' - V}{F} \tag{6.13}$$

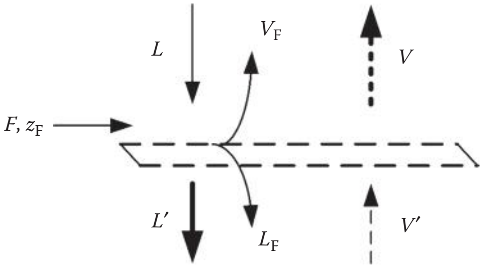


FIGURE 6.3
Material balance around feed tray.

Rearranging Equation 6.12,

$$y\left(\frac{V'-V}{F}\right) = x\left(\frac{L-L'}{F}\right) + z_F \tag{6.14}$$

Feed tray operating line:

$$y = x\left(\frac{q}{q-1}\right) - z_F\left(\frac{1}{q-1}\right) \tag{6.15}$$

q is the number of moles of the saturated liquid on the feed tray per mole of feed. If the feed enters at its boiling point, $q = 1$. If the feed enters as vapor at the dew point, $q = 0$. For a cold liquid feed, $q > 0$; for superheated vapor, $q < 1$; and for the feed being part liquid and part vapor, q is the fraction of the feed that is liquid ($0 < q < 1$).

$$q = \frac{H_V - H_F}{H_V - H_L} = \frac{(H_V - H_L) + C_{pL}(T_B - T_F)}{H_V - H_L} = \frac{\lambda + C_{pL}(T_B - T_F)}{\lambda} \tag{6.16}$$

where λ is the latent heat of vaporization (kJ/kg mol), C_{pL} is the heat capacity of the liquid feed (kJ/kg mol K), T_B is the boiling point of the feed, and T_F is the feed stream temperature.

6.3 Multicomponent Distillation

In multicomponent distillation, the equilibrium depends on all components. Complete composition of top and bottom products required trial-and-error calculations. Separation is between Light Key (LK) and Heavy Key (HK) components. Components lighter than LK are the main components in the head, and those heavier than HK are the main component in the bottom. Two methods are used in the design of multicomponent distillation: shortcut method and rigorous method.

6.3.1 Shortcut Distillation Method

The shortcut column performs Fenske–Underwood shortcut calculations for simple refluxed towers. The Fenske minimum number of trays and the Underwood minimum reflux are calculated. A specified reflux ratio can then be used to calculate the vapor and liquid traffic rates in the enriching and stripping sections, the condenser duty and reboiler duty, the number of ideal trays, and the optimal feed location. The shortcut column is only an estimate of the column performance and is restricted to simple refluxed columns. For more realistic results, the rigorous column operation should be used. This operation can provide initial estimates for most simple columns.

6.3.2 Minimum Number of Trays at Total Reflux Ratio, $N_{\min}$

The Fenske equation is used to determine the minimum number of equilibrium stages.

$$N_{\min} = \frac{\ln\left[(x_{\mathrm{LK}}/x_{\mathrm{HK}})_D (x_{\mathrm{HK}}/x_{\mathrm{LK}})_B\right]}{\log(\bar{\alpha}_{\mathrm{LK/HK}})} \tag{6.17}$$

where LK and HK, and $\bar{\alpha}_{\mathrm{LK/HK}}$ is the average geometric relative volatility defined by

$$\bar{\alpha}_{\mathrm{LK/HK}} = \left[(\alpha_{\mathrm{LK/HK}})_F (\alpha_{\mathrm{LK/HK}})_D (\alpha_{\mathrm{LK/HK}})_B\right]^{1/3} \tag{6.18}$$

D is distillate and *B* is the bottom products [3].

6.3.3 Minimum Reflux Ratio, $R_{\min}$

An approximate method for calculating the minimum reflux ratio, $R_{\min}$, is given by Underwood equations. Two equations must be solved:

$$1 - q = \sum_{i=1}^{n} \frac{\alpha_i \, x_{F,i}}{\alpha_i - \varphi} \tag{6.19}$$

where n is the number of individual components in the feed, α_i is the average geometric relative volatility of component i in the feed mixture to the HK component. $x_{F,i}$ is the mole fraction of component *i* in the feed, and *q* is the moles of saturated liquid on the feed tray per mole of feed.

$$R_{\min} + 1 = \sum_{i=1}^{n} \frac{\alpha_i \, x_{Di}}{\alpha_i - \varphi} \tag{6.20}$$

where α_i is equal to K_i / K_{HK} where K_{HK} is the *K* value for the HK. x_{Di} is the mole fraction of component *i* in the distillate. The correct value of ϕ lies between the values of α for the HKs and LKs, that is, solve for ϕ from the first Equation 6.3, then use this value to get $R_{\min}$ in the second Equation 6.4. The correct value is found by solving Equations 6.3 and 6.4 simultaneously.

6.3.4 Number of Equilibrium Stages, *N*

Gilliland correlation is used to calculate number of equilibrium stages, *N*. Select a reflux ratio that is $R = (1.1 - 1.5)R_{\min}$

$$\frac{N - N_{\min}}{N + 1} = 0.75\left(1 - \left(\frac{R - R_{\min}}{R + 1}\right)^{0.566}\right) \tag{6.21}$$

The Gilliland correlation is good for preliminary estimates, but has some restrictions

- Number of components must be between 2 through 11
- The *q* value must be between 0.28 and 1.42
- Pressure must be from vacuum to 600 psig
- α must be between 1.11 and 4.05
- $R_{\min}$ must be between 0.53 and 9.09
- $N_{\min}$ must be from 3.4 to 60.3

6.3.5 Best Feed Locations

The most popular method for determining the best feed locations are done using the Kirkbridge equation which is given in Equation 6.6. The ratio of trays above feed tray (N_D) and the ones below the feed tray (N_B) is calculated using the following equation:

$$\ln\left(\frac{N_D}{N_B}\right) = 0.206 \ln\left(\left(\frac{x_{\mathrm{HK}}}{x_{\mathrm{LK}}}\right)_F \left(\frac{x_{\mathrm{LK,in}B}}{x_{\mathrm{HK,in}D}}\right)^2 \left(\frac{B}{D}\right)\right) \tag{6.22}$$

where N_D is the number of equilibrium stages above the feed tray, while N_B is the number of equilibrium stages below the feed tray. B is the molar flow rate of bottom; D is the molar flow rate of distillate. Since $N_D + N_B = N$ where N is the total number of equilibrium stages, we can easily calculate the location of the feed plate.

6.3.6 Composition of Non-Key Components

The Fenske equation can be rearranged to help estimate the splits of other components, if the split of one is specified.

$$\frac{x_{Di}}{x_{Bi}} = (\bar{\alpha}_{ij}^{N_{\min}})\frac{(x_{\mathrm{HK}})_D}{(x_{\mathrm{HK}})_B} \tag{6.23}$$

where x_{Di} is the mole fraction of component i in the bottom; x_{Bi} is the mole fraction of component i in distillate. $N_{\min}$ is the minimum number of stages from the Fenske equation. $\bar{\alpha}_{ij}$ is the average geometric relative volatility of component i relative to HK component. The estimated splits are close to being correct even though N is not at minimum. If you multiply the equation by D/B:

$$\frac{d_i}{b_i} = \left(\bar{\alpha}_{ij}^{N_{\min}}\right)\frac{d_j}{b_j} \tag{6.24}$$

If j is the HK, $f_i = b_i + d_i$ (material balance on the column):

$$d_i = \frac{f_i(\bar{\alpha}_{ij}^{N_{\min}})(d_j/b_j)}{1 + (\bar{\alpha}_{ij}^{N_{\min}})(d_j/b_j)} \tag{6.25}$$

The distillate flow rate:

$$D = \sum d_i \tag{6.26}$$

6.4 Column Diameter

Most of the factors that affect column operation are due to vapor flow conditions; either excessive or too low. Vapor flow velocity is dependent on column diameter. Weeping determined the minimum vapor flow required, while flooding determines the maximum vapor flow allowed. The incorrect ratio of vapor/liquid flow conditions can cause foaming, entrainment, flooding, and weeping. Foaming is the expansion of liquid due to passage of vapor or gas, foaming is caused by high vapor flow rates, entrainment by excessively high vapor flow rates, flooding by excessive vapor flow, and weeping or dumping by excessively low vapor flow. Downcomer flooding is caused by excessively high liquid flow or a mismatch between the liquid flow rate and the downcomer area. The tower inside the cross-sectional area, A_T, is computed at a fraction f (typically 0.75–0.85) of the vapor flooding velocity, U_f, the vapor mass flow rate G:

$$G = f \times U_f \, (A_T - A_d) \, \rho_g \tag{6.27}$$

A_d is the cross-sectional area of the downcomer. Rearranging the equation for tower inside cross-sectional area:

$$A_T = \frac{G}{f \times U_f \times (1 - A_d/A_T)\rho_g} \tag{6.28}$$

The ratio of the down comer cross-sectional area to tray cross-sectional area:

$$\frac{A_d}{A_T} = 0.1 \quad \text{for } F_{LG} \le 0.1,$$

$$\frac{A_d}{A_T} = 1 + \frac{(F_{LG} - 0.1)}{9} \quad \text{for } 0.1 \le F_{LG} \le 1.0$$

$$\frac{A_d}{A_T} = 0.2 \quad \text{for } F_{LG} \ge 1.0$$

The tower inside diameter,

$$D_T = \sqrt{\frac{4A_T}{\pi}} \tag{6.29}$$

The flooding velocity (U_f) is computed based on a force balance on a suspended liquid droplet.

$$U_f = C\left(\frac{\rho_L - \rho_g}{\rho_g}\right)^{0.5} \tag{6.30}$$

where C, the capacity parameter is given by

$$C = C_{SB} F_{ST} F_F F_{HA} \tag{6.31}$$

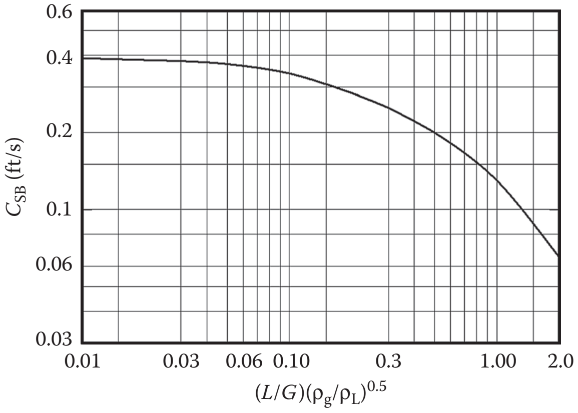


FIGURE 6.4
Capacity value, C_{SB} values for 24 in tray spacing (Adapted from Fair R. J., 1961. *Petro./Chem. Egn.*, 33: 45–52.)

The parameter C_{SB} is given by the correlation of Fair (1961). For 24 in tray spacing, Figure 6.4 shows C_{SB} as a function of the flow ratio parameter F_{LG}:

$$F_{LG} = \left(\frac{L}{G} \sqrt{\frac{\rho_g}{\rho_l}} \right) \tag{6.32}$$

L and G are the mass flow rate of liquid and vapor, respectively.

F_{ST} is the surface tension factor, $F_{ST} = (\sigma/20)^{0.2}$, σ = liquid surface tension (dyne/cm). F_F is the foaming factor, $F_F = 1$ for non-foaming systems, most distillation applications. $F_F = 0.5 - 0.75$ for foaming systems, absorption with heavy oils. F_{HA} is the hole–area factor, for valve and bubble cap:

$F_{HA} = 1,$ for sieve trays
$F_{HA} = 1,$ for $A_h / A_a \geq 1$
$F_{HA} = 5(A_h/A_a) + 0.5,$ for $0.06 \leq A_h/A_a \leq 0.1$

where A_h is the total whole area on a tray and A_a is the active area of the tray where bubbling area occurs:

$$A_a = (A_T - 2A_d)$$

Rectifying and stripping vapor and liquid flow rates:

- Rectifying liquid: $L_R = RD$

- Rectifying vapor: $V_R = (R + 1)D$
- Stripping liquid: $L_S = L_R + qF$
- Stripping vapor: $V_S = V_R - (1 - q)F$

where R is the reflux ratio, q is the feed index; 1 for boiling liquid and 0 for the saturated vapor. F is the feed flow rate.

Example 6.1: Tray Diameter Calculation

Compute the diameter of distillation column consists of valve trays, the liquid phase flow rate is 21,500 lb/h, vapor phase flow rate is 2440 lb/h, density of liquid is 32.4 lb/ft^3, gas-phase density is 1.095 lb/ft^3, liquid surface tension is 7.1 dyne/cm.

SOLUTION

First, the flooding velocity is determined:

$$U_f = C\left(\frac{\rho_L - \rho_g}{\rho_g}\right)^{0.5}$$

The capacity factor

$$C = C_{SB}F_{ST}F_F F_{HA}$$

C_{SB} is a function of F_{LG}:

$$F_{LG} = \left(\frac{L}{G}\sqrt{\frac{\rho_V}{\rho_l}}\right) = \left(\frac{21{,}500}{2440}\sqrt{\frac{1.095}{32.4}}\right) = 1.62$$

From Figure 6.4, for 24 in tray spacing, $C_{SB} = 0.09$ m/s; $F_F = 1$, for distillation column where no foaming exists; $F_{HA} = 1$, for valve trays.

$$F_{ST} = (\sigma/20)^{0.2} = (7.1/20)^{0.2} = 0.813$$

The flooding velocity for 24 in tray spacing,

$$U_f = C_{SB}F_{ST}F_F F_{HA}\left(\frac{\rho_L - \rho_g}{\rho_g}\right)^{0.5} = 0.09(0.813)(1)(1)\left(\frac{32.24 - 1.095}{1.095}\right)^{0.5}$$

$$= 0.39 \text{ ft/s}(1408 \text{ ft/h})$$

The ratio of downcomer cross-sectional area to tray cross-sectional area, A_d/A_T; since, $F_{LG} > 1$:

$$\frac{A_d}{A_T} = 0.2$$

Assuming the column is operating at 80% of flooding velocity the column cross-sectional area

$$A_T = \frac{G}{f \times U_f(1 - A_d/A_T)\rho_g} = \frac{2440}{0.8 \times 1408(1 - 0.2)1.095} = 2.47\,\text{ft}^2$$

The tower inside diameter

$$D_T = \sqrt{\frac{4A_T}{\pi}} = \sqrt{\frac{4 \times 2.47}{\pi}} = 1.78\ \text{ft}$$

Example 6.2: Binary Distillation Column

In 10 kmol/h of a saturated liquid consists of 40 mol% benzene (B) and 60% toluene (T). It is desired to have a distillate composition with 99.2 mol% of benzene and a bottom product composition with 98.6 mol% of toluene. The relative volatility, benzene/toluene (α_{BT}), is 2.354. The reflux is returned as a saturated liquid, and the column has a total condenser and a partial re-boiler.

a. Use Fenske equation to determine minimum number of trays, N_{min}
b. Determine optimum feed stage for the minimum number of stage
c. Using Underwood equations to find minimum reflux ratio, R_{min} or $(L/D)_{min}$
d. Calculate actual reflux ratio, R if $R = 1.1\ R_{min}$
e. Actual number of trays
f. Optimum feed tray
g. Rectifying liquid and vapor, stripping liquid and vapor flow rate

SOLUTION

HAND CALCULATIONS

a. Using Fenske equation to determine,

$$N_{min} = \frac{\ln((x_{LK}/x_{HK})_D(x_{HK}/x_{LK})_B)}{\ln(\bar{\alpha}_{LK/HK})}$$

Substituting required values:

$$N_{min} = \frac{\ln((0.992/0.008)_D(0.986/0.014)_B)}{\ln(2.354)} = \frac{9.075}{0.856} = 10.6$$

For binary component it can be also done such as

$$N_{min} = \frac{\ln((x/1 - x)_D/(x/1 - x)_B)}{\ln\alpha_{BT}}$$

$$= \frac{\ln((0.992/1 - 0.992)_D/(0.986/1 - 0.986)_B)}{\ln(2.354)} = 10.59$$

b. Optimum feed stage for the minimum number of stage:

$$N_{F\min} = \frac{\ln((x_{\text{LK}}/x_{\text{HK}})_D/(x_{\text{LK}}/x_{\text{HK}})_F)}{\ln\alpha_{\text{LK-HK}}} = \frac{\ln((0.992/0.008)_D/(0.4/0.6)_F)}{\ln(2.4)} = 6.1$$

c. Using Underwood equations to find the minimum reflux ratio, $R_{\min}$ or $(L/D)_{\min}$

$$1-q = \sum_{i=1}^{n}\frac{(\alpha_i\,x_i)_F}{\alpha_i-\varphi} = 1-1 = \sum_{i=1}^{n}\frac{(\alpha_i\,x_i)_F}{\alpha_i-\varphi}$$

Since feed is saturated liquid, $q = 1$,

$$0 = \sum\frac{\alpha_i\,x_{Fi}}{\alpha_i-\varphi} = \frac{\alpha_B\,x_{B,F}}{\alpha_B-\varphi} + \frac{\alpha_T\,x_{T,F}}{\alpha_T-\varphi} = \frac{2.354\times 0.4}{2.354-\varphi} + \frac{1\times 0.6}{1-\varphi}$$

Solving for φ

$$0 = 0.94(1-\phi) + 0.6(2.354-\phi) \Rightarrow \phi = 1.528$$

Substituting the value of $\phi = 1.528$ in the Underwood equation:

$$R_{\min}+1 = \sum\frac{(\alpha_i\,x_i)_D}{\alpha_i-\varphi} = \frac{(\alpha_B\,x_B)_D}{\alpha_B-\varphi} + \frac{(\alpha_T\;x_T)_D}{\alpha_T-\varphi} = \frac{(2.354)(0.992)}{2.354-1.528} + \frac{(1)(0.008)}{1-1.528}$$

$$R_{\min}+1 = 2.83 - 0.0152 = 2.82$$

$$R_{\min} = 1.82$$

d. Calculate actual reflux ratio, R, if $R = 1.1\ R_{\min}$

$$R = 1.1\times R_{\min} = 1.1\times 1.82 = 2.0$$

e. Actual number of trays N (or equilibrium number of trays) is calculated using Gilliland correlation to estimate number of stages and optimum feed location:

$$\frac{N-N_{\min}}{N+1} = 0.75\left(1-\left(\frac{R-R_{\min}}{R+1}\right)^{0.5668}\right)$$

Substituting values of $N_{\min}$, $R_{\min}$ and R in Gilliland correlation:

$$\frac{N-10.59}{N+1} = 0.75\left(1-\left(\frac{2-1.82}{2+1}\right)^{0.5668}\right)$$

$(N - 10.59)/N + 1 = 0.6$, solving for $N \Rightarrow N = 28$. Actual number of stages is 28 stages.

f. Optimum feed tray:

$$\frac{N_D}{N_B} = \left(\frac{x_{F,\mathrm{HK}} \times x_{B,\mathrm{LK}} \times B}{x_{F,\mathrm{LK}} \times x_{D,\mathrm{HK}} \times D}\right)^{0.206}$$

This needs knowing values of B and D:

$$D = \left(\frac{z - x_B}{x_D - x_B}\right) F$$

Benzene balance:

$$D = \left(\frac{0.4 - 0.014}{0.992 - 0.014}\right)(10\ \mathrm{kmol/h}) = 3.95\ \mathrm{kmol/h}$$

The bottom molar flow rate, B

$$F = D + B \Rightarrow B = 10 - 3.95 = 6.05\ \mathrm{kmol/h}$$

Then optimum feed tray location is calculated:

$$\frac{N_D}{N_B} = \left(\frac{0.6 \times 0.014 \times 6.05}{0.4 \times 0.008 \times 3.95}\right)^{0.206} = 1.33$$

$$\frac{N_D}{N_B} = 1.33\ \&\ N_D + N_B = 28$$

$$N_B + 1.33\ N_B = 28$$

Solving for N_B and N_D

$$N_B = 12 \quad \text{and} \quad N_D = 16$$

The feed tray is tray 16 from top. Using Kirkbride method:

$$\ln\left(\frac{N_D}{N_B}\right) = 0.206 \ln\left(\left(\frac{x_{\mathrm{HK}}}{x_{\mathrm{LK}}}\right)_F \left(\frac{x_{\mathrm{LK,in}B}}{x_{\mathrm{HK,in}D}}\right)^2 \left(\frac{B}{D}\right)\right)$$

Substituting values of mole fraction of LK and HK in feed stream distillate and bottom stream and mole flow rate of bottom and distillate in Kirkbride equation:

$$\ln\left(\frac{N_D}{N_B}\right) = 0.206 \ln\left(\left(\frac{0.6}{0.4}\right)_F \left(\frac{0.014}{0.008}\right)^2 \left(\frac{6.05}{3.95}\right)\right)$$

The number of trays above feed tray to those in the bottom trays:

$$N_D / N_B = 1.5$$

Since, $N_D/N_B = 1.5$ and $N_D + N_B = 28$

$$1.5N_B + N_B = 28$$

$$2.5N_B = 28 \Rightarrow N_B = 11$$

Solving for N_B and N_D

$$N_B = 11, \quad N_D = 17$$

The number of stages above the feed tray is 17 trays from top; this means that the feed tray is the tray number 17th from the top.

g. Rectifying vapor, $V_R = D(R + 1) = 3.95(2 + 1) = 11.58$ kmol/h.
Rectifying liquid, $L_R = D \times R = 3.95 \times 2 = 7.9$ kgmol/h.
Stripping liquid, $L_S = L_R + F = 7.9 + 10 = 17.9$ kgmol/h.
Stripping vapor, $V_s = V_R = 11.58$ kgmol/h.

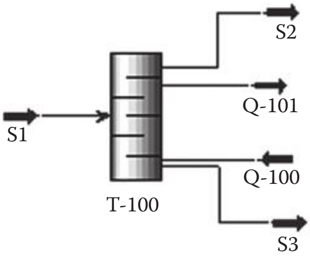
HYSYS/UNISIM SIMULATION

Distillation in Hysys can be performed using the shortcut column and continuous distillation column. The data from shortcut distillation column can be used as initial estimate to the rigorous distillation column. The specs needed are the number of stages, number of feed stage, reboiler and condenser pressure, reflux ratio and distillate rate. In the shortcut column there is no iterations, or advanced specs. The rigorous model takes more effort, but there are a number of ways to help the solver get to a solution. If the rigorous model does not converge with data provided from shortcut column, then more easily achieved specs need to be used.

Shortcut Column Method

Using Hysys shortcut distillation method; connecting feed stream, distillate and product streams, condenser and reboiler energy streams and fully specifying feed stream. While in *Design/Parameters* page the following data should be made available:

- LK in bottom: Benzene with mole fraction 0.014
- HK in distillate: toluene, mole fraction 0.008
- Condenser pressure: 1 atm
- Reboiler pressure: 1 atm
- External reflux ratio: 2

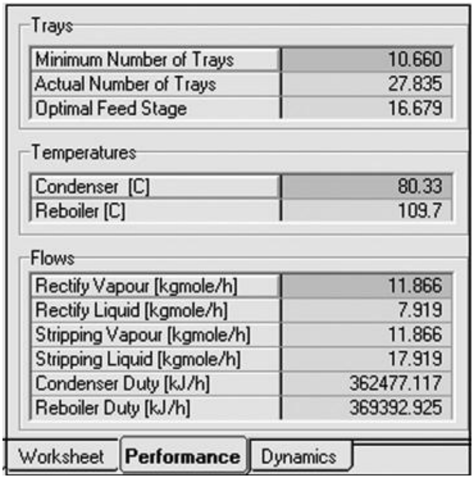


Streams				
		S1	S2	S3
Temperature	C	95.00	80.33	109.7
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	10.00	3.947	6.053
Comp molar flow (benzene)	kgmol/h	4.00	3.92	0.08
Comp molar flow (toluene)	kgmol/h	6.00	0.03	5.97

FIGURE 6.5
Hysys shortcut column process flow sheet and stream summary.

The process flowsheet and stream summary is shown in Figure 6.5.

Specify light and heavy components, top and bottom pressure (in the design, parameter's page). Specify the reflux ratio to be 1.1 times the minimum reflux ratio, $R = 1.1\ R_{\min}$, the shortcut results are obtained in the performance page, by clicking the *Performance* tab button. The results are shown in Figure 6.6.



Trays

Minimum Number of Trays	10.660
Actual Number of Trays	27.835
Optimal Feed Stage	16.679

Temperatures

Condenser [C]	80.33
Reboiler [C]	109.7

Flows

Rectify Vapour [kgmole/h]	11.866
Rectify Liquid [kgmole/h]	7.919
Stripping Vapour [kgmole/h]	11.866
Stripping Liquid [kgmole/h]	17.919
Condenser Duty [kJ/h]	362477.117
Reboiler Duty [kJ/h]	369392.925

FIGURE 6.6
Shortcut column performance page.

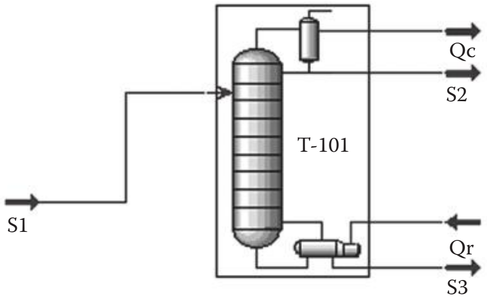
Minimum number of trays is 11 trays, the actual number of trays is 28 and optimum feed tray is tray 17 counting from top. Results are in good agreement with those obtained by hand calculations. The rectifying vapor is 11.866 kmol/h and the rectifying liquid molar flow rate is 7.919 kgmol/h.

Hysys/Unisim Rigorous Column

After selecting the *Distillation Column* from the object palate or Case (main), connecting feed stream, top and bottom product streams and two energy streams one for the condenser and one for the partial reboiler, the following data have to be provided:

- Feed stream is fully specified (i.e., providing feed flow rate and composition, and stream conditions, such as temperature and pressure or vapor/phase fraction and temperature or pressure)
- Feed stream inlet stage: 17
- Total number of trays: 28
- Condenser and reboiler pressure: 1 atm
- Reflux ratio: 2
- Distillate liquid rate: 3.947 kmol/h

In the *Monitor* page, it is necessary to make sure that the degree of freedom is zero and uncheck the check buttons for the unspecified variables. Providing all the above required data and running the system the results should look like that shown in Figure 6.7. The results show that molar flow rate of top and bottom product streams are as those obtained by hand calculation.



Streams				
		S1	S2	S3
Temperature	C	95.00	80.53	109.7
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	10.00	3.947	6.053
Comp molar flow (benzene)	kgmol/h	4.0000	3.8764	0.1236
Comp molar flow (toluene)	kgmol/h	6.0000	0.0710	5.9290

FIGURE 6.7
Rigorous column process flow sheet and stream summary generated with Hysys.

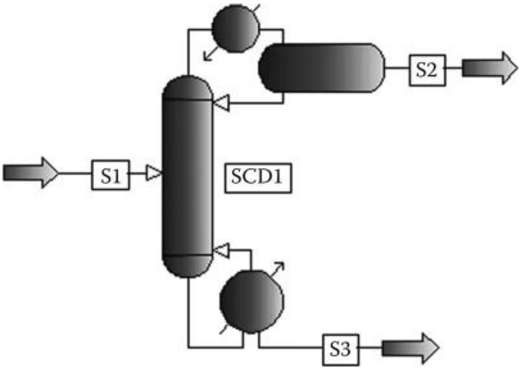


FIGURE 6.8
Shortcut distillation flow sheet in PRO/II.

PRO/II SIMULATION

Two distillation methods are available in PRO/II:

1. Shortcut distillation method
2. Continuous distillation method

Shortcut Distillation Method

From the object palette *Shortcut* is selected and placed in the PFD area. The reboiler and condenser in the popup window are selected. Feed stream and two product streams are connected as shown in Figure 6.8. Double clicking on the shortcut distillation block diagram, the required data windows are shown in Figure 6.9.

The following buttons are required in providing the necessary data:

Minimum Reflux: Double click on the minimum reflux button and perform minimum reflux calculation is checked, LK is benzene, HK is toluene, reflux ratio is 1.1.

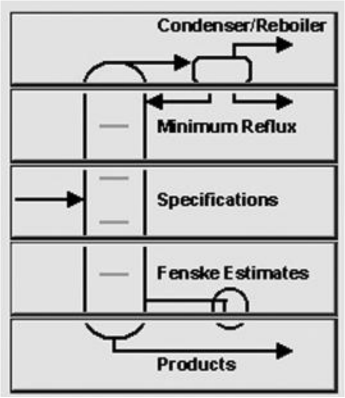
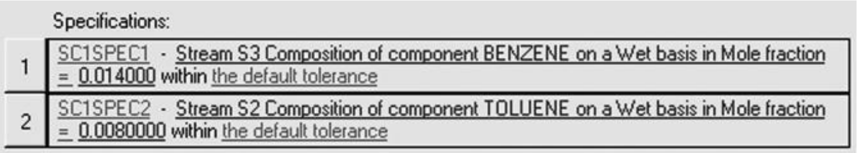


FIGURE 6.9
PROII shortcut distillation required data.



Specifications:

1	SC1SPEC1 - Stream S3 Composition of component BENZENE on a Wet basis in Mole fraction = 0.014000 within the default tolerance
2	SC1SPEC2 - Stream S2 Composition of component TOLUENE on a Wet basis in Mole fraction = 0.0080000 within the default tolerance

FIGURE 6.10
Specifications of shortcut distillation column.

Specifications: The composition of benzene in the bottom streams (S3) is set to be 0.014, and the toluene composition in the distillate is 0.008 (Figure 6.10).

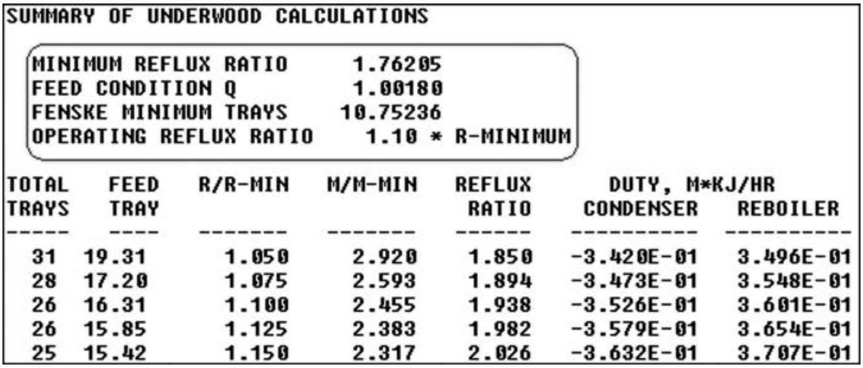
Products: The molar flow rate of the product stream S2 is set to 4 kgmol/h. One needs to enable the minimum reflux calculations in the shortcut column to see the minimum number of tray and feed location. Once this option is selected then running the simulation, generates a text report. The required results are under the *Summary of Underwood Calculations* section in the report as shown in Figure 6.11. The stream property table is shown in Figure 6.12 where exit streams molar flow rate and conditions are obtained.

PRO/II Rigorous Distillation Method

The *Distillation* unit in the object palette is selected and placed the PFD space assuming that the PFD is set up with the proper components and thermodynamic package. As soon as the column is placed a window will appear asking for the number of theoretical trays to be used and whether to include a condenser and reboiler (these can be changed after the column has been placed).

Connections: Press the *Streams* button to begin connecting streams. Connect the feed stream to the left side of the distillation column. Define the inlet stream name or keep the stream default name S1.

Condenser: The condenser has several port connections. The top port is normally vapor product while the bottom red port is liquid product and the



```
SUMMARY OF UNDERWOOD CALCULATIONS

   MINIMUM REFLUX RATIO      1.76205
   FEED CONDITION Q          1.00180
   FENSKE MINIMUM TRAYS     10.75236
   OPERATING REFLUX RATIO     1.10 * R-MINIMUM

TOTAL    FEED    R/R-MIN   M/M-MIN   REFLUX      DUTY, M*KJ/HR
TRAYS    TRAY                         RATIO    CONDENSER   REBOILER
-----    ----    -------   -------   ------   ----------  ----------
  31    19.31     1.050     2.920     1.850   -3.420E-01   3.496E-01
  28    17.20     1.075     2.593     1.894   -3.473E-01   3.548E-01
  26    16.31     1.100     2.455     1.938   -3.526E-01   3.601E-01
  26    15.85     1.125     2.383     1.982   -3.579E-01   3.654E-01
  25    15.42     1.150     2.317     2.026   -3.632E-01   3.707E-01
```

FIGURE 6.11
Summary of Underwood calculations.

Stream name		S1	S2	S3
Stream description				
Phase		Liquid	Liquid	Liquid
Temperature	K	368.2000	353.1469	383.0572
Pressure	kpa	101.3250	101.3250	101.3250
Enthalpy	M*kJ/h	0.1513	0.0464	0.1124
Molecular weight		86.5298	78.2259	91.9441
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	10.000	3.947	6.053
Fluid rates	kgmol/h			
Benzene		4.0000	3.9153	0.0847
Toluene		6.0000	0.0316	5.9684

FIGURE 6.12
Streams property table.

bottom green port is water. These identifications can also be seen by holding the stream cursor over the individual ports. For this example we will be connecting the liquid product port from the condenser.

To define the distillation column in PRO/II several factors need to be defined. Double click on the column to open the specification window. The following are required to be defined indicated by the red border (Figure 6.13):

- Pressure profile
- Feeds and products
- Performance specifications

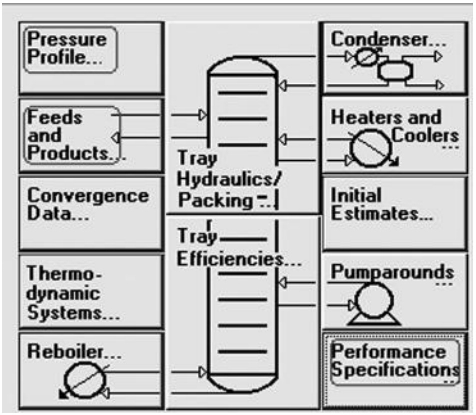


FIGURE 6.13
Column required data.

The *Condenser* and *Reboiler* are defined by defaults, indicated by the blue border. *Conversion Data*, *Thermodynamic Systems*, and *Initial Estimates* are all user optional, they can be defined or redefined but it is not necessary, indicated by the green border. *Heaters*, *Coolers*, and *Pumparounds* are optional additions to the distillation column. The column can be renamed by typing the desired name into the Unit: field, currently T1. Clicking on *Pressure Profile* will open this window:

Pressure Profile: The pressure in the column can be defined either by the *overall* or by *individual trays*. To change between these two systems select the appropriate radio button. *Overall* requires the top tray pressure and the overall pressure drop, either per tray or across the whole column. By *Individual trays* allow the user to specify the pressure on individual trays. The minimal trays to define are the top and bottom trays. Once the pressure profile for the column is defined, press *OK* to save the changes and return to the Column window. If the pressure profile is properly defined that box will now have a blue border (Figure 6.14).

Feeds and Products: In this window the user defines what tray the feed stream will flow to, the user can also set whether both vapor and liquid from the feed stream will go to the feed tray or the feed flashes when entering the column. If the feed is flashed the liquid portion of the feed stream will go to the feed tray, while the vapor will go to the tray above the feed tray (Figure 6.15). In addition, an estimate of one of the two product stream flow rates is needed. Both stream flows have red borders, but once one is defined the other becomes set. Setting both streams can lead to over specifications of the system. Once the feed tray and the product flow rate have been set click *OK* to save the changes and return to the column window. If the feed tray and product streams are properly defined that box will now have a blue border.

Performance Specifications: If *Performance Specifications* have not been set at this point PRO/II will prompt the user if they want to set the product flow rate as a specification. If the user does this the flow rate will not be an estimate but a factor that PRO/II will try to fit. Clicking "Performance Specifications" will open the window as shown in Figure 6.16.

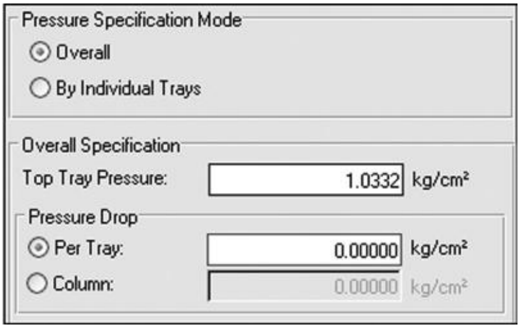
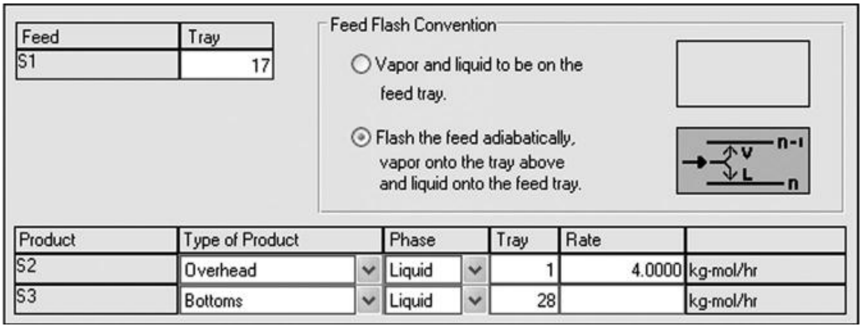

Pressure Specification Mode
● Overall
○ By Individual Trays
Overall Specification
Top Tray Pressure: 1.0332 kg/cm²
Pressure Drop
● Per Tray: 0.00000 kg/cm²
○ Column: 0.00000 kg/cm²

FIGURE 6.14
Pressure specification windows.



Feed	Tray
S1	17

Feed Flash Convention

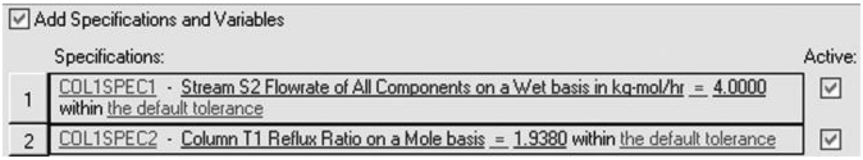
○ Vapor and liquid to be on the feed tray.

● Flash the feed adiabatically, vapor onto the tray above and liquid onto the feed tray.

Product	Type of Product	Phase	Tray	Rate	
S2	Overhead	Liquid	1	4.0000	kg-mol/hr
S3	Bottoms	Liquid	28		kg-mol/hr

FIGURE 6.15
Feed and products windows.

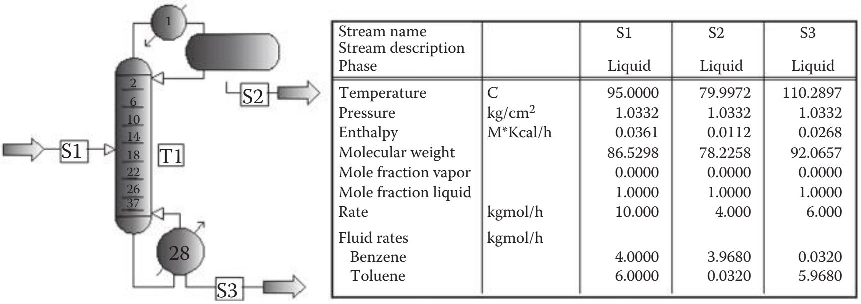
If condenser and/or reboiler have been added and/or removed since placing the distillation column they may not be preset as variables. The distillation column has a wide variety of possible parameter to fit. This example will use one parameter from the column and one parameter from a product stream; however, it is possible to define a distillation column just using column parameters or stream parameters. Start by clicking on *Parameter* in the *COL1SPEC1* line. Under the drop down menu select either *stream* or *column*; here column was selected; only the column being defined will appear under unit name, even if there are multiple distillation columns in the PFD. Then click *Parameter* to select the column parameter to fit and open this window. All possible parameters appear in the window. Each one has multiple subchoices and/or can be set for individual trays. This example will be using a fixed reflux ratio as a fitting parameter. Once the parameter has been selected, click *OK* to save the changes. The new parameter will appear highlighted in blue and the units that will be used are in green. If these are acceptable click *OK* again, if not either the parameter can be changed by clicking on it again, the units can be changed by clicking on them. Once the parameter has been set, the value can be set by clicking on *value* and entering the desired value in the string field that appears. Repeating this process for line COL1SPEC2, but instead selecting *Stream* and the desired stream name in the first parameter window that appears will open this window. In this window the parameter to be fit to in the selected stream can be chosen. This example is selecting composition of one of the product streams to be the parameter to fit (Figure 6.16).



☑ Add Specifications and Variables

	Specifications:	Active:
1	COL1SPEC1 - Stream S2 Flowrate of All Components on a Wet basis in kg-mol/hr = 4.0000 within the default tolerance	☑
2	COL1SPEC2 - Column T1 Reflux Ratio on a Mole basis = 1.9380 within the default tolerance	☑

FIGURE 6.16
Performance specifications page.



Stream name Stream description Phase		S1 Liquid	S2 Liquid	S3 Liquid
Temperature	C	95.0000	79.9972	110.2897
Pressure	kg/cm^2	1.0332	1.0332	1.0332
Enthalpy	M*Kcal/h	0.0361	0.0112	0.0268
Molecular weight		86.5298	78.2258	92.0657
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	10.000	4.000	6.000
Fluid rates	kgmol/h			
Benzene		4.0000	3.9680	0.0320
Toluene		6.0000	0.0320	5.9680

FIGURE 6.17
Process flow sheet and stream properties table.

Now the user can calculate the PFD by pressing *Run* in the Run Palette. The system will become colored blue if everything is able to be calculated (Figure 6.17).

ASPEN SIMULATION

There are two types of common interest for distillation in Aspen:

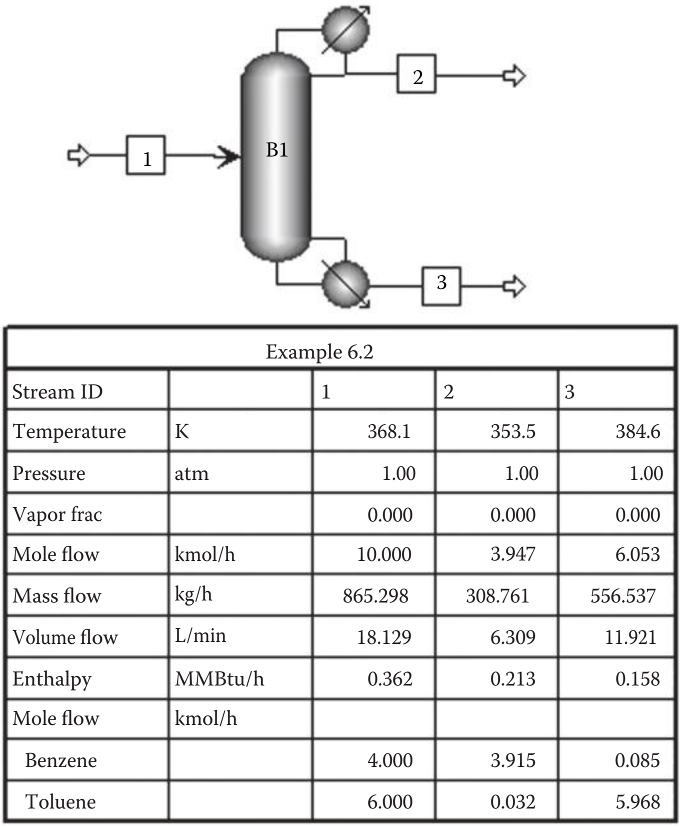
- DSTWU, which is the multicomponent shortcut distillation method.
- RadFrac, which is the rigorous simulation of a single column.

Press on the *Columns* tab in the *Equipment Model Library* and place a DSTWU column into the process flowsheet window. To create the inlet and exit streams, first click on the *Material Streams* button at the bottom left corner of the window. Red and blue arrows appear around the column. A red arrow signifies a stream that is required for a design specification; blue arrows signify an optional stream. Connect the feed and product streams where Aspen indicates they are required (Figure 6.18).

Now open up the Data Browser window. You will notice that we are only required to update our data input in the Blocks tab. For this simulation we will be inputting:

- The reflux ratio
- The key component recoveries
- The tower pressures

For our purposes, we will assume that the tower has no pressure drop throughout it. However, we will set the condenser and reboiler pressures to 1 atm to aid in our separation process. We will start with an input reflux ratio of $1.1*R_{\text{min}} = 1.84$. The component recovery values that are input are equal to the amount of each component in the distillate divided by the amount of each component in the feed. For this reason a recovery of 98% for benzene and 0.5% for the toluene are reasonable if our distillation tower is operating well, the results should look like that shown in Figure 6.19. Using Aspen short cut distillation column the minimum



Example 6.2				
Stream ID		1	2	3
Temperature	K	368.1	353.5	384.6
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	10.000	3.947	6.053
Mass flow	kg/h	865.298	308.761	556.537
Volume flow	L/min	18.129	6.309	11.921
Enthalpy	MMBtu/h	0.362	0.213	0.158
Mole flow	kmol/h			
Benzene		4.000	3.915	0.085
Toluene		6.000	0.032	5.968

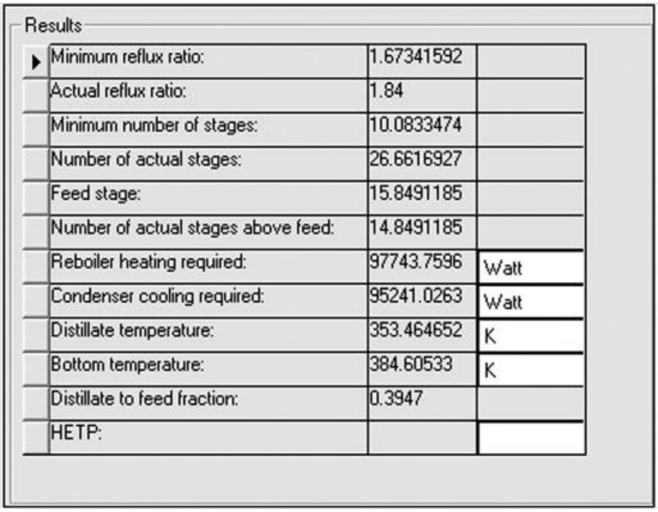
FIGURE 6.18
Process flow sheet for shortcut distillation.

reflux ratio is 1.67, actual reflux ratio is 1.84, minimum number of stages is 10, number of actual stages is 27, and feed stage is stage 16.

Aspen Rigorous Distillation Column

The rigorous distillation column in Aspen is *Radfrac* column in the model library. The following data obtained from the short cut column is used to provide the data required to the rigorous column:

- Fully specifying the feed stream (feed stream flow rate, composition and conditions)
- Number of stages: 28
- Condenser type: Total
- Distillate rate: 3.947
- Reflux rate: 2



Results

Minimum reflux ratio:	1.67341592	
Actual reflux ratio:	1.84	
Minimum number of stages:	10.0833474	
Number of actual stages:	26.6616927	
Feed stage:	15.8491185	
Number of actual stages above feed:	14.8491185	
Reboiler heating required:	97743.7596	Watt
Condenser cooling required:	95241.0263	Watt
Distillate temperature:	353.464652	K
Bottom temperature:	384.60533	K
Distillate to feed fraction:	0.3947	
HETP:		

FIGURE 6.19
Summary of shortcut distillation results.

- Stage of feed stream: 17
- Condenser pressure: 1 atm

Providing all required data and running the system, the material streams results should look like that in Figure 6.20.

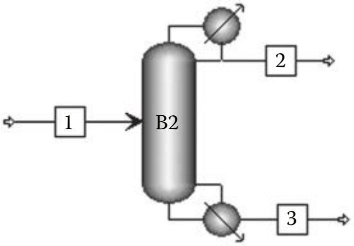
SUPERPRO SIMULATION

From toolbar, select *Unit Procedures*, then *Distillation* and then *Continuous (Shortcut)*. The shortcut distillation column is selected and added to the process flow sheet. Feed stream and two product streams are connected to the unit as shown in Figure 6.21. Feed stream is fully specified and in the operating conditions, relative volatiles of feed stream components and percentage in distillate are filled in as shown in Figure 6.22. The number of theoretical stages obtained with SuperPro designer is 28 and minimum reflux ratio is 1.748 (i.e., 1.923/1.1).

The data in top section of Figure 6.22 is a user supplied data. The relative vitalities should be calculated using Antoine equation or took from other softwares. Distillate stream composition is also needed, so pre material balance calculations are required. Reflux ratio to minimum reflux ratio (R/R_{min}), column pressure and feed quality (q) need to be provided. Vapor linear velocity and stage efficiency can be left as SuperPro default values.

Example 6.3: Multicomponent Distillation Column

In 2000 kmol/h of saturated liquid is feed to a distillation column at atmospheric pressure. The feed stream composition mole fractions are 0.056 *n*-propane, 0.321



Example 6.2c				
Stream ID		1	2	3
Temperature	K	369.0	353.5	384.6
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	10.000	3.947	6.053
Mass flow	kg/h	865.298	308.740	556.558
Volume flow	L/min	18.150	6.308	11.922
Enthalpy	MMBtu/h	0.364	0.213	0.158
Mole flow	kmol/h			
Benzene		4.000	3.917	0.083
Toluene		6.000	0.030	5.970

FIGURE 6.20
Rigorous column flow sheet and streams properties.

n-butane, 0.482 *n*-pentane, and 0.141 *n*-hexane. The mixture is to be separated in a distillation column. The column has a total condenser and a partial reboiler, the reflux ratio is 3.5, a fractional recovery of 99.4% of *n*-butane is desired in the distillate and 99.7% of *n*-pentane in the bottom stream. Calculate flow rate of distillate and bottom products using hand calculation, verify hand calculations with Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro designer.

SOLUTION

HAND CALCULATIONS

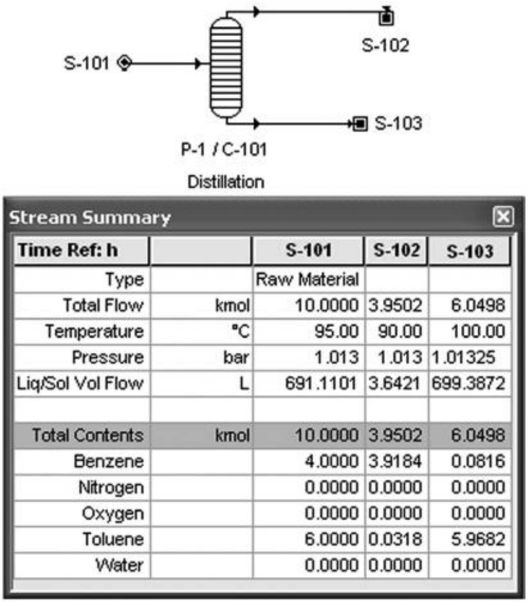
The *k*-values of the components in the feed stream (saturated liquid, 10.41°C) is calculated using Antoine equations and shown in Tables 6.1, 6.2, and 6.3 for feed stream, distillate, and bottom products, respectively.

The *k*-values of the components in distillate stream ($T_{bp} = -12°C$). The distillation *k*-values and relative volatilities are shown in Table 6.2.

The *k*-values of the components in the bottom stream ($T_{bp} = 41.6°C$) is shown in Table 6.3.

The order of the feed stream volatilities are:

Propane > *n*-butane > *n*-pentane > *n*-hexane



Time Ref: h		S-101	S-102	S-103
Type		Raw Material		
Total Flow	kmol	10.0000	3.9502	6.0498
Temperature	°C	95.00	90.00	100.00
Pressure	bar	1.013	1.013	1.01325
Liq/Sol Vol Flow	L	691.1101	3.6421	699.3872
Total Contents	kmol	10.0000	3.9502	6.0498
Benzene		4.0000	3.9184	0.0816
Nitrogen		0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000
Toluene		6.0000	0.0318	5.9682
Water		0.0000	0.0000	0.0000

FIGURE 6.21
Shortcut distillation process flow sheet and stream summary.

Since the fractional recovery of *n*-butane in the distillate is specified, it is the LK. Also, the fractional recovery of *n*-pentane in the bottom is specified, it is the HK. Accordingly, propane = LNK (light non key) and *n*-hexane = HNK (heavy non key). Thus we can assume that there is no propane in the bottom and there is no *n*-hexane in the distillate. From the giving information regarding fractional recovery, we can write the following equations:

Material Balance

The fractional recovery of *n*-butane in distillate:

$$0.994 = \frac{\text{moles } n\text{-butane in distillate}}{\text{moles } n\text{-butane in the feed}} = \frac{x_{c4.d} \times D}{z_{C4} \times F}$$

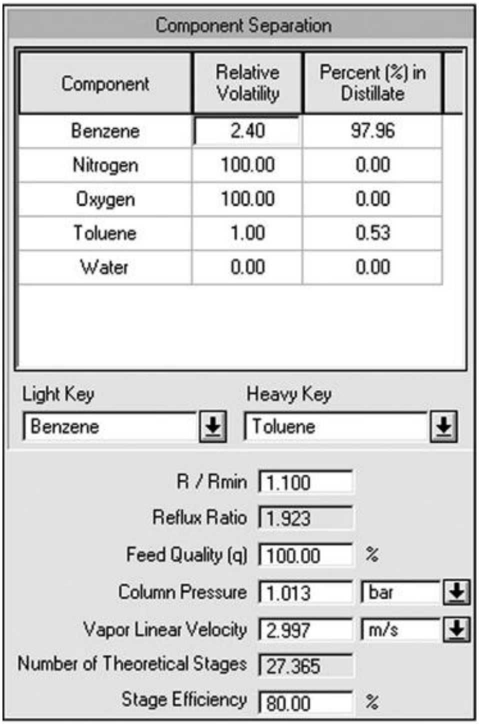
$$x_{C4,d}\, D = 0.994 \times F z_{C4}$$

$$x_{C4,b}\, B = (1 - 0.994) F z_{C4}$$

Fractional recovery of *n*-pentane in the bottom

$$0.997 = \frac{\text{moles } n\text{-pentane in bottom}}{\text{moles } n\text{-butane in the feed}} = \frac{x_{c5.b} \times B}{z_{C5} \times F}$$

$$x_{C5,b}\, B = 0.997 \times F z_{C5}$$


Component Separation

Component	Relative Volatility	Percent (%) in Distillate
Benzene	2.40	97.96
Nitrogen	100.00	0.00
Oxygen	100.00	0.00
Toluene	1.00	0.53
Water	0.00	0.00

Light Key: Benzene
Heavy Key: Toluene

R / Rmin: 1.100
Reflux Ratio: 1.923
Feed Quality (q): 100.00 %
Column Pressure: 1.013 bar
Vapor Linear Velocity: 2.997 m/s
Number of Theoretical Stages: 27.365
Stage Efficiency: 80.00 %

FIGURE 6.22
Shortcut distillation operating data.

$$x_{C5,d}\,D = (1 - 0.997)Fz_{C5}$$

Assuming all propane gone to distillate and no *n*-hexane exist in distillate:

$$x_{C3,d}D = Fz_{C3}$$

$$x_{C6,d}D = 0$$

Substitute values of known concentration and flow rates (Distillate).

TABLE 6.1
Feed Stream *k*-Value

Components	*k*-Values	Key Components	Relative Volatility
Propane	6.35	NLK	16.28
***n*-Butane**	**1.48**	**LK**	**3.8**
***n*-Pentane**	**0.39**	**HK**	**1**
n-Hexane	0.103	NHK	0.264

TABLE 6.2

Distillate Stream ***k***-Value

Components	*k*-Values	Key Components	Relative Volatility
Propane	3.18	NLK	23.21
***n*-Butane**	**0.63**	**LK**	**4.6**
***n*-Pentane**	**0.137**	**HK**	**1**
n-Hexane	0.031	NHK	0.226

$$x_{C3,d}\, D = 2000\ (0.056) = 112\ \text{kmol/h}$$

$$x_{C4,d}\, D = (0.994)\ (20{,}000)\ (0.321) = 638.5\ \text{kmol/h}$$

$$x_{C5,d}\, D = (1 - 0.994)\ (2000)\ (0.482) = 2.89\ \text{kmol/h}$$

$$x_{C6,d}\, D = 0\ \text{kmol/h}$$

The total distillate mass flow rate:

$$D = \sum(D\, x_{i,d}) = 112 + 638.5 + 2.90 = 753.4\ \text{kmol/h}$$

Repeating the same procedure for the bottom stream:

$$x_{C3,d}\, B = 0\ \text{kmol/h}$$

$$x_{C4,b}\, B = (1 - 0.994)\ (20{,}000)\ (0.321) = 3.85\ \text{kmol/h}$$

$$x_{C5,b}\, B = (0.997)\ (2000)\ (0.482) = 961.1\ \text{kmol/h}$$

$$x_{C6,bot}\, B = Fz_{C6} = 282\ \text{kmol/h}$$

The total molar flow rate of the bottom:

$$B = \sum(B\, x_{i,dist}) = 3.85 + 961.1 + 282 = 1247\ \text{kmol/h}$$

TABLE 6.3

Bottom Stream ***k***-Value

Components	*k*-Values	Key Components	Relative Volatility
Propane	13.88	NLK	11.81
***n*-Butane**	**3.83**	**LK**	**3.26**
***n*-Pentane**	**1.175**	**HK**	**1**
n-Hexane	0.382	NHK	0.325

Checking the mass balance:

$$D + B = 2000 \text{ OK},$$

Using Fenske equation to determine minimum number of trays, $N_{\min}$

$$N_{\min} = \frac{\ln((x_{LK}/x_{HK})_D(x_{HK}/x_{LK})_B)}{\ln(\bar{\alpha}_{LK/HK})}$$

$$\bar{\alpha}_{LK/HK} = \left(\alpha_{LK/HK,F} \times \alpha_{LK/HK,D} \times \alpha_{LK/HK,B}\right)^{1/3} = \left(3.8 \times 4.6 \times 3.26\right)^{1/3} = 2.514$$

$$N_{\min} = \frac{\ln\left(\left(0.8475/0.0038\right)_D \left(0.771/0.0031\right)_B\right)}{\ln(2.514)} = 8.106$$

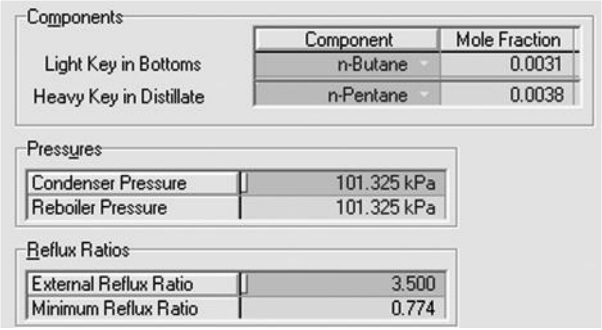
HYSYS/UNISIM SIMULATION

Two distillation methods are available in Hysys/Unisim:

- Shortcut distillation method
- Continuous distillation method

Shortcut Column

Selecting shortcut distillation method and connecting feed stream, two product streams and two energy streams. Peng–Robinson EOS is selected as the thermodynamic fluid package. The feed stream mole flow rate (2000 kmol/h) pressure (1 atm) and compositions were specified as given in the example, since the feed is saturated liquid, vapor/phase fraction in Hysys was set to zero. While in the *Design/Parameters* page, mole fraction of LK in bottom and HK in distillate were specified as shown in Figure 6.23.



Components

	Component	Mole Fraction
Light Key in Bottoms	n-Butane	0.0031
Heavy Key in Distillate	n-Pentane	0.0038

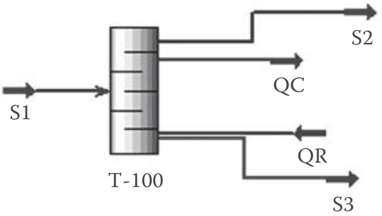
Pressures

Condenser Pressure	101.325 kPa
Reboiler Pressure	101.325 kPa

Reflux Ratios

External Reflux Ratio	3.500
Minimum Reflux Ratio	0.774

FIGURE 6.23
Shortcut distillation design parameters.



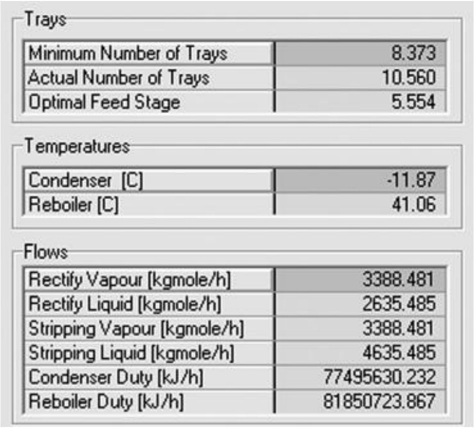
Streams				
		S1	S2	S3
Temperature	C	10	−12	41
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	2000	753.0	1247
Comp molar flow (propane)	kgmol/h	112.00	112.00	0.00
Comp molar flow (*n*-butane)	kgmol/h	642.00	638.13	3.87
Comp molar flow (*n*-pentane)	kgmol/h	964.00	2.86	961.14
Comp molar flow (*n*-hexane)	kgmol/h	282.00	0.00	282.00

FIGURE 6.24
Shortcut distillation process flow sheet and stream summary.

$$\text{The mole fraction of LK}(n-\text{butane})\text{ in bottom} = \frac{3.85}{1247} = 0.0031$$

$$\text{The mole fraction of HK}(n-\text{pentane})\text{ is distillate} = \frac{2.89}{753.4} = 0.0038$$

The process flow sheet and stream summary are shown in Figure 6.24. The performance of shortcut distillation method is shown in Figure 6.25.



Trays

Minimum Number of Trays	8.373
Actual Number of Trays	10.560
Optimal Feed Stage	5.554

Temperatures

Condenser [C]	-11.87
Reboiler [C]	41.06

Flows

Rectify Vapour [kgmole/h]	3388.481
Rectify Liquid [kgmole/h]	2635.485
Stripping Vapour [kgmole/h]	3388.481
Stripping Liquid [kgmole/h]	4635.485
Condenser Duty [kJ/h]	77495630.232
Reboiler Duty [kJ/h]	81850723.867

FIGURE 6.25
Performance of the shortcut distillation.

Hysys Rigorous Column

The data from shortcut distillation column is used as initial estimate to the rigorous distillation column. After connecting and specifying the feed stream, connecting top and bottom product streams and energy streams using total condenser, the following data are provided:

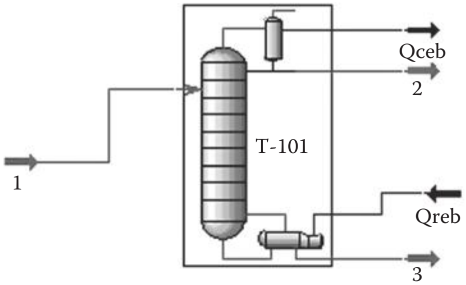
- Feed stream inlet stage: 6
- Total number of trays: 11
- Condenser and reboiler pressure: 1 atm
- Reflux ratio: 3.5
- Distillate liquid rate: 743 kmol/h

Providing all the above required data and running the system the results should look like that shown in Figure 6.26. In the *Monitor* page, the degree of freedom must be zero. The product streams conditions and molar flow rates are close to those obtained by the shortcut column and hand calculation.

PRO/II Simulation

Two distillation methods are available in PRO/II:

- Shortcut distillation method
- Continuous distillation method



Streams				
		1	2	3
Temperature	C	10.41	−11.89	41.13
Pressure	kPa	101.32	101.32	101.32
Molar flow	kgmol/h	2000	753.0	1247
Comp molar flow (propane)	kgmol/h	112.00	112.00	0.00
Comp molar flow (*n*-butane)	kgmol/h	642.00	639.30	2.70
Comp molar flow (*n*-pentane)	kgmol/h	964.00	1.70	962.30
Comp molar flow (*n*-hexane)	kgmol/h	282.00	0.00	282.00

FIGURE 6.26
Hysys rigorous column flow sheet and stream summary.

PRO/II Shortcut Simulation

Using the shortcut distillation method in PRO/II, Peng–Robinson was selected as the thermodynamic fluid package. *Perform minimum reflux calculations* should be selected so as to get the Underwood results summary. The following information is required: feed stream fully specified, the LK is *n*-butane, and the HK is *n*-pentane. The ratio of reflux ration to minimum reflux ratio is 3.98 (i.e., 3.5/0.87915).

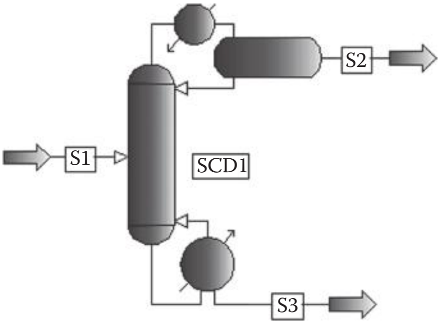
Providing above required data and running the system, the process flowsheet with stream summary is shown in Figure 6.27 and the Underwood summary is shown in Figure 6.28.

PRO/II Continuous Column

PRO/II *Distillation* column is used for continuous distillation. Peng–Robinson is employed as the thermodynamic fluid package.

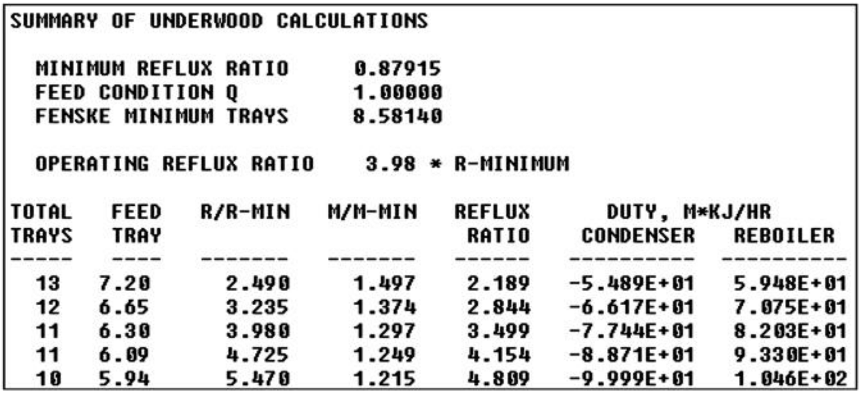
The following information is required to run the system:

- Feed stream is fully specified.
- Number of theoretical trays: 11
- Overall top tray pressure: 1 atm
- Pressure drop per tray: 0



Stream name		S1	S2	S3
Stream description				
Phase		Liquid	Liquid	Liquid
Temperature	K	281.5491	260.9497	314.1151
Pressure	kPa	101.3200	101.3200	101.3200
Enthalpy	M*kJ/h	3.4158	–0.8843	8.8855
Molecular weight		68.0544	56.0894	75.2822
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	2000.000	753.179	1246.821
Fluid rates	kgmol/h			
Propane		112.0000	112.0000	0.0000
n-butane		642.0001	638.3927	3.6074
Pentane		964.0001	2.7859	961.2139
Hexane		282.0000	0.0000	281.9999

FIGURE 6.27
Shortcut distillation process flow sheet and stream summary.



```
SUMMARY OF UNDERWOOD CALCULATIONS

  MINIMUM REFLUX RATIO      0.87915
  FEED CONDITION Q          1.00000
  FENSKE MINIMUM TRAYS      8.58140

  OPERATING REFLUX RATIO     3.98 * R-MINIMUM

TOTAL   FEED   R/R-MIN   M/M-MIN   REFLUX     DUTY, M*KJ/HR
TRAYS   TRAY                        RATIO   CONDENSER   REBOILER
-----   ----   -------   -------   ------   ----------  ----------
  13    7.20     2.490     1.497    2.189   -5.489E+01   5.948E+01
  12    6.65     3.235     1.374    2.844   -6.617E+01   7.075E+01
  11    6.30     3.980     1.297    3.499   -7.744E+01   8.203E+01
  11    6.09     4.725     1.249    4.154   -8.871E+01   9.330E+01
  10    5.94     5.470     1.215    4.809   -9.999E+01   1.046E+02
```

FIGURE 6.28
Summary of Underwood calculations.

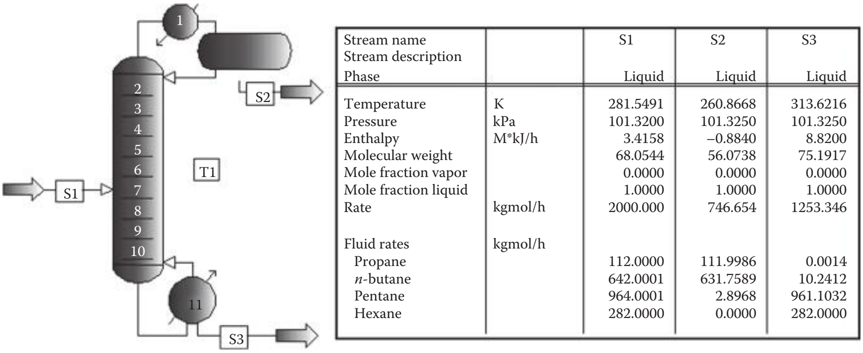
- Feed tray: 7
- Distillate (Stream S2) molar flow rate is 750 kmol/h. The molar flow rate of stream S2 is not used as specification but as initial guess.
- Reflux ratio is 3.5
- Mole fraction of *n*-propane in distillate is 0.15

Once all required information is completed, running the system should lead to the results shown in Figure 6.29. The rigorous column streams molar flow rates and conditions are similar to that obtained in the shortcut column.

Aspen Plus Simulation

Two distillation methods are considered:

- Shortcut distillation method
- Continuous distillation method



Stream name Stream description Phase		S1 Liquid	S2 Liquid	S3 Liquid
Temperature	K	281.5491	260.8668	313.6216
Pressure	kPa	101.3200	101.3250	101.3250
Enthalpy	M*kJ/h	3.4158	–0.8840	8.8200
Molecular weight		68.0544	56.0738	75.1917
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	2000.000	746.654	1253.346
Fluid rates	kgmol/h			
Propane		112.0000	111.9986	0.0014
n-butane		642.0001	631.7589	10.2412
Pentane		964.0001	2.8968	961.1032
Hexane		282.0000	0.0000	282.0000

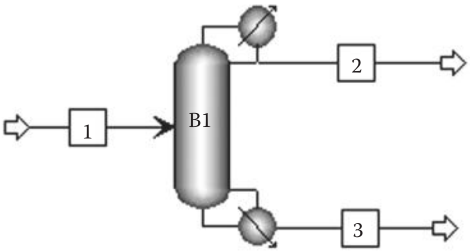
FIGURE 6.29
PRO/II results of continuous distillation column.

Shortcut Column Method

The process flowsheet and stream summary results using Aspen shortcut (DSTWU) distillation method is shown in Figure 6.30. The following data is provided to the shortcut distillation method in Aspen plus:

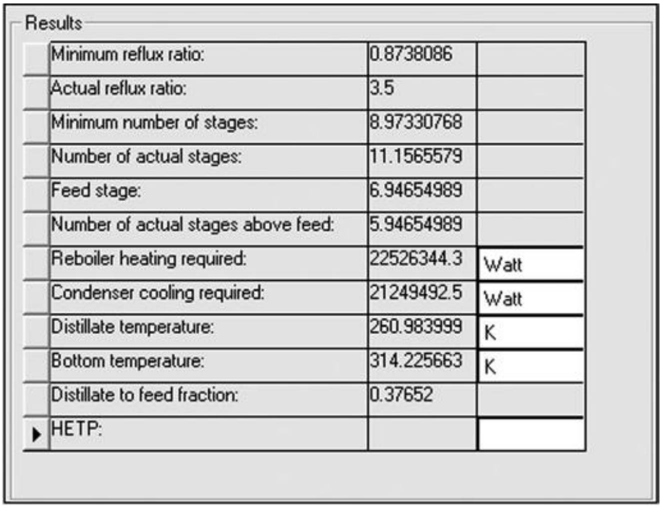
- Reflux ratio: 3.5
- LK: *n*-butane, fraction recovery in distillate: 0.994
- HK: *n*-pentane, fractional recovery in distillate: 0.003
- Condenser (total) and reboiler pressure: 1 atm

The column performance summary obtained using Aspen Plus short cut column is shown in Figure 6.31. The minimum reflux ratio is 0.873, actual reflux ratio is 3.5, minimum number of stage is 9, number of actual stages is 12, and feed stage is stage number 7. The result is within the range of those obtained with hand calculations, Hysys and PRO/II.



Example 6.3				
Stream ID		1	2	3
Temperature	K	281.6	261.0	314.2
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	2000.000	753.040	1246.960
Mass flow	kg/h	136108.863	42238.800	93870.063
Volume flow	L/min	3620.409	1159.523	2542.077
Enthalpy	MMBtu/h	−318.523	−105.925	−208.242
Mole flow	kmol/h			
Propa-01		112.000	112.000	Trace
n-but-01		642.000	638.148	3.852
n-pen-01		964.000	2.892	961.108
n-hex-01		282.000		282.000

FIGURE 6.30
Shortcut distillation process flow sheet and stream summary.



Results

Minimum reflux ratio:	0.8738086	
Actual reflux ratio:	3.5	
Minimum number of stages:	8.97330768	
Number of actual stages:	11.1565579	
Feed stage:	6.94654989	
Number of actual stages above feed:	5.94654989	
Reboiler heating required:	22526344.3	Watt
Condenser cooling required:	21249492.5	Watt
Distillate temperature:	260.983999	K
Bottom temperature:	314.225663	K
Distillate to feed fraction:	0.37652	
HETP:		

FIGURE 6.31
Summary of shortcut distillation method.

Rigorous Distillation Method

The rigorous column in Aspen is *RadFrac* under column tab in the model library. After building the process flowsheet the following data are provided:

- Number of trays: 11
- Condenser: Total
- Distillate rate: 753 kmol/h
- Reflux ratio: 3.5
- Feed stream: stage 6
- Top stage condenser pressure: 1 atm

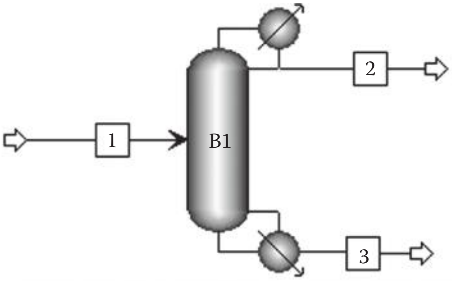
Running the system leads to the results shown in Figure 6.32.

SUPERPRO SIMULATION

The shortcut distillation column is used and added to the process flow sheet; from *Unit Procedures* in the toolbar, then *Distillation* and then *Continuous (Shortcut)*. Feed stream and two product streams are connected to the unit as shown in Figure 6.33. Feed stream is specified and in the operating conditions, relative volatiles of feed stream components and percentage in distillate are filled in as shown in Figure 6.34. The number of theoretical stages obtained with SuperPro (10.224) and minimum reflux 0.767 (i.e., 3.5/4.565).

Example 6.4: Multicomponent Separation

A mixture with 33% *n*-hexane, 37% *n*-heptane, and 30% *n*-octane is to be separated in a distillation column. The feed stream is 60% vapor (temperature is 105°C).



Example 6.3c				
Stream ID		1	2	3
Temperature	K	281.6	261.0	314.1
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	2000.000	753.000	1247.000
Mass flow	kg/h	136108.861	42265.572	93843.288
Volume flow	L/min	3620.409	1160.057	2540.989
Enthalpy	MMBtu/h	−318.523	−105.967	−208.227
Mole flow	kmol/h			
Propane		112.000	112.000	<0.001
n-butane		642.000	636.034	5.966
n-pen-01		964.000	4.966	959.034
n-hex-01		282.000	<0.001	282.000

FIGURE 6.32
Rigorous column PFD and stream table.

The distillate product should contain 0.01 mole fraction *n*-heptane and a bottom product with 0.01 mole fraction *n*-hexane. The column will operate at 1.2 atm. The feed molar flow rate is 100 mol/h.

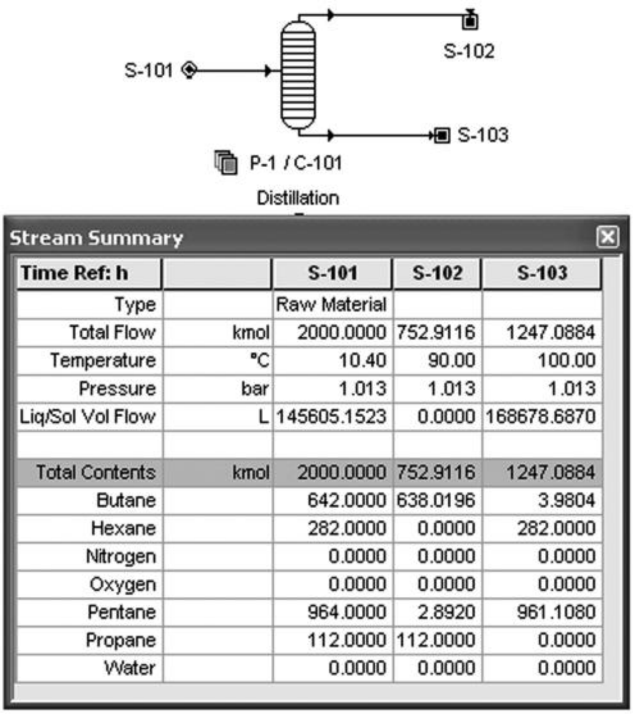
a. Calculate the complete product composition and minimum number of ideal palates at infinite reflux.
b. Estimate the number of ideal plates required for the separation if the reflux ratio is 1.5 R_{min}.
c. Find the optimum feed tray [5].

SOLUTION

HAND CALCULATIONS

The vapor pressure is estimated using Antoine coefficients:

$$\log(P) = \frac{A - B}{(T + C)}$$



Time Ref: h		S-101	S-102	S-103
Type		Raw Material		
Total Flow	kmol	2000.0000	752.9116	1247.0884
Temperature	°C	10.40	90.00	100.00
Pressure	bar	1.013	1.013	1.013
Liq/Sol Vol Flow	L	145605.1523	0.0000	168678.6870
Total Contents	kmol	2000.0000	752.9116	1247.0884
Butane		642.0000	638.0196	3.9804
Hexane		282.0000	0.0000	282.0000
Nitrogen		0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000
Pentane		964.0000	2.8920	961.1080
Propane		112.0000	112.0000	0.0000
Water		0.0000	0.0000	0.0000

FIGURE 6.33
Shortcut distillation process flow sheet and stream summary.

where P is in mmHg and T is in degree Celsius. The parameters of the Antoine equations for the feed stream components are shown in Figure 6.4 (Table 6.4).

For the feed temperature at 105°C, the vapor pressure of pure hexane,

$$\log(P) = \frac{A - B}{(T + C)} = \frac{6.87024 - 1168.72}{(224.210 + 105)}$$

The vapor pressure in atm is $P_i = 2.75$ atm

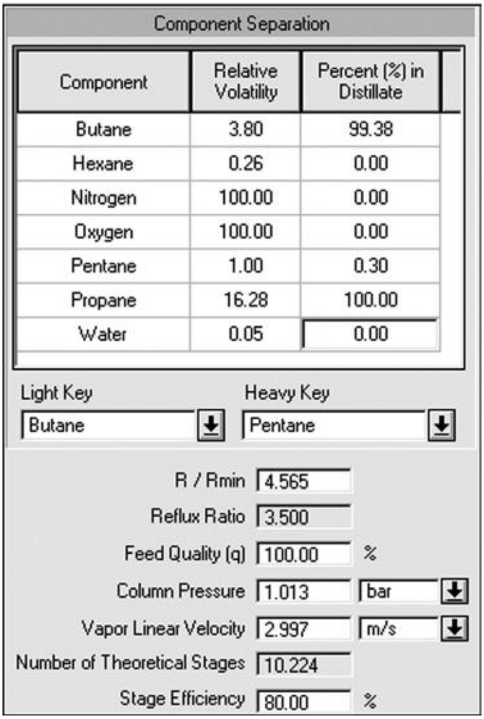
$$K_i = \frac{P_i}{P_{\text{tot}}}$$

Using simple material balance to determine top and bottom product stream components:

The boiling point of the bottom product is 115°C

The boiling point of the distillate is 75°C

The k-values values of feed, distillate and bottom stream are shown in Table 6.5.



Component Separation

Component	Relative Volatility	Percent (%) in Distillate
Butane	3.80	99.38
Hexane	0.26	0.00
Nitrogen	100.00	0.00
Oxygen	100.00	0.00
Pentane	1.00	0.30
Propane	16.28	100.00
Water	0.05	0.00

Light Key: Butane

Heavy Key: Pentane

R / Rmin: 4.565

Reflux Ratio: 3.500

Feed Quality (q): 100.00 %

Column Pressure: 1.013 bar

Vapor Linear Velocity: 2.997 m/s

Number of Theoretical Stages: 10.224

Stage Efficiency: 80.00 %

FIGURE 6.34
Operating conditions.

TABLE 6.4

Parameters Used in Antoine Equations

Formulae	**Component**	***A***	***B***	***C***
C_6H_{14}	Hexane	6.87024	1168.720	224.210
C_7H_{16}	Heptane	6.89385	1264.370	216.636
C_8H_{18}	Octane	6.90940	1349.820	209.385

TABLE 6.5

k-Values of Feed, Distillate, and Bottom Streams (1.2 atm)

Components		**Feed**		**Distillate**			**Bottom**		
Key		**(mol/h)**	***K* 105°C**	**(mol/h)**	***X***	***K* 75°C**	**(mol/h)**	***X***	***K* 115°C**
LK	*n*-Hexane	33	2.31	32.32	0.99	1.0	0.68	0.010	2.92
HK	*n*-Heptane	37	1.01	0.33	0.01	0.396	36.67	0.544	1.33
HNK	*n*-Octane	30	0.45	0	0	0.156	30	0.446	0.61

a. Using Fenske equation to determine minimum number of trays, $N_{\min}$

$$N_{\min} = \frac{\ln((x_{LK}/x_{HK})_D(x_{HK}/x_{LK})_B)}{\ln(\bar{\alpha}_{LK/HK})}$$

$$\bar{\alpha}_{LK/HK} = \left(\alpha_{Fij} \times \alpha_{Dij} \times \alpha_{Bij}\right)^{1/3} = \left(2.29 \times 2.52 \times 2.2\right)^{1/3} = 2.3$$

Substituting wanted values in Fenske equation:

$$N_{\min} = \frac{\ln\left((0.99/0.01)_D\,(0.544/0.01)_B\right)}{\ln(2.3)} = 9.5$$

b. The inlet feed stream liquid fraction, q
   Since 60% of the feed is vapor, and q is the liquid fraction hence, $q = 0.4$, also it can be calculated as

$$q = \frac{H_V - H_F}{H_V - H_L} = \frac{-1.72 \times 10^5 - (-1.861 \times 10^5)}{-1.72 \times 10^5 - (-2.065 \times 10^5)} = 0.4$$

$$1 - 0.4 = \sum_{i=1}^{n} \frac{\left(\alpha_i\, x_i\right)_F}{\alpha_i - \varphi} = 1 - 1 = \sum_{i=1}^{n} \frac{\left(\alpha_i\, x_i\right)_F}{\alpha_i - \varphi}$$

$$0.6 = \sum \frac{\alpha_i\, x_{Fi}}{\alpha_i - \varphi} = \frac{2.28 \times 0.33}{2.28 - \varphi} + \frac{1 \times 0.37}{1 - \varphi} + \frac{0.45 \times 0.30}{0.45 - \varphi}$$

$$0.6 = \frac{0.75}{2.27 - \varphi} + \frac{0.37}{1 - \varphi} + \frac{0.134}{0.446 - \varphi}$$

Solving for φ, there may be more than one value, select the one between the light and HK relative volatility.
By trial and error $\varphi = 1.68$

$$R_{\min} + 1 = \sum \frac{\left(\alpha_i\, x_i\right)_D}{\alpha_i - \varphi} = \frac{(2.525)(0.99)}{2.525 - 1.68} + \frac{(1)(0.01)}{1 - 1.68}$$

$$R_{\min} + 1 = 2.94$$

$$R_{\min} = 1.94$$

$$R = 1.5R_{\min} = 1.5 \times 1.94 = 2.92$$

The ideal number of plates, N

$$\frac{N - N_{\min}}{N + 1} = 0.75\left(1 - \left(\frac{R - R_{\min}}{R + 1}\right)^{0.5668}\right)$$

$$\frac{N - 9.5}{N + 1} = 0.75\left(1 - \left(\frac{2.92 - 1.94}{2.92 + 1}\right)^{0.5668}\right)$$

$$\frac{N - 9.5}{N + 1} = 0.41$$

$$N = 16.8$$

The actual number of trays is 17 trays.

c. Using Kirkbride method to calculate optimum feed tray:

$$\ln\left(\frac{N_D}{N_B}\right) = 0.206\ln\left(\left(\frac{x_{HK}}{x_{LK}}\right)_F \left(\frac{x_{LK,\text{in}B}}{x_{HK,\text{in}D}}\right)^2 \left(\frac{B}{D}\right)\right)$$

Substituting required values:

$$\ln\left(\frac{N_D}{N_B}\right) = 0.206\ln\left(\left(\frac{0.37}{0.33}\right)_F \left(\frac{0.01}{0.01}\right)^2 \left(\frac{67.35}{32.65}\right)\right)$$

The ratio of rectifying (N_D) to stripping number of trays (N_B) is

$$\frac{N_D}{N_B} = 1.2$$

$$N = 16.8 = N_D + N_B$$

Substituting values and rearranging:

$$16.8 = N_D + N_B = 1.2N_B + N_B$$

$$N_B = 7.6, \quad N_D = 9.2$$

The number of trays above the feed tray is 9 and that below the feed tray is 8 trays, the feed tray is tray number 10.

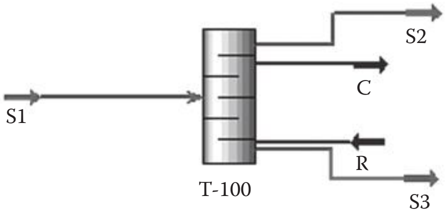
HYSYS SIMULATION

The process flow sheet is performed using shortcut distillation and utilizing Antoine package for thermodynamic properties calculations.

- LK in bottom: *n*-hexane, mole fraction is 0.01
- HK in distillate: *n*-heptane, mole fraction is 0.01
- The process flowsheet and stream summary is shown in Figure 6.35

External reflux ratio is 3.972 = 1.5 × R_{min}, and the value of minimum reflux ratio found by Hysys was found to be 2.648 (the value can be seen in the *Design/Parameters* page).

From the performance page the minimum number of trays is 10, the actual number of trays is 18 and the optimum feed tray is tray number 10 (Figure 6.36).



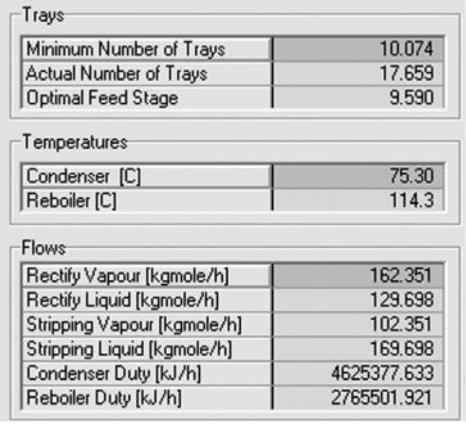
Streams				
		S1	S2	S3
Temperature	C	105.3	75.30	114.3
Pressure	kPa	121.6	121.6	121.6
Molar flow	kgmol/h	100.0	32.65	67.35
Comp mole frac (*n*-hexane)		0.33	0.99	0.01
Comp mole frac (*n*-heptane)		0.37	0.01	0.54
Comp mole frac (*n*-octane)		0.30	0.00	0.45

FIGURE 6.35
Process flow sheet and stream summary.

HYSYS RIGOROUS DISTILLATION COLUMN

The following data were obtained from the Hysys shortcut column and fed to the Hysys rigorous distillation column:

- Feed stream is fully specified by providing feed stream flow low rate, composition and feed conditions (i.e., temperature and pressure or vapor/phase ratio with either temperature or pressure).



Trays

Minimum Number of Trays	10.074
Actual Number of Trays	17.659
Optimal Feed Stage	9.590

Temperatures

Condenser [C]	75.30
Reboiler [C]	114.3

Flows

Rectify Vapour [kgmole/h]	162.351
Rectify Liquid [kgmole/h]	129.698
Stripping Vapour [kgmole/h]	102.351
Stripping Liquid [kgmole/h]	169.698
Condenser Duty [kJ/h]	4625377.633
Reboiler Duty [kJ/h]	2765501.921

FIGURE 6.36
Performance page of shortcut distillation.

- Feed stream inlet stage: 10
- Total number of trays: 18
- Condenser and reboiler pressure: 121.6 kPa
- Reflux ratio: 3.972
- Distillate liquid rate: 32.65 kmol/h

Providing all the above required data and running the system the results should look like that shown in Figure 6.37. The product streams molar flow rate is close to that obtained by Hysys shortcut method.

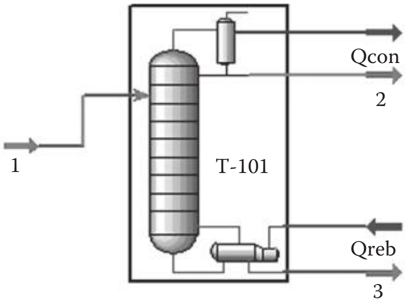
SIMULATION WITH PRO/II

The following two methods are considered in the design of distillation column:

- Shortcut method
- Rigorous distillation method are considered

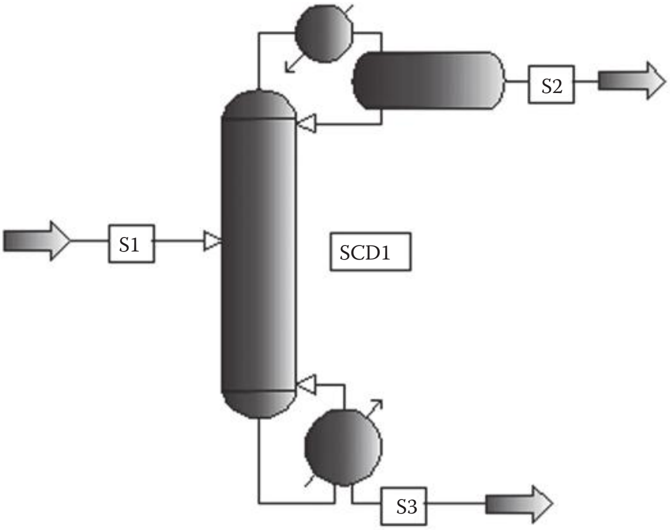
PRO/II Shortcut Column

Using PRO/II shortcut column, the process flow sheet is shown in Figure 6.38. After building the process flowsheet, the specifications page is shown in Figure 6.39. The mole fraction of LK (*n*-hexane) in bottom (S3) is 0.01. The mole fraction of HK (*n*-heptane) in distillate (S2) is 0.01.



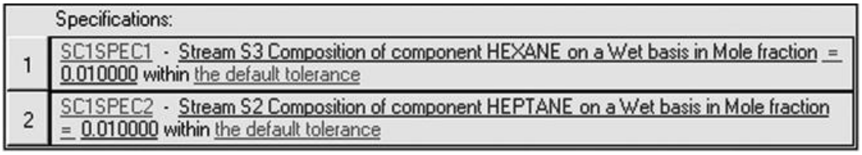
Streams				
		1	2	3
Temperature	C	105.3	75.22	114.4
Pressure	kPa	121.6	121.6	121.6
Molar flow	kgmol/h	100.0	32.65	67.35
Comp mole frac (*n*-hexane)		0.33	0.99	0.01
Comp mole frac (*n*-heptane)		0.37	0.01	0.55
Comp mole frac (*n*-octane)		0.30	0.00	0.45

FIGURE 6.37
PFD and stream table of Hysys continuous distillation column.



Stream name Stream description Phase		S1 Mixed	S2 Liquid	S3 Liquid
Temperature	K	378.7883	348.2527	387.6156
Pressure	kPa	121.6000	121.6000	121.6000
Enthalpy	M*kJ/h	4.3639	0.4908	1.9484
Molecular weight		99.7832	86.3175	106.3121
Mole fraction vapor		0.6118	0.0000	0.0000
Mole fraction liquid		0.3882	1.0000	1.0000
Rate	kgmol/h	100.000	32.653	67.347
Fluid rates	kgmol/h			
Hexane		33.0000	32.3266	0.6735
Heptane		37.0000	0.3265	36.6735
Octane		30.0000	0.0001	29.9999

FIGURE 6.38
Shortcut distillation process flow sheet and stream summary.



Specifications:

1 SC1SPEC1 - Stream S3 Composition of component HEXANE on a Wet basis in Mole fraction = 0.010000 within the default tolerance

2 SC1SPEC2 - Stream S2 Composition of component HEPTANE on a Wet basis in Mole fraction = 0.010000 within the default tolerance

FIGURE 6.39
Specifications page.

The summary of Underwood calculations shows the minimum reflux ratio is 2.74, feed conditions; $q = 0.388$, minimum number of trays is 12 and total number of trays is 19 based on ratio of total reflux to minimum reflux ratio ($R/R_{\min} = 1.5$). The result is shown in Figure 6.40.

PRO/II Rigorous Distillation Column

PRO/II *Distillation* column is used for continuous distillation, the Peng–Robinson EOS is engaged for the property estimation. The following values obtained from the shortcut column are filled in the PRO/II *Distillation* column:

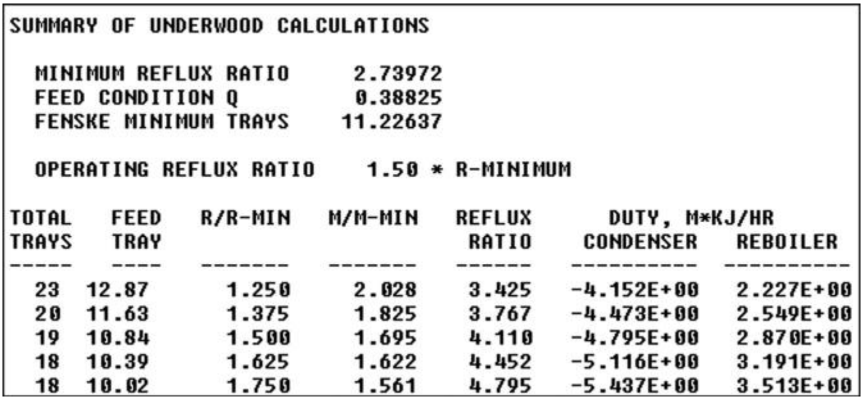
- Feed stream is fully specified by providing flow rate, composition, pressure and liquid fraction (i.e., $q = 0.4$).
- Number of theoretical trays: 19
- Overall top tray pressure: 121.6 kPa
- Pressure drop per tray: 0
- Feed tray: 11
- Distillate (Stream S2) molar flow rate is 32.65 kmol/h. The molar flow rate of stream S2 is not used as specification but as initial guess.
- Reflux ratio is 4.11 (i.e., 1.5 $R_{\min}$).
- Mole fraction of *n*-propane in distillate is 0.989.

Once all required information is completed, running the system should lead to the results shown in Figure 6.41.

ASPEN PLUS SIMULATIONS

Two methods available in Aspen are considered:

- Shortcut method
- Rigorous distillation column



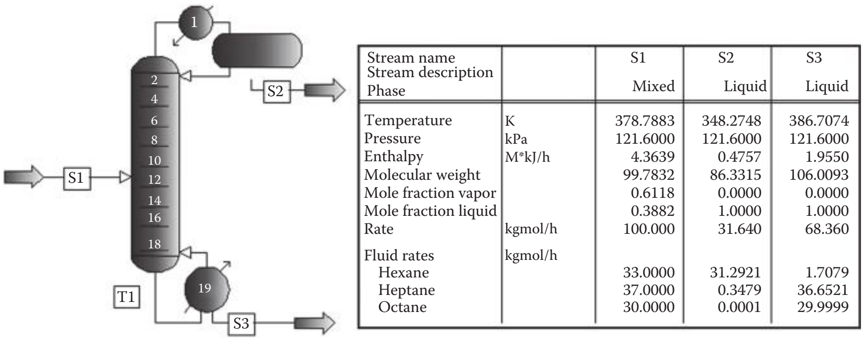
```
SUMMARY OF UNDERWOOD CALCULATIONS

  MINIMUM REFLUX RATIO      2.73972
  FEED CONDITION Q          0.38825
  FENSKE MINIMUM TRAYS     11.22637

  OPERATING REFLUX RATIO     1.50 * R-MINIMUM

TOTAL   FEED    R/R-MIN    M/M-MIN    REFLUX      DUTY, M*KJ/HR
TRAYS   TRAY                           RATIO    CONDENSER   REBOILER
-----   ----    -------    -------    ------   ----------  ----------
  23  12.87       1.250      2.028     3.425   -4.152E+00   2.227E+00
  20  11.63       1.375      1.825     3.767   -4.473E+00   2.549E+00
  19  10.84       1.500      1.695     4.110   -4.795E+00   2.870E+00
  18  10.39       1.625      1.622     4.452   -5.116E+00   3.191E+00
  18  10.02       1.750      1.561     4.795   -5.437E+00   3.513E+00
```

FIGURE 6.40
Summary of Underwood calculations.



Stream name Stream description Phase		S1 Mixed	S2 Liquid	S3 Liquid
Temperature	K	378.7883	348.2748	386.7074
Pressure	kPa	121.6000	121.6000	121.6000
Enthalpy	M*kJ/h	4.3639	0.4757	1.9550
Molecular weight		99.7832	86.3315	106.0093
Mole fraction vapor		0.6118	0.0000	0.0000
Mole fraction liquid		0.3882	1.0000	1.0000
Rate	kgmol/h	100.000	31.640	68.360
Fluid rates	kgmol/h			
Hexane		33.0000	31.2921	1.7079
Heptane		37.0000	0.3479	36.6521
Octane		30.0000	0.0001	29.9999

FIGURE 6.41
Distillation process flow sheet and stream summary.

Aspen Shortcut Simulations

The first step in the flow sheet simulation is to define process flow sheet connectivity by placing unit operations (blocks) and their connected streams. To define a process flow sheet block, select a model from the Model Library (Column and then DSTWU) and insert it in the workspace. To define a process stream, select Streams from the Model Library and click to establish each end of the steam connection on the available inlet and outlet locations of the existing blocks. Building process flow sheet using shortcut distillation form the model library, for fluid package, Peng–Robinson EOS is used. Date needed for simulation.

Reflux ratio is 3.972. Recovery of LK (*n*-hexane) in distillate is 0.98 (molar flow rate of *n*-hexane in distillate/molar flow rate of *n*-hexane in feed stream) and for HK (*n*-heptane) in distillate is 0.0088 (molar flow rate of *n*-heptane in distillate to molar flow rate of *n*-heptane in feed stream).

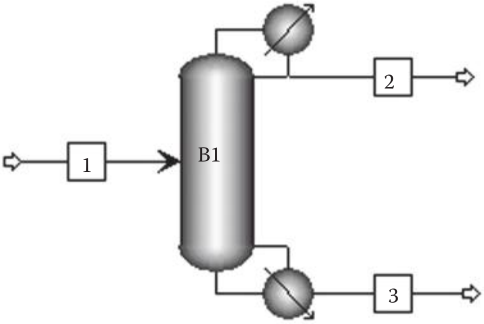
Condenser and reboiler pressure is 121.59. Filling in all required data, the simulation is ready, running the system leads to results shown in Figure 6.42. The unit specifications such as minimum reflux ratio are 2.72, actual reflux ratio is 3.972, minimum number of stages is 11, number of actual stages is 18 and optimum feed stage is stage 11. Results are shown in Figure 6.43.

Aspen Rigorous Simulations

The rigorous column in Aspen is *RadFrac* from the model library. After building the process flow sheet the following data are provided:

- Number of trays: 18
- Condenser: Total
- Distillate rate: 32.65 kmol/h
- Reflux ratio: 3.972
- Feed stream: stage 10
- Top stage condenser pressure: 121.6 kPa

Running the system leads to the results shown in Figure 6.44. The streams molar flow rate and conditions are similar to those obtained by Aspen shortcut method.



Example 6.4				
Stream ID		1	2	3
Temperature	K	378.7	348.2	387.7
Pressure	atm	1.20	1.20	1.20
Vapor frac		0.600	0.000	0.000
Mole flow	kmol/h	100.000	32.666	67.334
Mass flow	kg/h	9978.323	2819.605	7158.718
Volume flow	L/min	24754.524	75.838	195.276
Enthalpy	MMBtu/h	−17.621	−5.838	−13.569
Mole flow	kmol/h			
n-hexane		33.000	32.340	0.660
n-hep-01		37.000	0.326	36.674
n-oct-01		30.000	<0.001	30.000

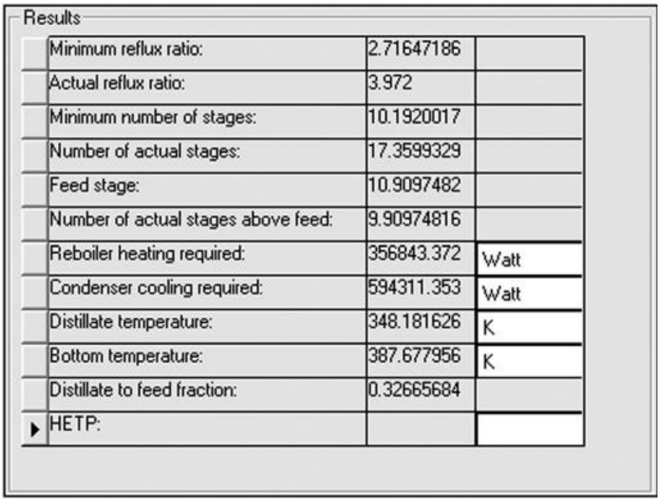
FIGURE 6.42
Process flow sheet and stream summary.

SuperPro Designer Simulations

The shortcut distillation column is used and added to the process flow sheet done in the previous examples. Feed stream and two product streams are connected to the unit as shown in Figure 6.45. Feed stream is specified and in the operating conditions, relative volatiles of feed stream components and percentage in distillate are filled in as shown in Figure 6.46. The number of theoretical stages obtained with SuperPro (20) and minimum reflux 1.588 (i.e., 2.382/1.5).

Example 6.5: Multicomponent Separation

A mixture of 100 kmol/h saturated liquid contains 30 mol% benzene, 25% toluene, and 45% ethyl benzene is to be separated by distillation column at atmospheric



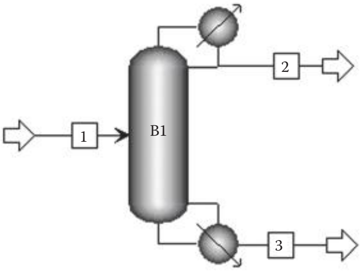
Results

Minimum reflux ratio:	2.71647186	
Actual reflux ratio:	3.972	
Minimum number of stages:	10.1920017	
Number of actual stages:	17.3599329	
Feed stage:	10.9097482	
Number of actual stages above feed:	9.90974816	
Reboiler heating required:	356843.372	Watt
Condenser cooling required:	594311.353	Watt
Distillate temperature:	348.181626	K
Bottom temperature:	387.677956	K
Distillate to feed fraction:	0.32665684	
HETP:		

FIGURE 6.43
Summary of shortcut results.

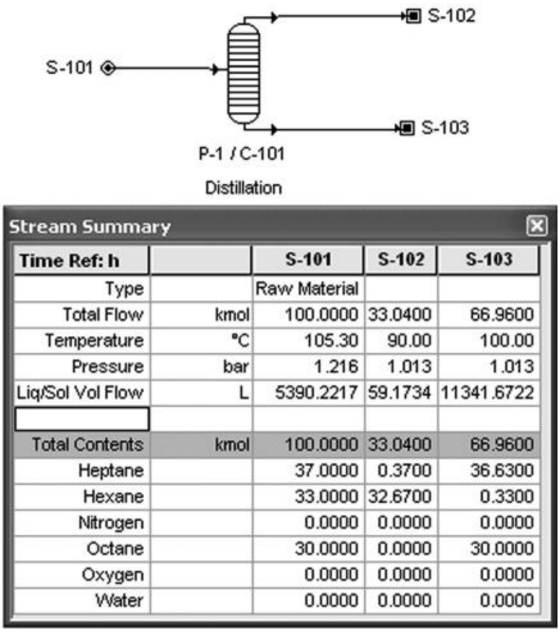
pressure, with 98% of the benzene and only 1% of the toluene is to be recovered in the distillate stream. The reflux ratio is 2. Calculate:

a. The minimum number of ideal plates
b. The approximate composition ×of the product
c. The actual number of trays
d. The minimum number of trays, if the distillation were carried out at 0.2 atm



Example 6.4c				
Stream ID		1	2	3
Temperature	K	378.7	348.6	387.2
Pressure	atm	1.20	1.20	1.20
Vapor frac		0.600	0.000	0.000
Mole flow	kmol/h	100.000	32.650	67.350
Mass flow	kg/h	9978.323	2826.883	7151.440
Volume flow	L/min	24754.524	76.038	194.983
Enthalpy	MMBtu/h	−17.621	−5.847	−13.567
Mole flow	kmol/h			
n-hexane		33.000	31.710	1.290
n-hep-01		37.000	0.939	36.061
n-oct-01		30.000	0.001	29.999

FIGURE 6.44
Aspen distillation flow sheet and stream table properties.



Time Ref: h		S-101	S-102	S-103
Type		Raw Material		
Total Flow	kmol	100.0000	33.0400	66.9600
Temperature	°C	105.30	90.00	100.00
Pressure	bar	1.216	1.013	1.013
Liq/Sol Vol Flow	L	5390.2217	59.1734	11341.6722
Total Contents	kmol	100.0000	33.0400	66.9600
Heptane		37.0000	0.3700	36.6300
Hexane		33.0000	32.6700	0.3300
Nitrogen		0.0000	0.0000	0.0000
Octane		30.0000	0.0000	30.0000
Oxygen		0.0000	0.0000	0.0000
Water		0.0000	0.0000	0.0000

FIGURE 6.45
Process flow sheet and stream summary.

SOLUTION

HAND CALCULATIONS

Table 6.6 shows the relative volatilities of components at feed conditions obtained using Antoine equation.

MATERIAL BALANCE

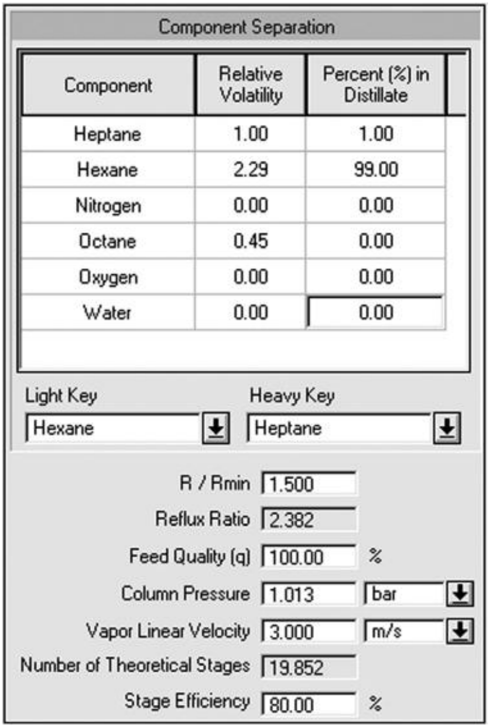
The following data are available:

- The molar flow rate of benzene in distillate is 0.98 × 30 = 29.4 mol/h.
- Molar flow rate of benzene in bottom: 30 – 29.4 = 0.6 mol/h.
- Molar flow rate of toluene in distillate: 0.01(25) = 0.25 mol/h.
- Molar flow rate of toluene in bottom: 25 – 0.25 = 24.75 mol/h.

At a first approximation all ethyl benzene goes to the bottom.

a. The minimum number of plates is obtained from the Fenske equation using the relative volatility of the LK to the HK, which is the ratio of the K factors (Tables 6.7 and 6.8).

$$N_{\min} = \frac{\ln\left((0.9916/0.0084)_D\,(0.3518/0.0085)_B\right)}{\ln(2.44)} = 9.52$$



Component Separation

Component	Relative Volatility	Percent (%) in Distillate
Heptane	1.00	1.00
Hexane	2.29	99.00
Nitrogen	0.00	0.00
Octane	0.45	0.00
Oxygen	0.00	0.00
Water	0.00	0.00

Light Key: Hexane

Heavy Key: Heptane

R / Rmin: 1.500

Reflux Ratio: 2.382

Feed Quality (q): 100.00 %

Column Pressure: 1.013 bar

Vapor Linear Velocity: 3.000 m/s

Number of Theoretical Stages: 19.852

Stage Efficiency: 80.00 %

FIGURE 6.46
Operating conditions.

The number of ideal plates including the partial reboiler is 9.52. A more accurate estimate of $N_{\min}$ can be obtained using a mean relative volatility based on values of top, feed and bottom of the column.

$$\bar{\alpha}_{LK/HK} = \left[(\alpha_{\mathrm{LK/HK}})_F (\alpha_{\mathrm{LK/HK}})_D (\alpha_{\mathrm{LK/HK}})_B\right]^{1/3} = \left[2.44 \times 2.42 \times 2.18\right]^{1/3} = 2.34$$

$$N_{\min} = \frac{\ln\left((0.9916/0.0084)_D (0.3518/0.0085)_B\right)}{\ln(2.34)} = 10.0$$

TABLE 6.6

Relative Volatilities of Feed Components

Key	Component	Feed Composition	Vapor Pressure (atm)	Relative Volatility (α)
LK	Benzene	0.3	2.37	2.44
HK	Toluene	0.25	0.97	1
	Ethyl benzene	0.45	0.47	0.49

TABLE 6.7

Composition and ***k***-Values of Distillate and Bottom Streams

Component	Feed (mol/h)	Distillate (mol/h)	Bottom (mol/h)	x_D	K	x_B	K
Benzene	30	29.4	0.6	0.9916	1.005	0.0085	3.125
Toluene	25	0.25	24.75	0.0084	0.4146	0.3518	1.437
Ethyl benzene	45	0	45	0		0.639	0.7312

Apply Fenske equation to benzene–ethyl benzene separation with $\alpha = 2.44/0.49 = 4.98$

$$N_{\min} = \frac{\ln\left((x_{LK}/x_{HK})_D (x_{HK}/x_{LK})_B\right)}{\ln(\bar{\alpha}_{LK/HK})}$$

$$N_{\min} = \frac{\ln\left((0.9916/x_{EB})_D (0.639/0.0085)_B\right)}{\ln(5)} = 9.52$$

$$\ln\left((0.9916/x_{EB})_D (0.639/0.0085)_B\right) = \ln(5) \times 9.52$$

$$\left(\frac{0.9916}{x_{EB}}\right)\left(\frac{0.639}{0.0085}\right) = 4.5 \times 10^6$$

From which the mole fraction of ethyl benzene in distillate, $x_{EB,D} = 1.7 \times 10^{-5}$, which is negligible.

b. Minimum reflux ration, $R_{\min}$
Since the feed is saturated liquid, $q = 1$

$$1 - q = \sum_{i=1}^{n} \frac{\alpha_i\, x_{F,i}}{\alpha_i - \varphi} = 1 - 1 = 0 = \frac{2.44 \times 0.3}{2.44 - \varphi} + \frac{1 \times 0.25}{1 - \varphi} + \frac{0.49 \times 0.45}{0.49 - \varphi}$$

Solving for φ, the value should be between 2.44 and 1, by trial and error:

$$\varphi = 1.471$$

TABLE 6.8

Feed Stream Relative Volatilities

	Component	Feed Composition	*k*-Value	Relative Volatility (α)
LK	Benzene	0.3	2.215	2.84
HK	Toluene	0.25	0.7791	1
	Ethyl benzene	0.45	0.3128	0.4

$$R_{\min} + 1 = \sum_{i=1}^{n} \frac{\alpha_i \, x_{Di}}{\alpha_i - \varphi} = \frac{2.424 \times 0.9916}{2.424 - 1.471} + \frac{1 \times 0.0084}{1 - 1.471} = 2.5$$

The minimum reflux ratio:

$$R_{\min} = 1.5$$

c. Gilliland correlation is used to calculate number of equilibrium stages, N. Select a reflux ratio that is $R = (1.1 \text{ to } 1.5)\, R_{\min}$

$$\frac{N - N_{\min}}{N + 1} = 0.75\left(1 - \left(\frac{R - R_{\min}}{R + 1}\right)^{0.566}\right)$$

Substituting required data:

$$\frac{N - 9.52}{N + 1} = 0.75\left(1 - \left(\frac{2 - 1.5}{2 + 1}\right)^{0.566}\right)$$

$$\frac{N - 9.52}{N + 1} = 0.48$$

$$0.522 \times N = 10 \Rightarrow N = 19 \text{ trays}$$

The actual number of stages is 19.

d. At 0.2 atm (the boiling point is 55°C) the relative volatilities are obtained using Antoine equation.
At a boiling point of 0.2 atm, the relative volatility of LK to HK is 2.84 compared to 2.44 at 1 atm.

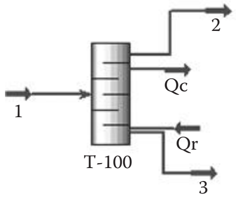
$$N_{\min} = \frac{\ln\left((0.9916/0.0084)_D\,(0.3518/0.0085)_B\right)}{\ln(2.84)} = 8.14$$

The heat of vaporization per mole is slightly higher at the low pressure, but for a given number of plates, less reflux is needed because of the higher relative volatility.

HYSYS/UNISIM SIMULATION

Two distillation methods available in Hysys are considered:

- Shortcut method
- Rigorous distillation method



Streams				
		1	2	3
Temperature	C	105.0	80.34	124.2
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	100.0	29.65	70.35
Comp molar flow (benzene)	kgmol/h	30.00	29.40	0.60
Comp molar flow (toluene)	kgmol/h	25.00	0.25	24.75
Comp molar flow (E-benzene)	kgmol/h	45.00	0.00	45.00

FIGURE 6.47
Process flow sheet and stream summary.

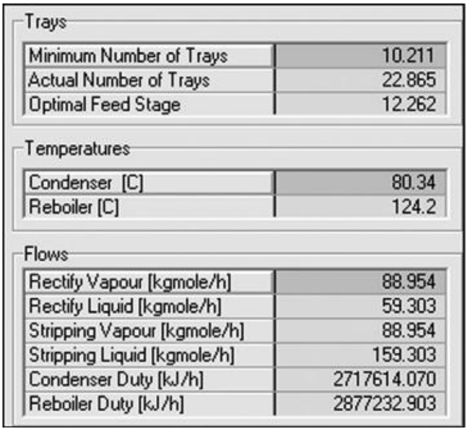
Hysys Shortcut

Select the shortcut distillation in Hysys, after connecting and fully specifying feed stream, connecting product and energy streams, selecting Peng–Robinson EOS as the thermodynamic fluid package (Figure 6.47). While in *Design/Parameters* page the following needs to be filled in:

- LK in the bottom is benzene with mole fraction 0.0085
- HK in distillate is toluene with mole fraction is 0.0084
- Condenser and reboiler pressure are 1 atm
- Reflux ratio is 2

The minimum reflux ratio is 1.629. Detailed performance of the column is shown in Figure 6.48. Minimum number of trays is 11, actual number of trays is 23; the optimum feed tray is tray number 13 from top.

The column performance is shown in Figure 6.48.



Trays

Minimum Number of Trays	10.211
Actual Number of Trays	22.865
Optimal Feed Stage	12.262

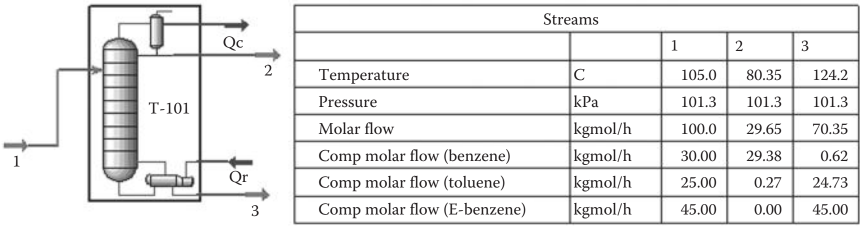
Temperatures

Condenser [C]	80.34
Reboiler [C]	124.2

Flows

Rectify Vapour [kgmole/h]	88.954
Rectify Liquid [kgmole/h]	59.303
Stripping Vapour [kgmole/h]	88.954
Stripping Liquid [kgmole/h]	159.303
Condenser Duty [kJ/h]	2717614.070
Reboiler Duty [kJ/h]	2877232.903

FIGURE 6.48
Performance of the distillation column.



Streams				
		1	2	3
Temperature	C	105.0	80.35	124.2
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmol/h	100.0	29.65	70.35
Comp molar flow (benzene)	kgmol/h	30.00	29.38	0.62
Comp molar flow (toluene)	kgmol/h	25.00	0.27	24.73
Comp molar flow (E-benzene)	kgmol/h	45.00	0.00	45.00

FIGURE 6.49
Process flow sheet of Hysys continuous distillation.

Hysys Continuous Distillation Column

The following data are required and provided from results obtained in the shortcut column:

- Feed stream is fully specified (i.e., filling in flow low rate and compositions, feed stream conditions; temperature and pressure or vapor to phase fraction with either temperature or pressure)
- Feed stream inlet stage: 12
- Total number of trays: 23
- Condenser and reboiler pressure: 101.3 kPa
- Reflux ratio: 2
- Distillate liquid rate: 29.65 kmol/h

Providing all the above required data and running the system the results should look like that shown in Figure 6.49. Streams molar flow rate are the same as those obtained by shortcut distillation method.

PRO/II SIMULATION

The following methods are used in simulating distillation column with Provision

- Shortcut method
- Rigorous methods are considered

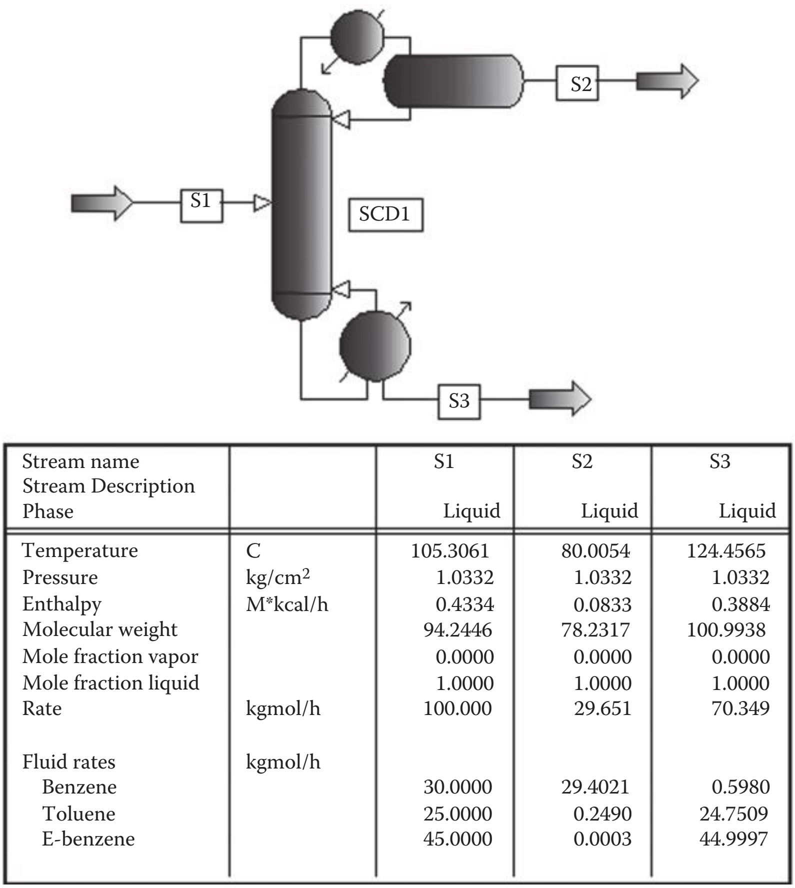
PRO/II Shortcut Column

Using shortcut method in PRO/II, Peng–Robinson EOS is used as a suitable property package. Process flowsheet and the product streams molar flow rates and compositions are shown in Figure 6.50. The summary of the Underwood calculations is shown in Figure 6.51. The minimum reflux ratio is 1.567, the minimum number of trays is 11 and the actual number of stages is 16 trays. Values are close to hand calculation results.

PRO/II Distillation Column

PRO/II *Distillation* column is used for continuous distillation, the Peng–Robinson EOS is engaged for the property estimation. The following values obtained from the shortcut column are filled in the PRO/II *Distillation* column:

- Feed stream is fully specified (filling in feed flow rate, compositions, pressure and feed at bubble point temperature).



Stream name Stream Description Phase		S1 Liquid	S2 Liquid	S3 Liquid
Temperature	C	105.3061	80.0054	124.4565
Pressure	kg/cm2	1.0332	1.0332	1.0332
Enthalpy	M*kcal/h	0.4334	0.0833	0.3884
Molecular weight		94.2446	78.2317	100.9938
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	100.000	29.651	70.349
Fluid rates	kgmol/h			
Benzene		30.0000	29.4021	0.5980
Toluene		25.0000	0.2490	24.7509
E-benzene		45.0000	0.0003	44.9997

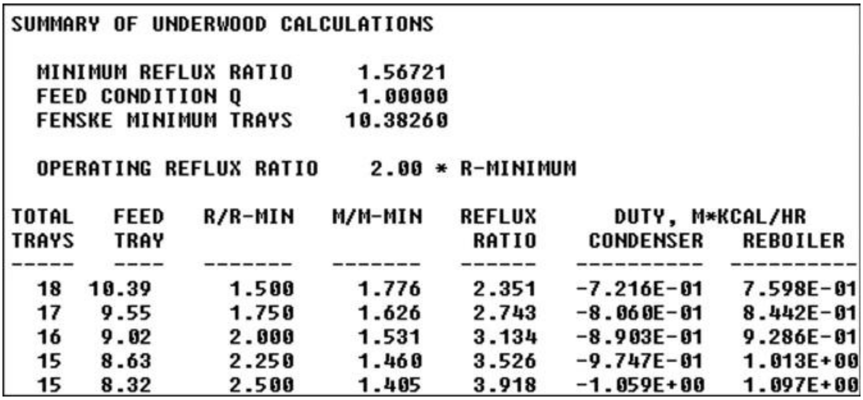
FIGURE 6.50
Process flow sheet and stream table properties.

- Number of theoretical trays: 16
- Overall top tray pressure: 1 atm
- Pressure drop per tray: 0
- Feed tray: 9
- Distillate (Stream S2) molar flow rate is 29.651 kmol/h. The molar flow rate of stream S2 is not used as specification but as initial guess.
- Reflux ratio is 3.134 (i.e., 2 R_{min}).
- Mole fraction of benzene in distillate is 0.992

Once all required information is completed, running the system should lead to the results shown in Figure 6.52.

ASPEN SIMULATION

Shortcut and rigorous method are considered.



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SUMMARY OF UNDERWOOD CALCULATIONS

  MINIMUM REFLUX RATIO     1.56721
  FEED CONDITION Q         1.00000
  FENSKE MINIMUM TRAYS    10.38260

  OPERATING REFLUX RATIO    2.00 * R-MINIMUM

TOTAL   FEED   R/R-MIN   M/M-MIN   REFLUX      DUTY, M*KCAL/HR
TRAYS   TRAY                        RATIO   CONDENSER   REBOILER
-----   ----   -------   -------   ------   ----------  ----------
  18  10.39     1.500     1.776    2.351   -7.216E-01   7.598E-01
  17   9.55     1.750     1.626    2.743   -8.060E-01   8.442E-01
  16   9.02     2.000     1.531    3.134   -8.903E-01   9.286E-01
  15   8.63     2.250     1.460    3.526   -9.747E-01   1.013E+00
  15   8.32     2.500     1.405    3.918   -1.059E+00   1.097E+00
```

FIGURE 6.51
Summary of Underwood calculations.

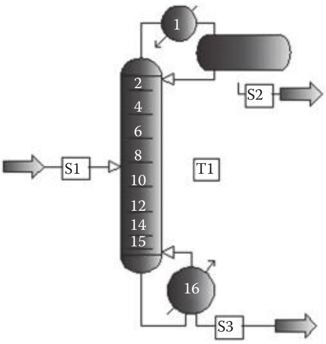
Shortcut Method

The process flow sheet with the stream summary is shown in Figure 6.53. Detailed column specifications are shown in Figure 6.54.

Aspen Continuous Distillation Column Method

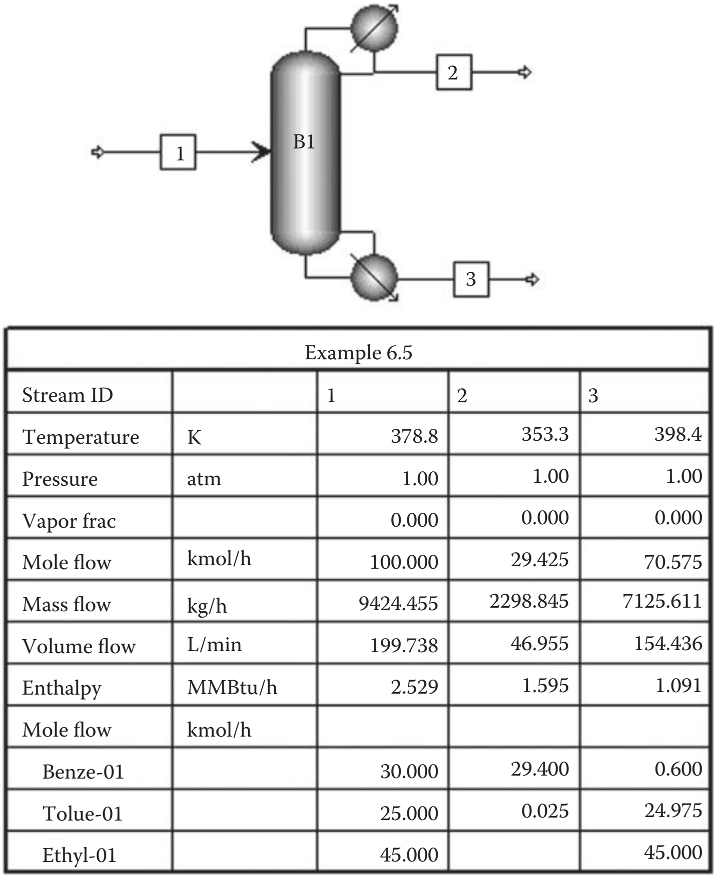
The rigorous column in Aspen is *RadFrac* from the model library. After building the process flow sheet the following data are provided:

- Number of trays: 13
- Condenser: Total
- Distillate rate: 29.56 kmol/h
- Reflux ratio: 2
- Feed stream stage: 12
- Top stage condenser pressure: 1 atm



Stream name		S1	S2	S3
Stream description				
Phase		Liquid	Liquid	Liquid
Temperature	C	105.3061	79.9976	124.1926
Pressure	kg/cm^2	1.0332	1.0332	1.0332
Enthalpy	M*kcal/h	0.4334	0.0826	0.3885
Molecular weight		94.2446	78.2263	100.9174
Mole fraction vapor		0.0000	0.0000	0.0000
Mole fraction liquid		1.0000	1.0000	1.0000
Rate	kgmol/h	100.000	29.408	70.592
Fluid rates	kgmol/h			
Benzene		30.0000	29.1720	0.8280
Toluene		25.0000	0.2349	24.7651
E-benzene		45.0000	0.0007	44.9993

FIGURE 6.52
PRO/II distillation column PFD and stream table.



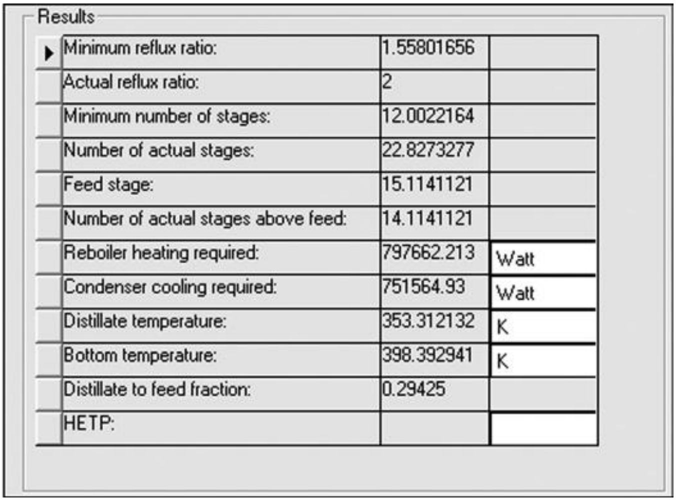
Example 6.5				
Stream ID		1	2	3
Temperature	K	378.8	353.3	398.4
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	100.000	29.425	70.575
Mass flow	kg/h	9424.455	2298.845	7125.611
Volume flow	L/min	199.738	46.955	154.436
Enthalpy	MMBtu/h	2.529	1.595	1.091
Mole flow	kmol/h			
Benze-01		30.000	29.400	0.600
Tolue-01		25.000	0.025	24.975
Ethyl-01		45.000		45.000

FIGURE 6.53
Process flow sheet and stream summary.

Running the system leads to the results shown in Figure 6.55. The product streams molar flow rate and conditions is the same as that obtained using Aspen shortcut method.

SUPERPRO DESIGNER SIMULATION

The shortcut distillation column is used and added to the process flow sheet done in the previous examples. Feed stream and two product streams are connected to the unit as shown in Figure 6.56. Relative volatilities and distillate stream composition is shown in Figure 6.57. Feed stream is specified and in the operating conditions, relative volatiles of feed stream components and percentage in distillate are filled in as shown in Figure 6.58. The number of theoretical stages obtained with SuperPro is 19 and minimum reflux ratio is 1.238 (i.e., 2.0/1.615).



Results

Minimum reflux ratio:	1.55801656	
Actual reflux ratio:	2	
Minimum number of stages:	12.0022164	
Number of actual stages:	22.8273277	
Feed stage:	15.1141121	
Number of actual stages above feed:	14.1141121	
Reboiler heating required:	797662.213	Watt
Condenser cooling required:	751564.93	Watt
Distillate temperature:	353.312132	K
Bottom temperature:	398.392941	K
Distillate to feed fraction:	0.29425	
HETP:		

FIGURE 6.54
Column detailed performance.

PROBLEMS

6.1 Shortcut Distillation

The feed to a distillation column is at 405°F and 100 psia enters at 1272 lbmol/h with the following compositions in mole fraction: Ethane 0.0148, propane 0.7315, *i*-butane 0.0681, *n*-butane 0.1462, *i*-Pentane 0.0173, *n*-pentane 0.015, *n*-hexane 0.0071. HK in distillate is *i*-butane 0.02 mole fraction; LK in bottom is propane 0.025 mole fraction for reflux ratios of 1.5. Calculate the minimum reflux ratio and column performance?

6.2 Rigorous Distillation

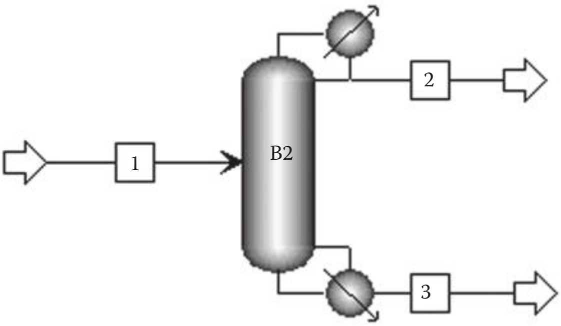
The feed to a distillation column is at room conditions ($T = 25$°C, $P = 1$ atm). The concentration of the feed stream is 50% ethanol, 50% iso-propanol in mass fractions. The feed is at a rate of 163 lb/h. For the reboiler heat duty, we will assume a load of 120,000 Btu/h, assume number of trays to be 24 and reflux ratio equal 3. Find the conditions of the exit streams.

6.3 Continuous Distillation

Repeat Example 6.2; assume that the reboiler duty is unknown. The overhead ethanol concentration is 0.55. What is the amount of the reboiler load in Btu/h?

6.4 Continuous Distillation with Known Reboiler Duty

Repeat Example 6.2; in this case calculate the reflux ratio that would give an ethanol concentration of 80% with a reboiler duty of 300,000 Btu/h (8.069e + 4 kcal/h) is to be calculated.



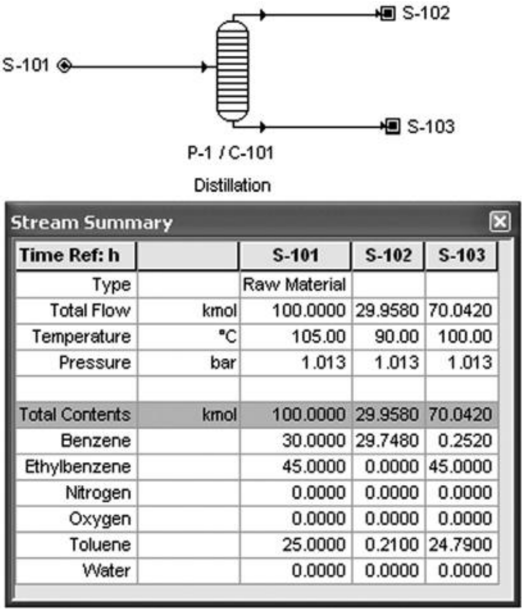
Example 6.5c				
Stream ID		1	2	3
Temperature	K	378.1	353.4	398.5
Pressure	atm	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000
Mole flow	kmol/h	100.000	29.650	70.350
Mass flow	kg/h	9424.455	2318.897	7105.558
Volume flow	L/min	199.563	47.377	154.017
Enthalpy	MMBtu/h	2.517	1.602	1.084
Mole flow	kmol/h			
Benze-01		30.000	29.449	0.551
Tolue-01		25.000	0.201	24.799
Ethyl-01		45.000	<0.001	45.000

FIGURE 6.55
Distillation column process flow sheet and stream conditions generated by Aspen Plus.

6.5 Separation of Benzene, Toluene, and Trimethyl-Benzene

A distillation column with a partial reboiler and a total condenser is being used to separate a mixture of benzene, toluene, and trimethyl-benzene. The feed consists of 0.4 mole fraction benzene, 0.3 mole fraction toluene and the balance is trimethyl-benzene. The feed enters the column as a saturated vapor. It is desired to separate 95% of the toluene in the distillate and 95% of the trimethyl benzene in the bottom. The column operates at 1 atm, the top and bottom temperatures are 390 and 450 K respectively.

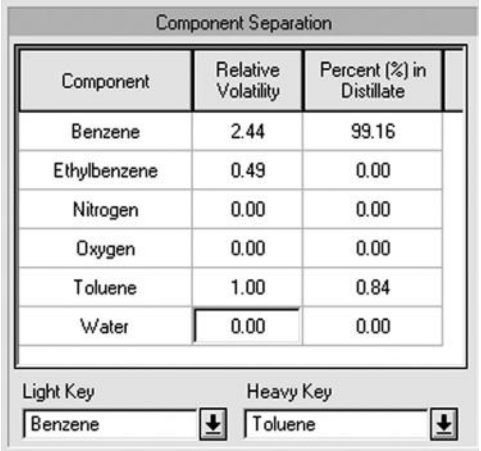
a. Find the number of equilibrium stages required at total reflux.
b. Find the minimum reflux ratio for the previous distillation problem using Underwood method.



Stream Summary

Time Ref: h		S-101	S-102	S-103
Type		Raw Material		
Total Flow	kmol	100.0000	29.9580	70.0420
Temperature	°C	105.00	90.00	100.00
Pressure	bar	1.013	1.013	1.013
Total Contents	kmol	100.0000	29.9580	70.0420
Benzene		30.0000	29.7480	0.2520
Ethylbenzene		45.0000	0.0000	45.0000
Nitrogen		0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000
Toluene		25.0000	0.2100	24.7900
Water		0.0000	0.0000	0.0000

FIGURE 6.56
Process flow sheet and stream summary.



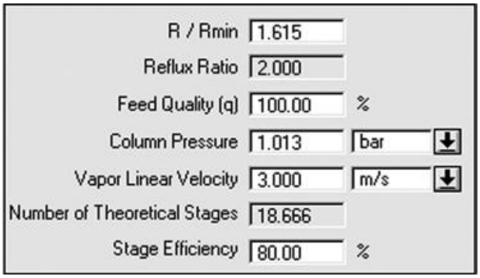
Component Separation

Component	Relative Volatility	Percent (%) in Distillate
Benzene	2.44	99.16
Ethylbenzene	0.49	0.00
Nitrogen	0.00	0.00
Oxygen	0.00	0.00
Toluene	1.00	0.84
Water	0.00	0.00

Light Key: Benzene

Heavy Key: Toluene

FIGURE 6.57
Column operating conditions.



R / Rmin 1.615

Reflux Ratio 2.000

Feed Quality (q) 100.00 %

Column Pressure 1.013 bar

Vapor Linear Velocity 3.000 m/s

Number of Theoretical Stages 18.666

Stage Efficiency 80.00 %

FIGURE 6.58
Number of theoretical stages.

c. Estimate the total number of equilibrium stages and the optimum feed-stage location if the actual reflux ratio *R* equals 1.

6.6 Separation of Hydrocarbon Mixtures

A mixture with 4% n-C_5, 40% n-C_6, 50% n-C_7, and 6% n-C_8 is to be distilled at 1 atm with 98% of n-C_6 and 1 % of n-C_7 recovered in the distillate. What is the minimum reflux ratio for a liquid feed at its bubble point?

6.7 Separation of Multicomponent Gas Mixture

A feed at its bubble point temperature is fed to a distillation column. The feed contains propane (C_3), *n*-butane (n-C_4), *i*-butane (i-C_4), *n*-pentane (n-C_5) and *i*-pentane(i-C_5). The mole % of components in the feed is respectively 5%, 15%, 25%, 20%, and 35%. The operating pressure of the column is 405.3 kPa. Ninety-five percent of the i-C_4 is recovered in the distillate (top) and 97% of the *n*-C5 us recovered in the bottom. Determine the top and bottom flow rats and composition, minimum reflux ratio and minimum number of trays at a reflux ratio of 2.25.

References

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5. McCabe, W., J. Smith, and P. Harriott, 2004. *Unit Operations of Chemical Engineering*, 7th edn, McGraw-Hill, New York, NY.
6. Fair, J. R., 1961. How to predict sieve tray entrainment and flooding. *Petro./Chem. Egn.*, 33: 45–52.

7

Gas Absorption

At the end of this chapter you should be able to

1. Familiarize yourself with the factors to be considered in designing absorbers.
2. Explain the importance of exhaust gas characteristics and liquid flow.
3. Compute the minimum liquid flow rate required for separation.
4. Determine the diameter and the packing height of a packed-bed column.
5. Find the number of theoretical plates and the height of a plate tower.

7.1 Introduction

Absorption is a process that refers to the transfer of a gaseous pollutant from the gas phase to the liquid phase. Absorbers are used extensively in the chemical industry for separation and purification of gas streams, as product recovery and as pollution control devices. The absorption process can be categorized as physical or chemical. Physical absorption occurs when the absorbed compounds dissolves in the solvent. Chemical absorption occurs when the absorbed compounds and the solvent react. Examples are separations of acid gases such as CO_2 and H_2S from natural gas using amine as solvents. Chemical engineers need to be able to design gas absorbers that produce a treated gas of a desired purity with an optimal size and liquid flow. This can be based on existing correlations and, when required, laboratory and/or pilot plant data. For gas absorption, the two most frequently used devices are the packed tower and the plate tower. Both these devices, if designed and operated properly, can achieve high collection efficiencies for a wide variety of gases. The primary outcomes of the design procedures are to determine the diameter of the column and the tower height [1–3].

7.2 Packed-Bed Absorber

The design of an absorber used to reduce gaseous pollutants from process streams is affected by many factors such as the pollutant gathering efficiency, contaminant solubility in the absorbing liquid, liquid-to-gas ratio, stream flow rate, pressure drop, and construction details of the absorbers such as packing materials, plates, liquid distributors, entrainment separators, and corrosion-resistant materials. Solubility is an important factor affecting the amount of a pollutant, or solute, which can be absorbed. Solubility is a function of both the temperature and pressure. As temperature increases, the volume of a gas also increases; therefore, less gas is absorbed due to the large gas volume. By increasing the pressure of a system, the amount of gas absorbed generally increases. Solubility data are obtained at equilibrium conditions. This involves filling measured amounts of a gas and a liquid into a closed vessel and allowing it to sit for a period of time. Henry's law is used to express equilibrium solubility of a gas–liquid system. Henry's law is expressed as

$$y = Hx$$

where y is the mole fraction of gas in equilibrium with liquid; H is Henry's law constant, mole fraction in vapor per mole fraction; and x is the mole fraction of the solute in equilibrium.

Henry's law, which depends on total pressure, can be used to predict solubility only when the equilibrium line is straight, the case when the solute concentration is very dilute. Another form of Henry's law is

$$p = k_H c$$

where p is the partial pressure of the solute in the gas above the solution, c is the concentration of the solute, and k_H is a constant with the dimensions of pressure units divided by concentration units. The constant, known as Henry's law constant, depends on the solute, the solvent, and the temperature. Some values for k_H for gases dissolved in water at 298 K include [4]

- Oxygen (O_2): 769.2 L atm/mol
- Carbon dioxide (CO_2): 29.4 L atm/mol
- Hydrogen (H_2): 1282.1 L atm/mol
- Acetone (CH_3COCH_3): 28 L atm/mol

Example 7.1: Henry's Law for Solubility Data

Calculate Henry's law constant (H) from the solubility of SO_2 in pure water at 30°C and 1 atm. The data are given in Table 7.1.

TABLE 7.1

Equilibrium Data of SO_2/H_2O at 30°C and 101.32 kPa

C_{SO2} (g of SO_2 per 100 g of H_2O)	P_{SO2} (kPa) (Partial Pressure of SO_2)
0.5	6
2.0	24.3

Source: Data from Peytavy, J. L. et al. 1990. *Chemical Engineering and Processing*, 27(3), 155–163.

SOLUTION

HAND CALCULATION

The mole fraction of SO_2 in the gas phase, y, is calculated by dividing the partial pressure of SO_2 by the total pressure of the system:

$$y_1 = \frac{P_{SO_2}}{P_T} = \frac{6\ \text{kPa}}{101.3\ \text{kPa}} = 0.06$$

$$y_2 = \frac{P_{SO_2}}{P_T} = \frac{24.3\ \text{kPa}}{101.3\ \text{kPa}} = 0.239$$

The mole fraction of the SO_2 in the liquid phase, x, is calculated by dividing the moles of SO_2 dissolved in the solution by the total moles of liquid.

$$x = \frac{\text{Moles of } SO_2 \text{ in solution}}{\text{Moles of } SO_2 \text{ in solution} + \text{Moles of } H_2O}$$

$$x_1 = \frac{(0.5\,\text{g}\,SO_2)/(64\,\text{g/mol})}{(0.5\,\text{g}\,SO_2)/(64\,\text{g/mol}) + (100\,\text{g}\,H_2O)/(18\,\text{g/mol})} = 0.0014$$

$$x_2 = \frac{(2.0\,\text{g}\,SO_2)/(64\,\text{g / mol})}{(2.0\,\text{g}\,SO_2)/(64\,\text{g/mol}) + (100\,\text{g}\,H_2O)/(18\,\text{g/mol})} = 0.0056$$

Henry's constant

$$H = \frac{y}{x} \Rightarrow \text{slope} = \frac{\Delta y}{\Delta x} = \frac{0.239 - 0.06}{0.0056 - 0.0014} = 42.62$$

Example 7.2: Minimum Liquid Flow Rate

Compute the minimum liquid mass flow rate of pure water required to cause 90% reduction in the composition of SO_2 from a gas stream of 85 m^3/min containing 3% SO_2 by volume. The temperature is 303 K and the pressure is 101.32 kPa.

SOLUTION

HAND CALCULATIONS

The mole fraction of SO_2 in the gas phase:

y_1 = 3% SO_2 by volume; inlet pollutant gas mole percent.
= 0.03 mole fraction of SO_2

y_2 = 90% reduction of SO_2 from inlet concentration
= (10%) y_1
= (0.1) (0.03)
= 0.003 mole fraction of SO_2

At the minimum liquid flow rate, the gas mole fraction of the pollutants moving into the absorber, y_1, will be in equilibrium with the liquid mole fraction of pollutants released from the absorber, x_1, and the liquid will be saturated with SO_2. At equilibrium

$$y_1 = Hx_1$$

$$H = 42.62\frac{\text{Mole fraction of } SO_2 \text{ in air}}{\text{Mole fraction of } SO_2 \text{ in water}}$$

The mole fraction of SO_2 in the liquid released from the absorber to achieve the required removal efficiency:

$$x_1 = \frac{y_1}{H} = \frac{0.03}{42.67} = 0.0007$$

The minimum liquid-to-gas ratio

$$y_1 - y_2 = \frac{L_m}{G_m}(x_1 - x_2)$$

Therefore,

$$\frac{L_m}{G_m} = \frac{y_1 - y_2}{x_1 - x_2} = \frac{0.03 - 0.003}{0.0007 - 0} = 38.4\frac{\text{gmol of water}}{\text{gmol of air}}$$

The molar flow rate of the inlet gas is calculated by converting inlet stream volumetric flow rate to gas molar flow rate. At 0°C and 101.3 kPa there are 0.0224 m^3/gmol of an ideal gas. The volume of gas at 30°C is

$$Q\big|_{\text{at}\,30\,°\text{C}} = 0.0224\ \text{m}^3/\text{gmol}\left(\frac{303\ \text{K}}{273\ \text{K}}\right) = 0.025\ \text{m}^3/\text{gmol}$$

Therefore,

$$G_m = Q_E\left(\frac{1\ \text{gmol of air}}{0.025\ \text{m}^3}\right)$$

We have

$$Q_G = 85\ \text{m}^3/\text{min} \quad \text{at } 30\,°\text{C}$$

Hence,

$$G_m = 85\ \text{m}^3/\text{min}\left(\frac{1\ \text{gmol}}{0.025\ \text{m}^3}\right) = 3400\ \text{gmol of air/min}$$

The minimum liquid flow rate is denoted as L_m.
The calculated minimum liquid-to-gas ratio

$$\left(\frac{L_m}{G_m}\right)_{\text{min}} = 38.4\,\frac{\text{gmol of water}}{\text{gmol of air}}$$

Therefore,

$$(L_m)_{\text{min}} = G_m(38.4)$$

$$(L_m)_{\text{min}} = 3400\,\frac{\text{gmol of air}}{\text{min}}\left(38.4\,\frac{\text{gmol of water}}{\text{gmol of air}}\right) = 1.3\times 10^5\,\frac{\text{gmol of water}}{\text{min}}$$

Converting to units of mass,

$$(L_m)_{\text{min}} = \left(130.0\,\frac{\text{kgmol of water}}{\text{min}}\right)\left(\frac{18\ \text{kg}}{\text{kgmol}}\right) = 2340\ \text{kg/min}$$

7.3 Number of Theoretical Stages

The height of a transfer unit is a function of the type of packing, liquid and gas flow rates, pollutant concentration and solubility, liquid properties, and system temperature. Tower height is primarily a function of packing depth. For most packed-tower applications, the height of a transfer unit can be estimated as 0.3–1.2 m (1–4 ft). The required depth of packing (H_{pack}) is determined from the theoretical number of overall transfer units (N_{tu}) needed to achieve specific removal efficiency, and the height of the overall transfer unit (H_{tu}) [2]:

$$H_{\text{pack}} = N_{\text{tu}}H_{\text{tu}} \tag{7.1}$$

The number of overall transfer units may be estimated graphically by stepping off stages on the equilibrium-operating line graph from inlet conditions to outlet conditions, or by the following equation:

$$N_{\text{tu}} = \frac{\ln[(y_i - mx_i/y_o - mx_i)(1-(1/\text{AF})) + 1/\text{AF}]}{1-(1/\text{AF})} \tag{7.2}$$

where the absorption factor

$$\mathrm{AF} = \frac{L_\mathrm{m}}{mG_\mathrm{m}} \tag{7.3}$$

where AF is the absorption factor, m is the slope of the equilibrium line on a mole fraction basis. The value of m may be obtained from available literature on vapor–liquid equilibrium data for specific systems. Since the equilibrium curve is typically linear in the concentration ranges usually encountered in air pollution control, the slope m would be constant for all applicable inlet and outlet liquid and gas streams. The slope may be calculated from mole fraction values using the following equation [5]:

$$m = \frac{y_\mathrm{o}^* - y_\mathrm{i}^*}{x_\mathrm{o} - x_i} \tag{7.4}$$

where y_i^* and y_o^* are the mole fractions of the pollutant in the vapor phase in equilibrium with the mole fractions of the pollutant entering and exiting the absorber in the liquid, x_i and x_o, respectively. The equation is based on several assumptions [6,7]:

- Henry's law applies for a dilute gas mixture.
- The equilibrium curve is linear from x_i to x_o.
- The pollutant concentration in the solvent is dilute enough such that the operating line can be considered a straight line.

If $x_i = 0$ (i.e., a negligible amount of pollutant enters the absorber in the liquid stream) and $1/\mathrm{AF} = 0$ (i.e., the slope of the equilibrium line is very small and/or the $L_\mathrm{m}/G_\mathrm{m}$ ratio is very large), Equation 1.26 simplifies to

$$N_\mathrm{tu} = \ln\left(\frac{y_i}{y_\mathrm{o}}\right) \tag{7.5}$$

There are several methods that may be used to calculate the height of the overall transfer unit: all are based on empirically determined packing constants [7–9]. One commonly used method involves determining the overall gas and liquid mass transfer coefficients; k_G, k_L. A major difficulty in using this approach is that the values of k_G and k_L is frequently unavailable for specific pollutant–solvent systems of interest. For this purpose, the method used to calculate the height of the overall transfer unit is based on estimating the height of the gas and liquid film transfer units, H_L and H_G, respectively [8–13].

7.4 Number of Theoretical Stages Using Graphical Technique

Graphical technique is used to estimate the number of theoretical stages using material balance on a differential element from the absorbers.

Mass Balance:

$$-V\,dy = K_y a S\,dz(y - y^*)$$

$$\frac{K_y a\,S}{V}\int dz = \int_{y_1}^{y_{N+1}} \frac{dy}{y - y^*}$$

Final design equation for dilute solutions

$$Z = \left(\frac{V}{K_y a S}\right)\left(\int_{y_1}^{y_{N+1}} \frac{dy}{y - y^*}\right)$$

$$Z = \mathrm{HTU_{OG}} * \mathrm{NTU_{OG}}$$

where a is the interfacial area, m^2/m^3; V is the total gas molar flow rate, kgmol/s; S is the cross-sectional area of the tower, m^2; and K_y is the volumetric film mass transfer coefficient, kgmol/s.

The integral part of the equation is the total number of trays as shown in Figure 7.1.

Example 7.3: Number of Theoretical Stages

A gas absorber is used to remove 90% of the SO_2 from a gas stream with pure water. The inlet gas stream molar flow rate is 206 kmol/h. The gas stream contains

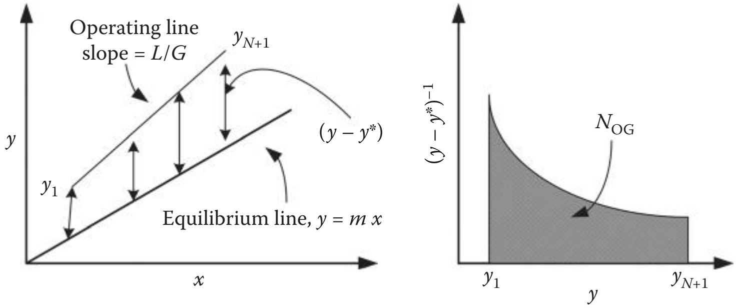


FIGURE 7.1
Operating and equilibrium.

3 mol% SO_2. The liquid water molar flow rate is 12,240 kmol/h. The temperature is 20°C and the pressure is 1 atm. The packing material is 2 in. ceramic Intalox Saddles randomly packed. Determine the number of theoretical stages required to achieve the required exit gas stream specifications. Henry's constant at the absorber operating conditions is 26.

SOLUTION

HAND CALCULATIONS

The number of theoretical stages

$$N_{OG} = \frac{\ln[(y_1 - mx_2/y_2 - mx_2)(1 - (mG_m/L_m)) + mG_m/L_m]}{1 - mG_m/L_m}$$

The absorption factor

$$AF = \frac{mG_m}{L_m} = \frac{26 \times 206\,\text{kmol/h}}{12240\,\text{kmol/h}} = 0.438$$

Substituting the absorption factor into the above equation,

$$N_{OG} = \frac{\ln[(0.03 - 0/0.003 - 0)(1 - 0.438) + 0.438]}{1 - 0.387} = 3.2$$

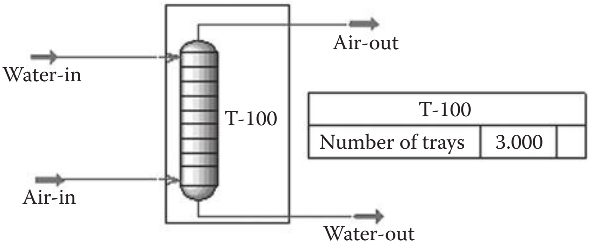
The total number of stages is rounded off to 4.

HYSYS SIMULATION

After opening a new case in Hysys, select all components involved and the appropriate fluid package (PR), then in the simulation environment select the absorber from the object palette. The absorber icon from the object palette is selected for this purpose. The feed streams are fully specified (i.e., air-in and water-in streams). Selection of the thermodynamic fluid package is very important. Using other fluid packages will result in different results. After trying different number of stages, three stages were found to give the desired exit molar fraction of SO_2. The stream summary and the process flow sheet are shown in Figure 7.2.

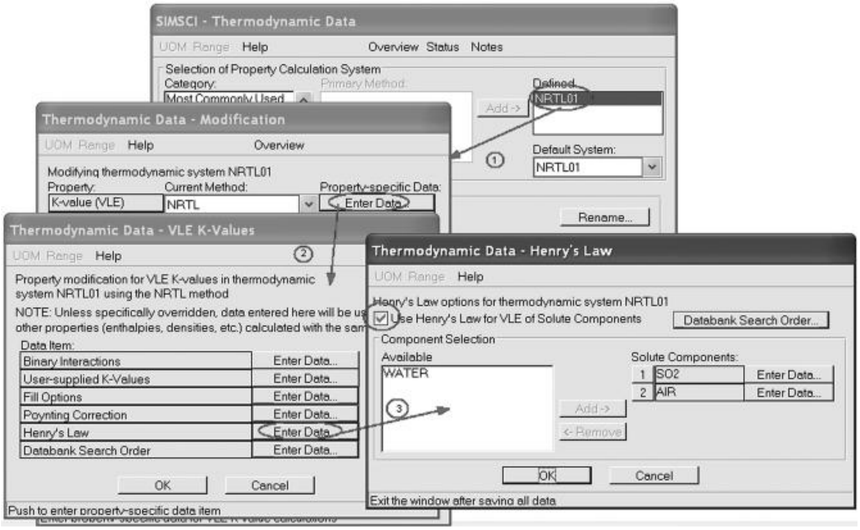
PRO/II SIMULATION

Selection of appropriate thermodynamic model for the simulation of CO_2 or SO_2 in gas absorbers using water as a solvent is very important. Nonrandom two liquids (NRTL) activity coefficient model is chosen to explain the nonideal phase behavior of a liquid mixture between H_2O and SO_2. Henry's law option is also selected for the calculation of noncondensable supercritical gases such as H_2, CO, CO_2, CH_4, and N_2 in a liquid mixture. In this example, NRTL was selected. Double click on NRTL01, the thermodynamic data modification window pops up. Click on *Enter Data*, vapor liquid equilibria (VLE) *K*-values window pops up, and then click on Henry's law *Enter Data* as shown in Figure 7.3. Check use Henry's law for VLE of solute components.



Streams					
		Water-in	Water-out	Air-in	Air-out
Temperature	C	20.00	19.89	19.85	20.02
Pressure	kPa	101.3	101.3	101.3	101.3
Molar flow	kgmol/h	12240	12243	206	203
Comp flow frac (SO_2)		0.000	0.000	0.030	0.003
Comp mole frac (air)		0.000	0.000	0.970	0.974
Comp mole frac (H_2O)		1.000	0.999	0.000	0.023

FIGURE 7.2
Process flow sheet and stream summary.



Selection of Property Calculation System
Category: Most Commonly Used
Primary Method:
Defined: NRTL01
Default System: NRTL01

Modifying thermodynamic system NRTL01
Property: K-value (VLE)
Current Method: NRTL
Property-specific Data: Enter Data...

Property modification for VLE K-values in thermodynamic system NRTL01 using the NRTL method
NOTE: Unless specifically overridden, data entered here will be us… other properties (enthalpies, densities, etc.) calculated with the sam…

Data Item:	
Binary Interactions	Enter Data...
User-supplied K-Values	Enter Data...
Fill Options	Enter Data...
Poynting Correction	Enter Data...
Henry's Law	Enter Data...
Databank Search Order	Enter Data...

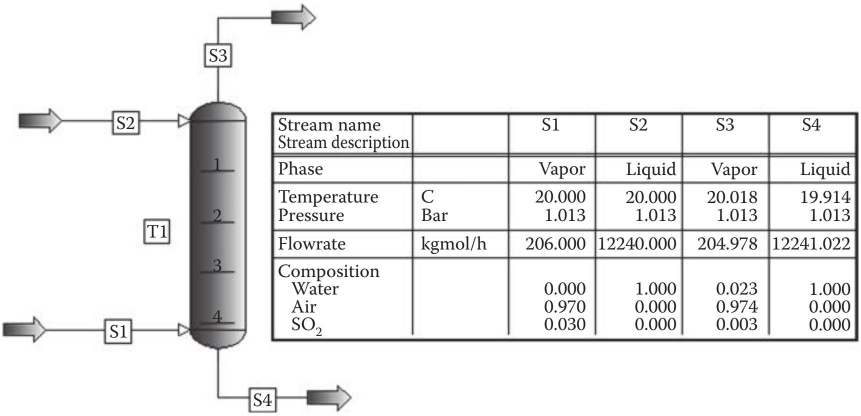
Push to enter property-specific data item

Henry's Law options for thermodynamic system NRTL01
☑ Use Henry's Law for VLE of Solute Components
Component Selection
Available: WATER

Solute Components:		
1	SO2	Enter Data...
2	AIR	Enter Data...

Exit the window after saving all data

FIGURE 7.3
Selection of the thermodynamic model.



Stream name Stream description		S1	S2	S3	S4
Phase		Vapor	Liquid	Vapor	Liquid
Temperature Pressure	C Bar	20.000 1.013	20.000 1.013	20.018 1.013	19.914 1.013
Flowrate	kgmol/h	206.000	12240.000	204.978	12241.022
Composition					
Water		0.000	1.000	0.023	1.000
Air		0.970	0.000	0.974	0.000
SO_2		0.030	0.000	0.003	0.000

FIGURE 7.4
Stream summaries.

The stream summary result is shown in Figure 7.4; the number of stages required to achieve the desired separation (i.e., mole fraction of 0.003 in exit air stream) is 4. The result obtained by PRO/II is closer to the hand-calculated results. This is attributed to the Henry's law constants used.

Henry's law constant generated by PRO/II is shown in Figure 7.5.

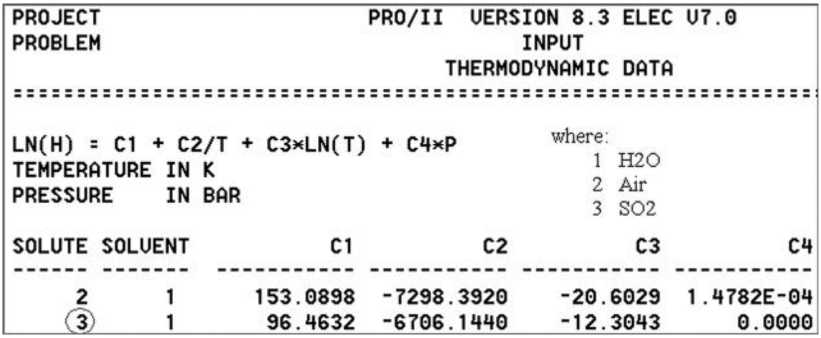
Henry's law constant is

$$H = \exp(96.46 - (6706.144/293) - 12.3043 * \ln(293)) = 39.5$$

The value obtained by PRO/II is close to that obtained in Example 7.2 ($H = 42.6$).

Aspen Simulation

Choose the *RateFrac* block from the *Columns* subdirectory. Clicking on the down arrow next to the *RateFrac* block, a set of icons will pop up. These icons represent

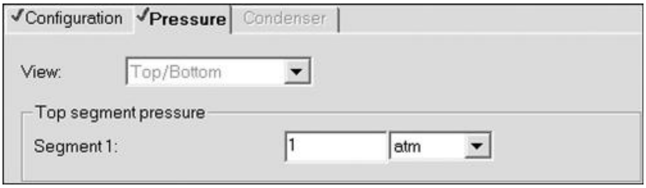


```
PROJECT                          PRO/II  VERSION 8.3 ELEC V7.0
PROBLEM                                       INPUT
                                       THERMODYNAMIC DATA
==================================================================

LN(H) = C1 + C2/T + C3*LN(T) + C4*P          where:
TEMPERATURE  IN K                              1  H2O
PRESSURE     IN BAR                            2  Air
                                               3  SO2

SOLUTE SOLVENT          C1          C2          C3          C4
------ -------  ----------- ----------- ----------- -----------
     2       1     153.0898  -7298.3920    -20.6029  1.4782E-04
     3       1      96.4632  -6706.1440    -12.3043      0.0000
```

FIGURE 7.5
Henry's law constants.



View: Top/Bottom

Top segment pressure

Segment 1: 1 atm

FIGURE 7.6
Pressure specification.

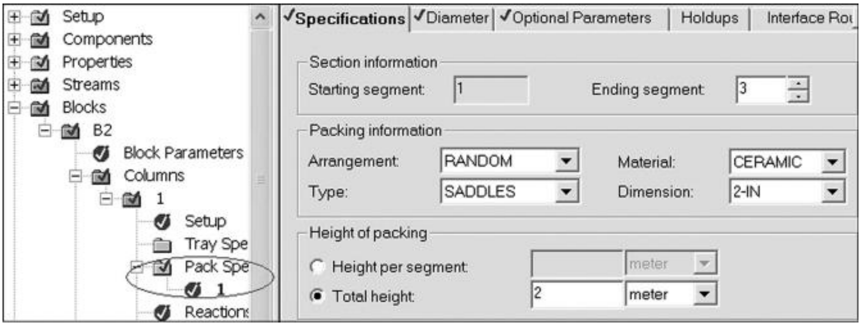
the same calculation procedure and are for different schematic purposes only. *RateFrac* is a rate-based nonequilibrium model for simulating all types of multistage vapor–liquid operations such as absorption, stripping, and distillation. *RateFrac* simulates actual tray and packed columns, rather than the idealized representation of equilibrium stages. The next screen allows you to select the type of pressure specification that you want to enter. Choose *Top/Bottom* and enter 1 atm pressure from the problem statement for segment 1. Segment 1 will refer to the first segment at the top of the tower (Figure 7.6). Click on *Next*.

The packing material is 2 in. ceramic Intalox Saddles randomly packed. The packing height that gives the desired separation is the value found from hand calculation. The required height of packing necessary to achieve the separation is 2 m as shown in Figure 7.7. Click on *Next* to continue.

The screen shown below asks to specify the location of feed inlets and outlets. Note that the inlet of gas stream should be entered in outside the bottom segment (number of segment + 1), because the convention for stream location is above the segment (Figure 7.8).

The following data (obtained from hand calculation) should be entered in the column block specifications window:

- Property method: NRTL
- Number of stages: 3
- Diameter: 1 m (initial estimate)
- Height: 2 m



Section information

Starting segment: 1

Ending segment: 3

Packing information

Arrangement: RANDOM

Material: CERAMIC

Type: SADDLES

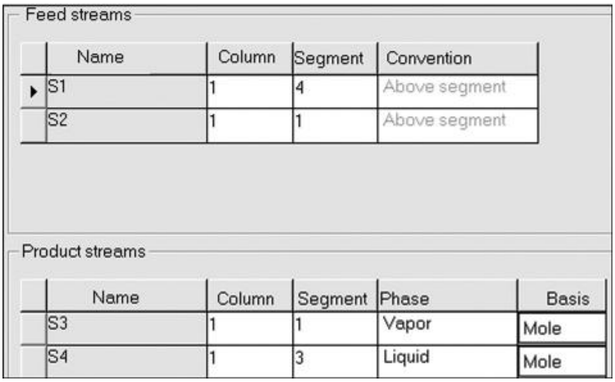
Dimension: 2-IN

Height of packing

○ Height per segment: meter

● Total height: 2 meter

FIGURE 7.7
Packed-specifications window.



Feed streams

Name	Column	Segment	Convention
S1	1	4	Above segment
S2	1	1	Above segment

Product streams

Name	Column	Segment	Phase	Basis
S3	1	1	Vapor	Mole
S4	1	3	Liquid	Mole

FIGURE 7.8
Feed and product stream locations.

- Packing type: 2 in. ceramic Intalox saddles
- Column pressure: 1 atm

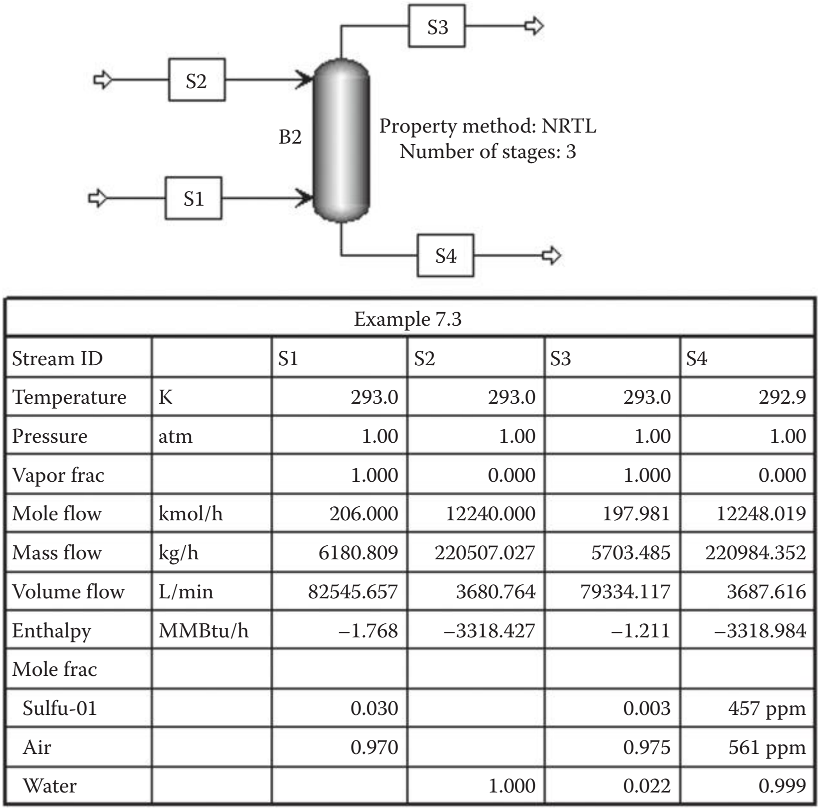
The required inputs are now entered and the simulation is ready to run. The results can be browsed by clicking on the double arrow next to the *Results* header. The Aspen Plus simulation result is shown in Figure 7.9.

SuperPro Designer Simulation

SuperPro Designer simulates the absorber tower in two modes; design mode and rating mode. In *Design Mode* calculation, the user can specify the column diameter or the pressure drop/length. In *User-Defined* (*Rating Mode*), the user specifies values for number of units, column diameter, and height. In *Design Mode*, the material balances are specified by the user (as % removed) and the separation specifications drive the equipment sizing calculation. In *Rating Mode*, the removal efficiency is either set by the user or calculated by the model.

The basic steps for creating a design case:

1. Specify *Mode of Operation* (i.e., continuous or batch)
2. Register *Components* and *Mixtures*;
    a. Tasks >> Register Components and Mixtures >> Pure Components
    b. To register pure components available in database:
        i. Select chemical compounds needed for the simulation either by:
            A. Typing the name of a chemical in the entry box.
            B. Scrolling up/down in *Pure Component Database* and selecting a chemical.
3. Click *Register*.
4. Unit procedures:
    a. To add a unit procedure select:
        i. Unit Procedures >> [Type of Procedure] >> [Procedure]
    b. For example, to add Absorber, select:
        i. Unit Procedures >> Absorption/Stripping >> Absorber

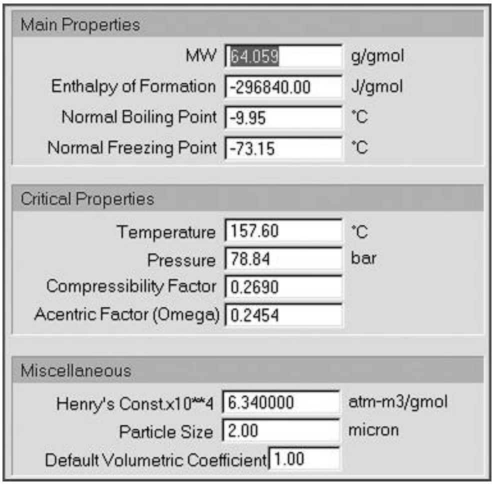


Example 7.3					
Stream ID		S1	S2	S3	S4
Temperature	K	293.0	293.0	293.0	292.9
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		1.000	0.000	1.000	0.000
Mole flow	kmol/h	206.000	12240.000	197.981	12248.019
Mass flow	kg/h	6180.809	220507.027	5703.485	220984.352
Volume flow	L/min	82545.657	3680.764	79334.117	3687.616
Enthalpy	MMBtu/h	−1.768	−3318.427	−1.211	−3318.984
Mole frac					
Sulfu-01		0.030		0.003	457 ppm
Air		0.970		0.975	561 ppm
Water			1.000	0.022	0.999

FIGURE 7.9
Stream summary using *RateFrac* columns in Aspen.

5. Input and output streams
   There are two modes in which the user can draw streams, *Connect Mode* and *Temporary Connect Mode*. *Connect Mode* is more convenient for drawing several streams at a time. To enter the connect mode, click on *Connect Mode* on the main toolbar; when in the connect mode, the cursor will change to the Connect Mode Cursor. The simulation will remain in the connect mode after you draw the stream(s). To leave the connect mode and return to select mode, click on *Arrow* next to *Connect Mode*. In the *Connect Mode*:
   a. Click once on an open area to begin drawing the stream.
   b. To change the direction of the stream, click once on the open area. The stream will bend at a 90° angle. Click once more to change the direction again. These direction changes are called stream elbows.
   c. Click once on an input port to connect the stream to the unit operation

The value of Henry's law constant should be provided. The value obtained from the literature is entered in *Physical (constants)* and then double click on the solute component name in the miscellaneous section (Figure 7.10).



Main Properties

MW 64.059 g/gmol

Enthalpy of Formation -296840.00 J/gmol

Normal Boiling Point -9.95 °C

Normal Freezing Point -73.15 °C

Critical Properties

Temperature 157.60 °C

Pressure 78.84 bar

Compressibility Factor 0.2690

Acentric Factor (Omega) 0.2454

Miscellaneous

Henry's Const.x10**4 6.340000 atm-m3/gmol

Particle Size 2.00 micron

Default Volumetric Coefficient 1.00

FIGURE 7.10
Henry's constant inlet menu.

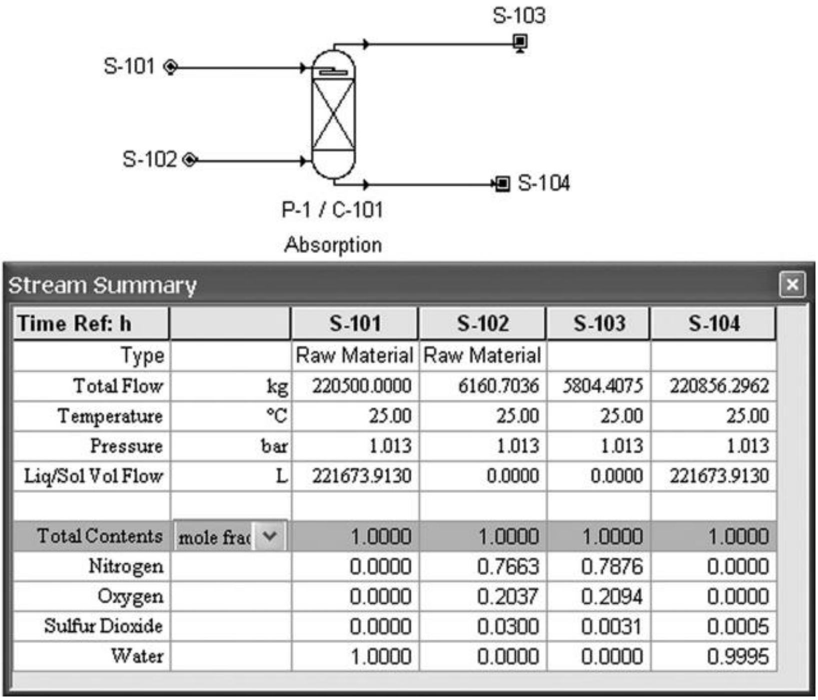
Tasks >> Edit Pure Components >> double click on the solute component

The inlet and exit streams are connected as shown in Figure 7.11. The design components calculated with SuperPro is shown in Figure 7.12.

The estimated number of transfer units (NTUs) is rounded off to 4.

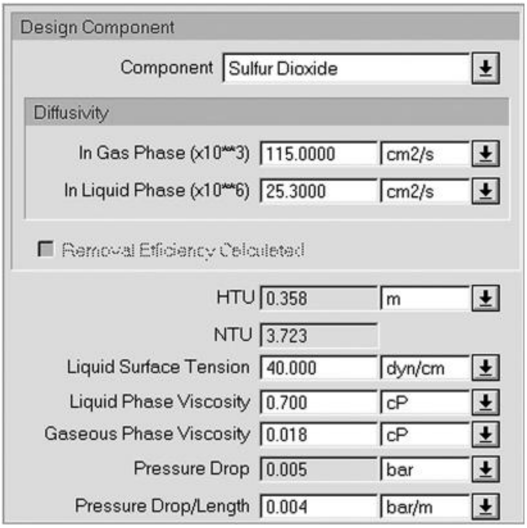
7.5 Packed-Bed Column Diameter

The main parameter affecting the size of a packed column is the gas velocity. At a fixed column diameter, when the gas flow rate through the column is gradually increased, a point will be reached where the liquid flowing down over the packing begins to be held in the void spaces between the packing. This gas-to-liquid ratio is termed as the loading point. The pressure drop of the column begins to increase and the degree of mixing between the phases decreases. A further increase in gas velocity will cause the liquid to completely fill the void spaces in the packing. The liquid forms a layer over the top of the packing and no more liquid can flow down through the tower. The pressure drop increases substantially, and mixing between the phases is minimal. This condition is referred to as flooding, and the gas velocity at which it occurs is the flooding velocity [9]. A typical operating range for the gas velocity through the columns is 50–75% of the flooding velocity, operating in this range; the gas velocity will be below the loading point. A common and relatively simple procedure for estimating flooding velocity is to use a generalized flooding and pressure drop correlation shown in Figure 7.1 [10]. Another factor influencing the tower diameter is the packing factor of the



Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	kg	220500.0000	6160.7036	5804.4075	220856.2962
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Liq/Sol Vol Flow	L	221673.9130	0.0000	0.0000	221673.9130
Total Contents	mole frac	1.0000	1.0000	1.0000	1.0000
Nitrogen		0.0000	0.7663	0.7876	0.0000
Oxygen		0.0000	0.2037	0.2094	0.0000
Sulfur Dioxide		0.0000	0.0300	0.0031	0.0005
Water		1.0000	0.0000	0.0000	0.9995

FIGURE 7.11
Process flow sheet and stream summary.



Component: Sulfur Dioxide

In Gas Phase (x10**3): 115.0000 cm2/s

In Liquid Phase (x10**6): 25.3000 cm2/s

☐ Removal Efficiency Calculated

HTU: 0.358 m

NTU: 3.723

Liquid Surface Tension: 40.000 dyn/cm

Liquid Phase Viscosity: 0.700 cP

Gaseous Phase Viscosity: 0.018 cP

Pressure Drop: 0.005 bar

Pressure Drop/Length: 0.004 bar/m

FIGURE 7.12
Column design component.

packing material used. The packing factor is inversely proportional to the packing size, the tower diameter requirements decrease as the size of packing material increases for the same inlet gas flow rate. The design is based on the gas flow rate at flooding conditions: the superficial gas flow rate entering the absorber, G_f (lb/s ft^2), or the gas flow rate per cross-sectional area is based on the L/G ratio. The cross-sectional area (A) of the column and the column diameter (D_t) can then be determined from G_f. Figure 7.1 presents the relationship between G_f and the L/G ratio at the tower flood point. The abscissa value (X-axis) in the graph is expressed as

$$X_{\text{axis}} = \left(\frac{L}{G}\right)\sqrt{\frac{\rho_G}{\rho_L}} \tag{7.6}$$

where L and G are the mass flow rate of the liquid stream and gas stream, respectively; ρ_G is the density of the gas stream; and ρ_L is the density of the absorbing liquid.

The ordinate value (Y-axis) in the graph is expressed as

$$Y_{\text{axis}} = \frac{G_f^2 \psi F_p \mu_L^{0.2}}{\rho_L \rho_G g} \tag{7.7}$$

where G_f is the mass flow rate of the gas, kg/s m^2 (lb/s ft^2); ψ is the ratio of the density of the scrubbing liquid to water; F_p is the packing factor, m^2/m^3, ft^2/ft^3; μ_L is the viscosity of the solvent, cP; ρ_L is the liquid density, kg/m^3; ρ_G is the gas density, kg/m^3; and g is the gravitational constant, 9.82 m/s^2 (32.2 ft/s^2).

The value of the packing factor, F_p, is obtained from Table 7.2 or from vendors.

TABLE 7.2

Design Data for Various Random Packing

Packing Type	Size in. (mm)	Weight (kg/m^3)	Surface Area a (m^2/m^3)	Packing Factor F_p m^{-1}
Ceramic *Raschig* rings	1/2 (13)	881	368	2100
	1 (25)	673	190	525
	1 1/2 (38)	689	128	310
	2 (51)	651	95	210
	3 (76)	561	69	120
Ceramic Intalox Saddles	1/2 (13)	737	480	660
	1 (25)	673	253	300
	1 1/2 (38)	625	194	170
	2 (51)	609	108	130

Source: Data from Sinnott, R. K. 1999. *Coulson & Richardson's Chemical Engineering.* Vol. 6, 3rd edn. Butterworth Heinemann, Oxford.

After calculating the *Abscissa* (X_{axis}) value, a corresponding *Ordinate* (Y_{axis}) value may be determined from the flooding curve. The *Ordinate* may also be calculated using the following equation:

$$Y_{\text{axis}} = 10^{\xi} \tag{7.8}$$

where $\xi = -1.668 - 1.085(\log X_{\text{axis}}) - 0.297(\log X_{\text{axis}})^2$.

Equation 7.2 may then be rearranged to solve for G_f:

$$G_f = \left[\frac{\rho_L \rho_G\, g(Y_{\text{axis}})}{F_p \psi\, \mu_L^{0.2}}\right]^{0.5} \tag{7.9}$$

where ρ_G and ρ_L in kg/m^3, $g = 9.82$ m/s^2, F_P packing factor in m^2/m^3 and μ_L in cP; ψ is the ratio of specific gravity of the scrubbing liquid to that of water.

The cross-sectional area of the tower is calculated as

$$A = \frac{G_m}{f\, G_f} \tag{7.10}$$

f is a flooding factor. To prevent flooding, the column is operated at a fraction of G_f. The value of f typically ranges from 0.60 to 0.85. The diameter of the column can be calculated from the cross-sectional area [9,10]:

$$D_t = \sqrt{\frac{4A}{\pi}} \tag{7.11}$$

As a rule of thumb, the diameter of the column should be at least 15 times the size of the packing used in the column. If this is not the case, the column diameter should be recalculated using a smaller-diameter packing [10]. The superficial liquid flow rate entering the absorber, L_f (lb/h-ft^2) based on the cross-sectional, is

$$L_f = \frac{L}{A} \tag{7.12}$$

For the absorber to operate properly, the liquid flow rate entering the column must be high enough to effectively wet the packing so that mass transfer between the gas and liquid can occur. The minimum value of $(L_f)_{\min}$ that is required to wet the packing effectively can be calculated using the equation

$$(L_f)_{\min} = \text{MWR}\,\rho_L\, a \tag{7.13}$$

where MWR is the minimum wetting rate (ft^2/h) and *a* is the surface area-to-volume ratio of packing (ft^2/ft^3). An MWR value of 0.85 ft^2/h is recommended for ring packing larger than 3 in. and for structured grid packing. For other packing; MWR of 1.3 ft^2/h is recommended [7,13].

Example 7.4: Absorption of SO_2 from Air with Pure Water

A gas absorber is used to remove 90% of the SO_2 from a gas stream with pure water. The stream mass flow rate is 103 kg/min. The gas stream contains 3% SO_2 by volume. The minimum liquid flow rate was 2450 kg/min. The temperature is 293 K and the pressure is 101.32 kPa. The gas velocity should be no greater than 70% of the flooding velocity, and the randomly packed material is 2 in. Ceramic Intalox Saddles. The liquid mass flow rate is 1.5 times the minimum liquid mass flow rate. Determine the packed-column diameter.

SOLUTION

HAND CALCULATIONS

The liquid mass flow rate is 1.5 times the minimum liquid flow rate:

$$L = 1.5 \times L_m = 1.5 \times 2450 = 3675 \text{ kg/min}$$

The superficial flooding velocity is the flow rate per unit of cross-sectional area of the tower.

$$\text{Abscissa} = \left(\frac{L}{G}\right)\left(\frac{\rho_g}{\rho_l}\right)^{0.5} = \left(\frac{3{,}675\text{ kg/min}}{103\text{ kg/min}}\right)\left(\frac{1.17\text{ kg/m}^3}{1000\text{ kg/m}^3}\right)^{0.5} = 1.22$$

Using Figure 7.13, with the abscissa of 1.22, move up to the flooding line, the value is on the ordinate ($Y_{\text{axis}} = 0.02$).

$$G_f = \left[\frac{\rho_L \rho_G\, g(Y_{\text{axis}})}{F_p \psi \mu_L^{0.2}}\right]^{0.5}$$

where $\rho_G = 1.17$ kg/m^3, density of air at 30°C; $\rho_L = 1000$ kg/m^3, density of water at 30°C; $g = 9.82$ m/s^2, the gravitational constant; $F_P = 131$ m^2/m^3, the packing factor for 2 in.; Ceramic Intalox Saddles; $\psi = 1.0$, the ratio of specific gravity of the scrubbing liquid to that of water; and $\mu_L = 0.8$ cP, the viscosity of liquid.
The superficial flooding velocity at flooding:

$$G_f = \left[\frac{(1.17\text{ kg/m}^3)(1000\text{ kg/m}^3)(9.82\text{ m/s}^2)(0.02)}{(131\text{m}^2/\text{m}^3)(1)(0.8\text{ cP})^{0.2}}\right]^{0.5} = 1.354\text{ kg/sm}^2$$

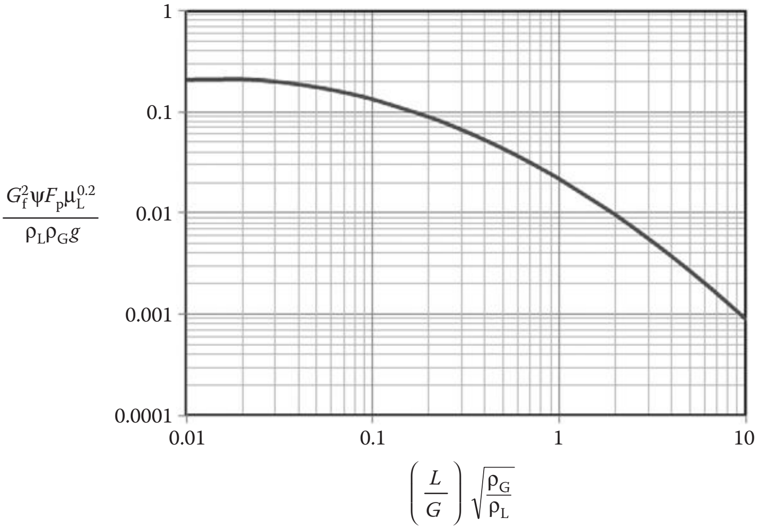


FIGURE 7.13
Eckert's correlation at flooding rate.

The superficial gas velocity at operating conditions (G_{op}), where the absorber operates at 70% of the flooding velocity, hence

$$G_{op} = f \times G_f, \quad \text{where } f = 0.70$$

$$G_{op} = 0.70 \times 1.354 \text{ kg/s m}^2 = 0.95 \text{ kg/sm}^2$$

The cross-sectional area of the packed tower is

$$A = \frac{G}{G_{op}} = \frac{103 \text{ kg/min} \,\big|\, 1 \text{min}/60\, s}{0.95 \text{ kg/s m}^2} = 1.81 \text{m}^2$$

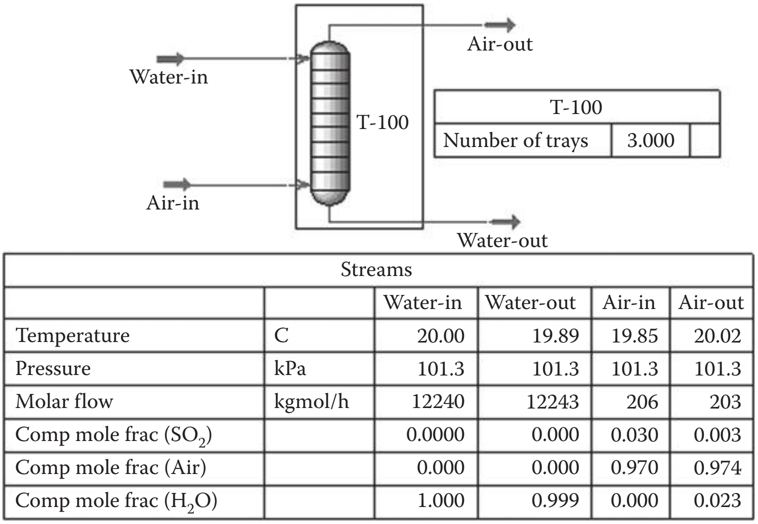
The tower diameter

$$D_t = \left(\frac{4A}{\pi}\right)^{0.5} = \left(\frac{4 \times 1.81 \text{m}^2}{3.14}\right)^{0.5} = 1.52 \text{ m}$$

Hysys Simulation

The *Absorber* icon from the object palette is selected for this purpose. The feed streams are fully specified (i.e., air-in and water-in streams). The number of stages is set to 3. The process flow sheet and the stream summary are shown in Figure 7.14.

The diameter of the tower is determined using Tools/utilities/trays sizing. The diameter obtained by Hysys is different from that obtained by hand calculations; the Hysys result is shown in Figure 7.15.



T-100		
Number of trays	3.000	

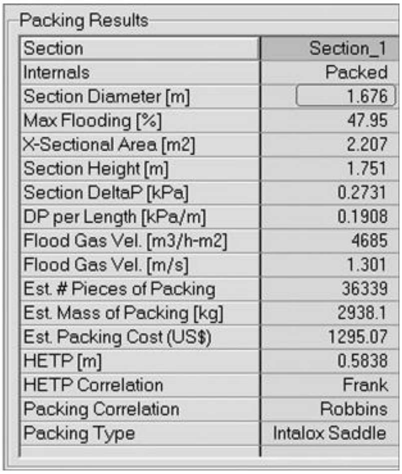
Streams					
		Water-in	Water-out	Air-in	Air-out
Temperature	C	20.00	19.89	19.85	20.02
Pressure	kPa	101.3	101.3	101.3	101.3
Molar flow	kgmol/h	12240	12243	206	203
Comp mole frac (SO_2)		0.0000	0.000	0.030	0.003
Comp mole frac (Air)		0.000	0.000	0.970	0.974
Comp mole frac (H_2O)		1.000	0.999	0.000	0.023

FIGURE 7.14
Process flow sheet and stream summary.

PRO/II SIMULATION

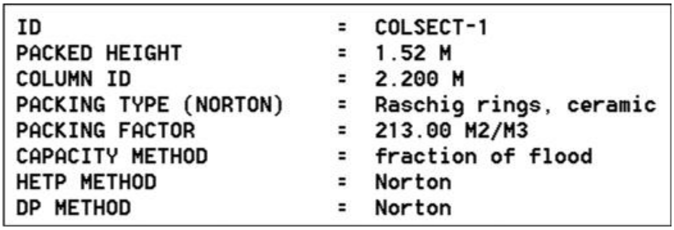
Using the data obtained in the hand calculations obtained in Example 7.3, the diameter calculated with PRO/II is shown in Figure 7.16. The data are found from the generated text report.

Output >> Generate text report



Section	Section_1
Internals	Packed
Section Diameter [m]	1.676
Max Flooding [%]	47.95
X-Sectional Area [m2]	2.207
Section Height [m]	1.751
Section DeltaP [kPa]	0.2731
DP per Length [kPa/m]	0.1908
Flood Gas Vel. [m3/h-m2]	4685
Flood Gas Vel. [m/s]	1.301
Est. # Pieces of Packing	36339
Est. Mass of Packing [kg]	2938.1
Est. Packing Cost (US$)	1295.07
HETP [m]	0.5838
HETP Correlation	Frank
Packing Correlation	Robbins
Packing Type	Intalox Saddle

FIGURE 7.15
Packed-column performance page.



```
ID                          =   COLSECT-1
PACKED HEIGHT               =   1.52 M
COLUMN ID                   =   2.200 M
PACKING TYPE (NORTON)       =   Raschig rings, ceramic
PACKING FACTOR              =   213.00 M2/M3
CAPACITY METHOD             =   fraction of flood
HETP METHOD                 =   Norton
DP METHOD                   =   Norton
```

FIGURE 7.16
Column diameter.

Aspen Simulation

The *Absorber* column is selected from *Ratefrac* in the *Column* subdirectory. After specifying feed streams, the following data (obtained from hand calculation) should be entered in the column block specifications window:

- Property method: NRTL
- Number of stages: 3
- Diameter: 1 m (initial estimate)
- Height: 2 m
- Packing type: ceramic Intalox saddles, 2 in.
- Column pressure: 1 atm

After the required data are entered, the system is ready to be run. The Aspen Plus simulation results are shown in Figure 7.17. The packed-bed diameter is obtained from design specifications of the *Flow sheet*ing options in the *Browser* menu.

Flow sheeting Options >> Design Spec >> New >> OK >>

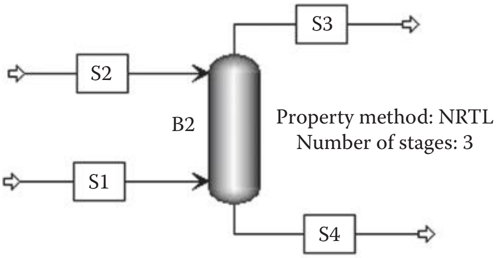
Enter the flow sheet name; CONC was entered for this example. Click on *Edit* and enter the variable component as shown in Figure 7.18. Click on the *Spec* tab and enter the design specification expressions as shown in Figure 7.19. Click on the *Vary* tab to enter the manipulated variable information and manipulated limit as shown in Figure 7.20. Run the system and explore the data for the final design specification of the diameter. If everything is done correctly the diameter converged value is obtained as shown in Figure 7.21.

SuperPro Designer Simulation

Follow the same procedure of example 7.3; Section 7.3.5. The value of Henry's law constant 6.34×10^{-4},atm m^3/mol should be provided; this value obtained from the literature is entered in the *Physical (constants)* and then double click on the solute component name in the miscellaneous section (Figure 7.22).

Tasks >> Edit Pure Components >> double click on the solute component

The inlet and exit streams are connected as shown in Figure 7.23. The design components calculated with SuperPro is shown in Figures 7.23 through 7.26. The packing material is 2 in. ceramic Intalox Saddles [10].



Example 7.4					
Stream ID		S1	S2	S3	S4
Temperature	K	293.0	293.0	293.0	292.9
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		1.000	0.000	1.000	0.000
Mole flow	kmol/h	206.000	12240.000	191.053	12254.947
Mass flow	kg/h	6180.809	220507.027	5508.313	221179.523
Volume flow	l/min	82545.657	3680.764	76556.458	3692.213
Enthalpy	MMBtu/h	−1.768	−3318.427	−1.163	−3319.031
Mole frac					
Sulfu-01		0.030		0.003	451 ppm
Air		0.970		0.975	0.001
Water			1.000	0.022	0.998

FIGURE 7.17
Stream summary using *RateFrac* columns in Aspen.

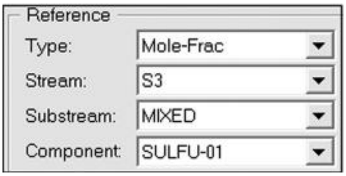
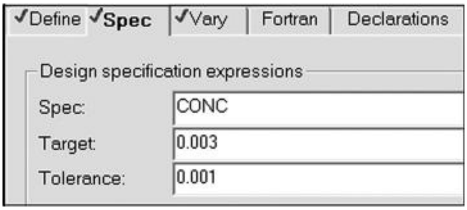
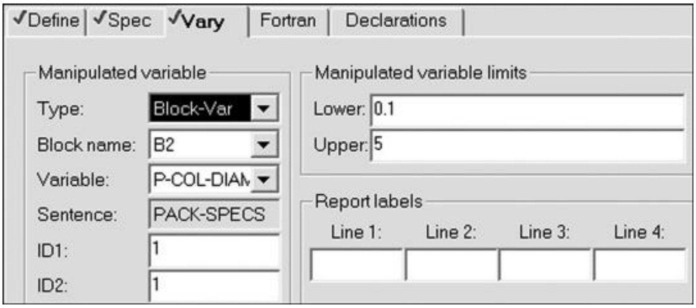

Reference
Type: Mole-Frac
Stream: S3
Substream: MIXED
Component: SULFU-01

FIGURE 7.18
Design specification page.



Design specification expressions
Spec: CONC
Target: 0.003
Tolerance: 0.001

FIGURE 7.19
Design specification.



Manipulated variable

Type: Block-Var
Block name: B2
Variable: P-COL-DIAM
Sentence: PACK-SPECS
ID1: 1
ID2: 1

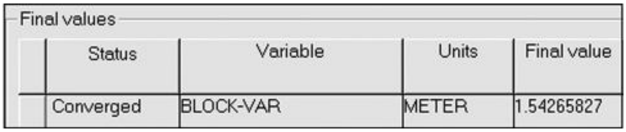
Manipulated variable limits

Lower: 0.1
Upper: 5

Report labels

Line 1:
Line 2:
Line 3:
Line 4:

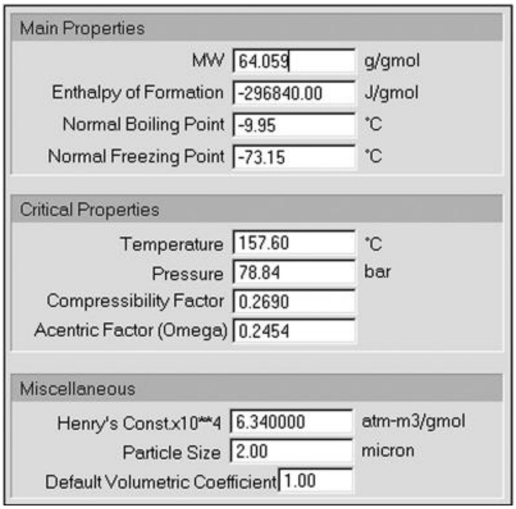
FIGURE 7.20
Manipulated variable, packed-column diameter.



Final values

Status	Variable	Units	Final value
Converged	BLOCK-VAR	METER	1.54265827

FIGURE 7.21
Diameter of packed column.



Main Properties

MW 64.059 g/gmol
Enthalpy of Formation -296840.00 J/gmol
Normal Boiling Point -9.95 °C
Normal Freezing Point -73.15 °C

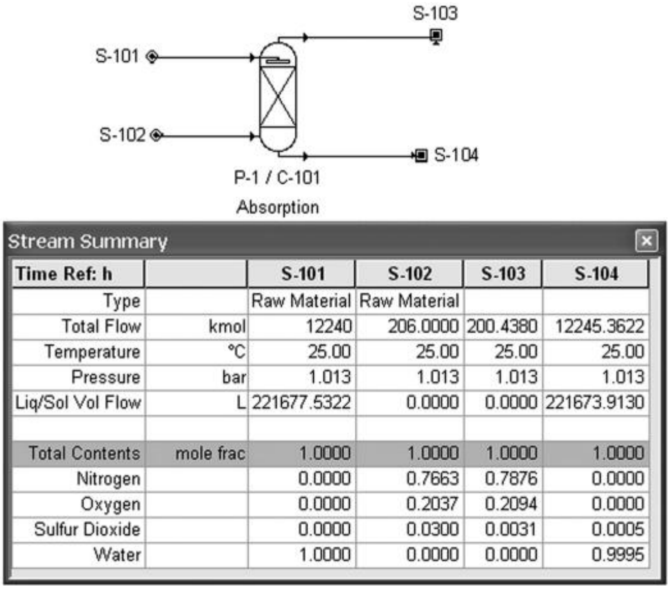
Critical Properties

Temperature 157.60 °C
Pressure 78.84 bar
Compressibility Factor 0.2690
Acentric Factor (Omega) 0.2454

Miscellaneous

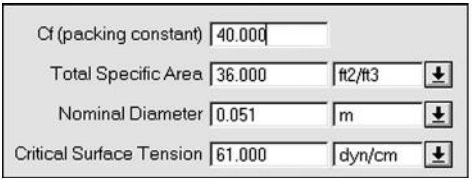
Henry's Const.x10**4 6.340000 atm-m3/gmol
Particle Size 2.00 micron
Default Volumetric Coefficient 1.00

FIGURE 7.22
Henry's constant inlet menu.



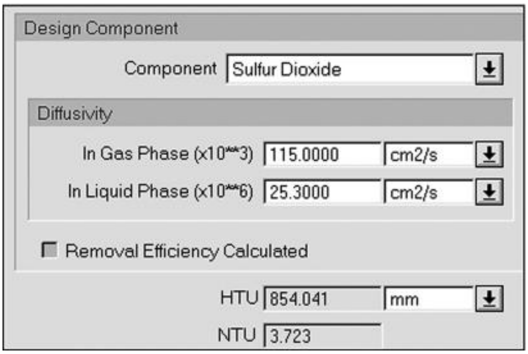
Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	kmol	12240	206.0000	200.4380	12245.3622
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Liq/Sol Vol Flow	L	221677.5322	0.0000	0.0000	221673.9130
Total Contents	mole frac	1.0000	1.0000	1.0000	1.0000
Nitrogen		0.0000	0.7663	0.7876	0.0000
Oxygen		0.0000	0.2037	0.2094	0.0000
Sulfur Dioxide		0.0000	0.0300	0.0031	0.0005
Water		1.0000	0.0000	0.0000	0.9995

FIGURE 7.23
Process flow sheet and stream summary.



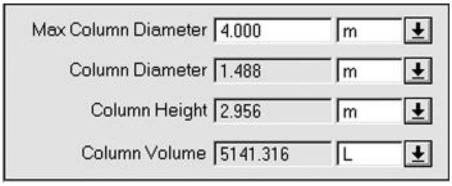
Cf (packing constant) 40.000
Total Specific Area 36.000 ft2/ft3
Nominal Diameter 0.051 m
Critical Surface Tension 61.000 dyn/cm

FIGURE 7.24
Specifications of packing material.



Design Component
Component Sulfur Dioxide
Diffusivity
In Gas Phase (x10**3) 115.0000 cm2/s
In Liquid Phase (x10**6) 25.3000 cm2/s
☐ Removal Efficiency Calculated
HTU 854.041 mm
NTU 3.723

FIGURE 7.25
Column design component.



Max Column Diameter 4.000 m

Column Diameter 1.488 m

Column Height 2.956 m

Column Volume 5141.316 L

FIGURE 7.26
Column design options.

7.6 Packed-Tower Height

The height of a packed column refers to the depth of packing material needed to accomplish the required removal efficiency. The more difficult the separation, the larger the packing height required. Determining the proper height of packing is important since it affects both the rate and the efficiency of absorption. A number of theoretical equations are used to predict the required packing height. These equations are based on diffusion principles [4].

7.6.1 Estimation of H_{OG} Using Onde's Method

The film mass-transfer coefficient k_G and k_L and effective wetted area of packing a_w are calculated using the correlation developed by Onda et al. [11], which can be used to calculate H_G and H_L

$$a_w = a_P\left\{1 - \exp\left[(-1.45)\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{L}{a_P\,\mu_L}\right)^{0.1}\left(\frac{L^2 a_P}{\rho_L^2 g}\right)^{-0.05}\left(\frac{L^2}{\rho_L\,\sigma\,a_P}\right)^{0.2}\right]\right\} \tag{7.14}$$

k_G and k_L are calculated from the following correlations:

$$k_G\left(\frac{RT}{a_P D_G}\right) = 5.23\left(\frac{G}{a_P\mu_G}\right)^{0.70}(Sc_G)^{1/3}(a_P d_P)^{-2} \tag{7.15}$$

$$k_L\left(\frac{\rho_L}{g\mu_L}\right)^{1/3} = 0.0051\left(\frac{L}{a_w\mu_L}\right)^{2/3}(Sc_L)^{-1/2}(a_P d_P)^{0.40} \tag{7.16}$$

where k_G is the gas film mass transfer coefficient, kmol/m^{2}s atm; k_L is the liquid film mass transfer coefficient, kmol/m^{2}s (kmol/m^3) [=] m/s; a_P is the total packing surface area per packed-bed volume, m^2/m^3; d_P is the packing size, m; L, G are the superficial mass velocity of liquid and gas, kg/m^{2}s; μ_L is the liquid phase viscosity, kg/m s; ρ_L is the liquid phase density, kg/m^3; σ_L is the water surface tension, N/m; $\sigma_c = 61$ dyne/cm for ceramic packing, 75 dyne/cm for steel packing, and 33 dyne/cm for plastic packing; D_G and D_L are diffusivity in the gas and liquid phase, respectively, m^2/s; $R = 0.08314$ m^3 bar/kmol K; and $g = 9.81$ m/s^2, d_P is the equivalent diameter of the packing and is calculated using the following equations:

$$d_P = \frac{6}{a_p}(1-\varepsilon)\left[=\right]m \tag{7.17}$$

The diffusion coefficient for the gas

$$D_{AB,G} = \frac{0.001T^{1.75}[M_{WA} + M_{WB}/M_{WA}.M_{WB}]}{P(a^{1/3}.b^{1/3})}\left[=\right]\frac{\text{cm}^2}{\text{s}} \tag{7.18}$$

where a and b are the atomic diffusion volumes of solute A in inert gas phase B, cm^3/mol; M_{WA} and M_{WB} are the molecular weights of A and B, respectively; and P is the pressure, atm.

$$D_{AB,L} = \frac{9.89 \times 10^{-8}.V_B^{0.265}.T}{V_A^{0.45}\mu_L^{0.907}}\left[=\right]\frac{\text{cm}^2}{\text{s}} \tag{7.19}$$

where V_A and V_B are the molar volume at normal boiling point of solute A in liquid phase B, cm^3/mol; T is the liquid stream temperature, K; μ_L is the liquid viscosity, kg/m s; and μ_G is the gas viscosity, kg/m s; the heights of transfer unit for the gas phase (H_G) and the liquid phase (H_L) are

$$H_G = \frac{G_m}{k_G.a_w.P}\left[=\right]\frac{(\text{kmol/m}^2\,\text{s})}{(\text{kmol/m}^2\,\text{s bar})(1/\text{m})(\text{bar})}\left[=\right]\text{m} \tag{7.20}$$

$$H_L = \frac{L_m}{k_L.a_w.C_T}\left[=\right]\frac{(\text{kmol/m}^2\,\text{s})}{(\text{m/s})(1/\text{m})(\text{kmol/m}^3)}\left[=\right]\text{m} \tag{7.21}$$

where P is the column pressure, atm; C_T is the total concentration, kmol/m^3 (ρ_L/molecular weight of solvent); G_m is the molar gas flow rate per cross-sectional area, kmol/m^2 s; and L_m is the molar liquid flow rate per unit cross-sectional area, kmol/m^2 s.

The overall height of transfer units (HTUs),

$$H_{OG} = H_G + \frac{mG_m}{L_m}H_L \tag{7.22}$$

7.6.2 Estimation of H_{OG} Using Cornell's Method

The empirical equations for predicting the height of the gas and liquid film transfer units [9]:

The height of the liquid film transfer units

$$H_L = 0.305 \times \phi_h (\mathrm{Sc_L})^{0.5} \times K_3 \left(\frac{Z}{3.05}\right)^{0.15} \tag{7.23}$$

The height of the gas film transfer units

$$H_G = \frac{0.011 \times \psi_h (\mathrm{Sc_G})^{0.5} \left(\frac{D_c}{3.05}\right)^{1.11} \left(\frac{Z}{3.05}\right)^{0.33}}{\left(L f_1 f_2 f_3\right)^{0.5}} \tag{7.24}$$

The term of diameter correction is taken as fixed 2.3 for diameter greater than 0.6 m.

$$H_G = \frac{0.011 \times \psi_h (\mathrm{Sc_G})^{0.5} (2.3) \left(\frac{Z}{3.05}\right)^{0.33}}{\left(L f_1 f_2 f_3\right)^{0.5}} \tag{7.25}$$

where K_3, ϕ_h, and ψ_h can be found elsewhere [9,10], the following correlation can also be used:

The percentage flooding correction factor, K_3.

$K_3 = 1$ for percentage flooding less than 45, and the following approximate equation can be used for a higher percentage of flooding F;

$$K_3 = -0.014F + 1.685 \tag{7.26}$$

Factors for H_G using Berl saddles, particle size $1\frac{1}{2}$ in. (38 mm), ψ_h

$$\psi_h = 9 \times 10^{-4} F^3 - 0.12F^2 + 5.29F + 0.834 \tag{7.27}$$

Factor for H_L using particle size $1\frac{1}{2}$ in. (38 mm), ϕ_h

$$\phi_h = 0.034 L_f^{0.4} \tag{7.28}$$

where L_f is the liquid mass velocity; kg/m² s.

Schmidt numbers for gas and liquid phases

$$\mathrm{Sc_G} = \frac{\mu_G}{\rho_g D_G}, \quad \mathrm{Sc_L} = \frac{\mu_L}{\rho_L D_L}$$

Liquid properties correction factor:

$$f_1 = \left(\frac{\mu_L}{\mu_W}\right)^{0.16} \tag{7.29}$$

$$f_2 = \left(\frac{\rho_W}{\rho_L}\right)^{1.25} \tag{7.30}$$

$$f_3 = \left(\frac{\sigma_W}{\sigma_L}\right)^{0.8} \tag{7.31}$$

where $\mu_w = 1.0$ mPa s(1 cP), $\rho_w = 1000$ kg/m^3, $\sigma_w = 72.8$ mN/m.

The height of the overall transfer unit

$$H_{OG} = H_G + \frac{mG_m}{L_m} \times H_L \tag{7.32}$$

Multiplying both sides of the equation by N_{OG},

$$N_{OG} \times H_{OG} = N_{OG} \times \left[H_G + \frac{mG_m}{L_m} \times H_L\right] \tag{7.33}$$

Since $Z = H_{pack} = N_{OG} \times H_{OG}$

The total height of the column may be calculated from the following correlation:

$$H_{tower} = 1.4\, H_{pack} + 1.02\, D + 2.81 \tag{7.34}$$

Equation 7.34 was developed from information reported by gas absorber vendors, and is applicable for column diameters from 2 to 12 feet and packing depths from 4 to 12 ft. The surface area (S) of the gas absorber can be calculated using the equation

$$S = \pi D\left(H_{tower} + \frac{D}{2}\right) \tag{7.35}$$

Example 7.5: Absorber Total Packing Height

It was determined that the H_{OG} of the SO_2/H_2O system is 0.6 m. Calculate the total height of packing required to achieve 90% reduction in the inlet concentration.

The packing is *Raschig* ring ceramic, 2 in. The process operating conditions is 20°C and 1 atm.

The following data were taken from the previous examples:

Henry's constant, $H = 26$.
G_m, molar flow rate of gas = 206 kmol/h.
L_m, molar flow rate of liquid = 12,240 kmol/h.
x_2, mole fraction of solute in entering liquid = 0 (no recycle liquid).
y_1, mole fraction of solute in entering gas = 0.03.
y_2, mole fraction of solute in existing gas = 0.003.

SOLUTION

HAND CALCULATIONS

The number of theoretical transfer units

$$N_{OG} = \frac{\ln\left[(y_1 - mx_2/y_2 - mx_2)(1 - mG_m/L_m) + mG_m/L_m\right]}{1 - (mG_m/L_m)}$$

The value of the inverse of the slope of the operating line to the equilibrium line:

$$\frac{mG_m}{L_m} = \frac{26 \times 206}{12{,}240} = 0.438$$

Substituting values:

$$N_{OG} = \frac{\ln\left[(0.03 - 0/0.003 - 0)(1 - 0.438) + 0.438\right]}{1 - 0.438} = 3.2$$

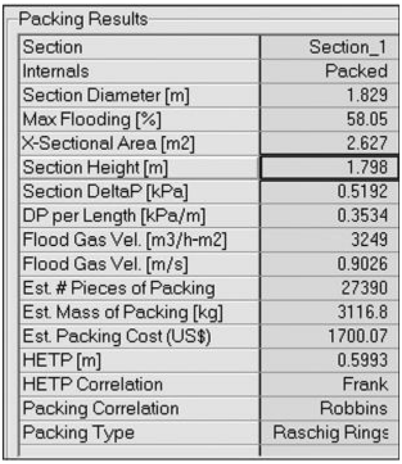
Rounding off the number of transfer stages to 4
The total packing height, Z,

$$Z = H_{OG} \times N_{OG}$$

Given; $H_{OG} = 0.60$ m is the overall height of a transfer unit.
$Z = (0.6 \text{ m})\ (3.2) = 1.922$ m of packing height.

HYSYS/UNISIM SIMULATION

Following the same procedure in simulating Example 7.3, and employing tray sizing utilities in Hysys, the HTUs is 0.6 m as shown in Figure 7.27. The simulated packing height is 3 m (Figure 7.27). Trying three stages it was possible to achieve a mole fraction in the exit air is 0.003.



Packing Results

Section	Section_1
Internals	Packed
Section Diameter [m]	1.829
Max Flooding [%]	58.05
X-Sectional Area [m2]	2.627
Section Height [m]	1.798
Section DeltaP [kPa]	0.5192
DP per Length [kPa/m]	0.3534
Flood Gas Vel. [m3/h-m2]	3249
Flood Gas Vel. [m/s]	0.9026
Est. # Pieces of Packing	27390
Est. Mass of Packing [kg]	3116.8
Est. Packing Cost (US$)	1700.07
HETP [m]	0.5993
HETP Correlation	Frank
Packing Correlation	Robbins
Packing Type	Raschig Rings

FIGURE 7.27
Absorber packed-bed height.

PRO/II SIMULATION

Using the converged file in Example 7.3 with three stages, the packed height is estimated by clicking on *Tray Hydraulics/Packin*g and entering in the packing internals as shown in Figure 7.28.

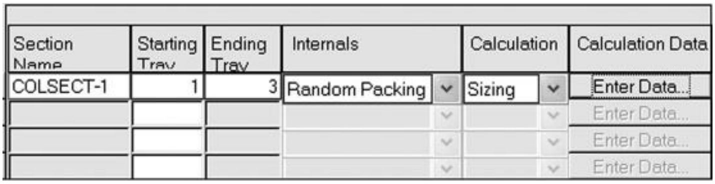
Click on *Enter Data* and enter the type of packing, packing size, and packing factor as shown in Figure 7.29.

The results are extracted from the output generated text report as shown in Figure 7.30.

ASPENPLUS SIMULATION

In this case, *RateFrac* absorber from the *Column* subdirectory is selected. Feed streams and outlet streams are connected. NRTL was selected for the property method. The number of stages is three trays. The packed height of the column is the manipulated variable (Figure 7.31).

The simulated packed-bed column with three stages achieves 0.003 mol fraction of SO_2 in the exit air stream as shown in Figure 7.32 (the conditions are the same as Example 7.3). The final results converged when a packing height of 1.39 m is reached.



Section Name	Starting Tray	Ending Tray	Internals	Calculation	Calculation Data
COLSECT-1	1	3	Random Packing	Sizing	Enter Data...
					Enter Data...
					Enter Data...
					Enter Data...

FIGURE 7.28
Tray hydraulics' page.

Packing Characteristics

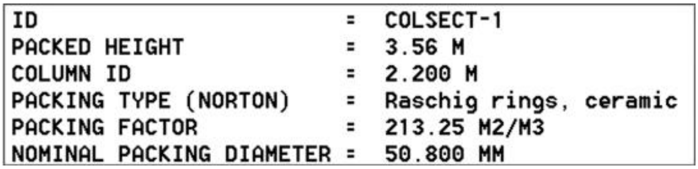
Manufacturer: Norton

Type: Raschig Rings (Ceramic)

Packing Size: 50.8 mm

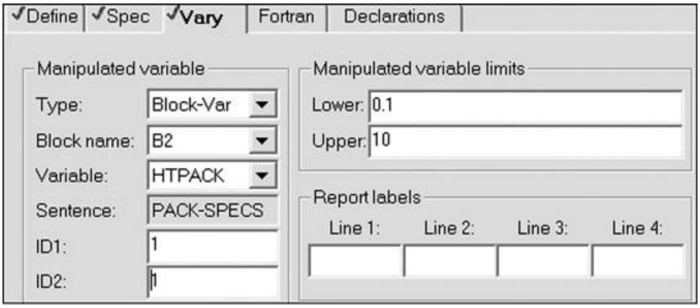
Packing 213.25 m2/m3

FIGURE 7.29
Packing characterization menu.



```
ID                       =  COLSECT-1
PACKED HEIGHT            =  3.56 M
COLUMN ID                =  2.200 M
PACKING TYPE (NORTON)    =  Raschig rings, ceramic
PACKING FACTOR           =  213.25 M2/M3
NOMINAL PACKING DIAMETER =  50.800 MM
```

FIGURE 7.30
Height of the packed column.



Manipulated variable

Type: Block-Var

Block name: B2

Variable: HTPACK

Sentence: PACK-SPECS

ID1: 1

ID2: 1

Manipulated variable limits

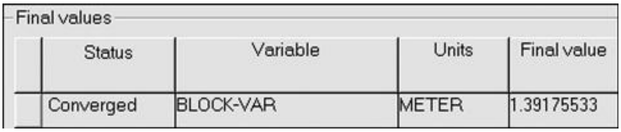
Lower: 0.1

Upper: 10

Report labels

Line 1: Line 2: Line 3: Line 4:

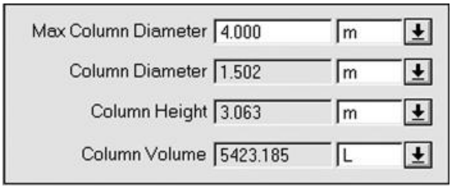
FIGURE 7.31
Manipulated variable.



Final values

Status	Variable	Units	Final value
Converged	BLOCK-VAR	METER	1.39175533

FIGURE 7.32
Absorber backing height calculated by Aspen Plus.



Max Column Diameter 4.000 m

Column Diameter 1.502 m

Column Height 3.063 m

Column Volume 5423.185 L

FIGURE 7.33
Diameter of the packed tower obtained by SuperPro Designer.

SuperPro Designer

Following the same procedure in Example 7.3, from the equipment data the diameter and the column height are shown in Figure 7.33.

Example 7.6: Number of Theoretical Stages

Sulfur dioxide in air is absorbed by pure water at 1 atm and 20°C. The gas feed stream is 5000 kg/h containing 8 mol% SO_2 in air. A 95% recovery of the sulfur dioxide is required. The inlet solvent is pure water with inlet mass flow rate of 29.5 kg/s. The solubility of SO_2 in water is shown in Table 7.3. For packing material, 1 1/2 in. ceramic Intalox Saddles is used. Design an absorber column for this purpose [9].

SOLUTION

Hand Calculations

The equilibrium mole fraction of SO_2 in liquid

$$x = \frac{(0.05/64)}{0.05/64 + (100 - 0.05)/18} = 0.00014$$

The equilibrium mole fraction of SO_2 in the gas phase

$$y = \frac{1.2\,\text{mmHg}}{760\,\text{mmHg}} = 0.002$$

TABLE 7.3
Solubility Data of SO_2

Mass Fraction SO_2 in Water	SO_2 Partial Pressure in Air (mmHg)
0.05	1.2
0.15	5.8
0.30	14
0.50	26
0.70	39
1.00	59

Source: Data from Perry, J.H. 1973. *Chemical Engineers' Handbook*, 5th edn, McGraw-Hill, New York, NY.

TABLE 7.4

Mole Fraction of SO_2 in Liquid Phase and Gas Phase at Equilibrium

Mole Fraction of SO_2 in Water (x)	Mole Fraction of SO_2 in Air (y)
0.00014	0.002
0.00042	0.008
0.00085	0.018
0.00141	0.034
0.00198	0.051
0.00283	0.077

Other values are calculated in the same manner as shown in Table 7.4.

The plot of the equilibrium line is shown in Figure 7.34.

The slope of the equilibrium line is the Henry's law constant is 26 (i.e., $m = 26$). In this section the number of theoretical stages, the column diameter, and column height are to be calculated.

The number of theoretical stages:

The liquid molar flow rate, L_m

$$\text{Gas molar flow rate}\,(G_m) = \frac{5000}{3600} = 1.39\ \text{kg/s} = \frac{1.39}{29} = 0.048\ \text{kmol/s}$$

$$\text{Liquid molar flow rate}\ (L_m) = \left(29.5\ \text{kg/s}\right)\left(\frac{\text{kmol}}{18\ \text{kg}}\right) = 1.64\ \text{kmol/s}$$

$$N_{OG} = \frac{\ln\left[(y_1 - mx_2/y_2 - mx_2)(1 - mG_m/L_m) + mG_m/Lm\right]}{1 - mG_m/L_m}$$

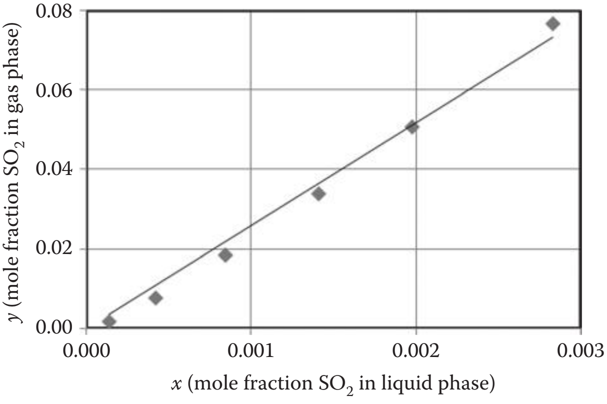


FIGURE 7.34

Plot of mole fraction in gas phase versus liquid phase at equilibrium.

Substituting values in the above equation:

$$N_{OG} = \frac{\ln\left[\left(0.08 - 0/0.004 - 0\right)\left(1 - (26)(0.048)/1.64\right) + (26)(0.048)/1.64\right]}{1 - (26)(0.048)/1.64}$$

$$= 6.15$$

The number of theoretical palettes is rounded off to seven trays.

COLUMN DIAMETER

The physical properties of the gas can be taken as those for air, as the concentration of SO_2 is low. The packing material: 38 mm (1 1/2 in.) ceramic Intalox saddles, $F_p = 170\ \text{m}^{-1}$

$$\text{Gas density } (\rho_g) \text{ at } (20°\text{C} = \frac{29}{22.4} \times \frac{273}{293} = 1.21\,\text{kg/m}^3$$

$$\text{Liquid density } (\rho_L) \;(\cong 1000\,\text{kg/m}^3$$

$$\text{Liquid viscosity } (\mu_L) = 10^{-3}\,\text{Pa s} = \text{Ns/m}^2$$

$$\frac{L}{G}\sqrt{\frac{p_g}{p_L}} = \frac{29.5\,\text{kg/s}}{1.39\,\text{kg/s}}\sqrt{\frac{1.21\,\text{kg/m}^3}{10^3\ \text{kg/m}^3}} = 0.74$$

Design for a pressure drop of 20 mm H_2O/m packing from Figure 11.44 [9].

$$Y_{\text{axis}} = 0.34$$

$$\text{At flooding}, Y_{\text{axis}} = 0.8$$

$$\text{Percentage of flooding} = \sqrt{\frac{0.34}{0.8}} \times 100 = 66\%, \text{satisfactory.}$$

The gas mass velocity at flooding

$$G_f = \left[\frac{Y_{\text{axis}}\,\rho_G(\rho_L - \rho_G)}{13.1 F_p(\mu_L/\rho_L)}\right]^{1/2} = \left[\frac{0.34 \times 1.21(1000 - 1.21)}{13.1 \times 170(10^{-3}/10^3)^{0.1}}\right]^{1/2} = 0.87\ \text{kg/m}^2\text{s}$$

For 66% of flooding:

$$\text{Column area required} = A_c = \frac{G}{G_f} = \frac{1.39\,\text{kg/s}}{0.87\,\text{kg/m}^2\,\text{s}} = 1.6\,\text{m}^2$$

$$\text{Diameter of the packed-bed tower} = D_t = \sqrt{\frac{4}{\pi} \times A_c} = \sqrt{\frac{4}{\pi} \times 1.6} = 1.41\text{m}$$

The calculated diameter is rounded off to 1.5 m

$$\text{Corrected column cross-sectional area} = A_{c,c} = \frac{4}{\pi} \times 1.5^2 = 1.77\ \text{m}^2$$

$$\text{The ratio of column diameter to packing size} = \frac{D_t}{D_p} = \frac{1.5\ \text{m}}{38 \times 10^{-3}\ \text{m}} = 39$$

$$\text{Corrected percentage flooding at selected diameter} = 66\% \times \frac{A_c}{A_{c,c}}$$

$$= 66\% \times \frac{1.6}{1.77} = 60\%$$

Using Figure 7.1, the value of the Y-axis, $Y_{\text{axis}} = 0.01$

$$G_f = \left[\frac{\rho_L \rho_G\, g(Y_{\text{axis}})}{F_p \psi \mu_L^{0.2}}\right]^{0.5} = \left[\frac{10^3\ \text{kg / m}^3 \times 1.21\,\text{kg/m}^3 \times 9.82\ \text{m/s}^2 \times 0.01}{170\ \text{m}^{-1} \times 1 \times (1\text{cP})^{0.2}}\right]^{0.2} = 0.83$$

$$\text{Column area required} = A_c = \frac{G}{f\,G_f} = \frac{1.39\ \text{kg/s}}{0.66 \times 0.87\ \text{kg/m}^2\,\text{s}} = 1.76\ \text{m}^2$$

$$\text{Diameter of the packed-bed tower} = D_t = \sqrt{\frac{4}{\pi} \times A_c} = \sqrt{\frac{4}{\pi} \times 1.76} = 1.498\ \text{m}$$

The calculated diameter is rounded off to 1.5 m.

OVERALL HEIGHT OF TRANSFER UNITS, H_{OG}

The overall HTUs is calculated using Cornell's method and Onda's method [9–11] the higher value among the two methods will be considered in the design.

CORNELL'S METHOD

The diffusivities of solute in liquid and gas phases are

$$D_L = 1.7 \times 10^{-9}\ \text{m}^2/\text{s}$$

$$D_G = 1.45 \times 10^{-5}\ \text{m}^2/\text{s}$$

The gas and liquid densities are

$$\rho_g = 1.21\ \text{kg/m}^3$$

$$\rho_L = 1000\ \text{kg/m}^3$$

The gas viscosity, $\mu_G = 0.018 \times 10^{-3}\ \text{Ns/m}^2$
Substituting values in Schmidt number for gas Sc_G and liquid Sc_L,

$$Sc_G = \frac{\mu_G}{\rho_S D_G} = \frac{0.018 \times 10^{-3}}{1.21 \times 1.45 \times 10^{-5}} = 1.04$$

Liquid-phase Schmidt number

$$Sc_L = \frac{\mu_L}{\rho_L D_L} = \frac{10^{-3}}{1000 \times 1.7 \times 10^{-9}} = 588$$

The gas velocity

$$G = \frac{29.5}{1.77} = 16.7 \text{ kg/sm}^2$$

Using Figures 11.40 through 11.43 [9] or Equations 7.26 through 7.28, the following values are obtained:

For 60% flooding, $K_3 = 0.85$ and $\psi_h = 80$
for $G = 16.7$, $\phi_h = 0.1$

H_L is calculated as follows:

$$H_L = 0.305 \times \phi_h (Sc)_L^{0.5} \times K_3 \left(\frac{Z}{3.05}\right)^{0.15}$$

Substituting values into the above equation

$$H_L = 0.305 \times 0.1(588)^{0.5} \times 0.85\left(\frac{Z}{3.05}\right)^{0.15} = 0.53Z^{0.15}$$

Since the column diameter is greater than 0.6 m, the diameter correction term will be taken as 2.3.

$$H_G = \frac{0.011 \times \psi_h (Sc)_G^{0.5} (2.3)\left(\frac{Z}{3.05}\right)^{0.33}}{\left(L f_1 f_2 f_3\right)^{0.5}}$$

At liquid water temperature 20°C,

$$f_1 = f_2 = f_3 = 1$$

Substituting values into H_G,

$$H_G = \frac{0.011 \times 80(1.04)^{0.5} (2.3)\left(\frac{Z}{3.05}\right)^{0.33}}{(16.7)^{0.5}} = 0.35Z^{0.33}$$

The overall HTUs in the gas phase

$$H_{OG} = H_G + \frac{mG_m}{L_m} \times H_L$$

Multiplying both sides of the equation by N_{OG}

$$N_{OG} \times H_{OG} = N_{OG} \times \left[H_G + \frac{mG_m}{L_m} \times H_L\right]$$

Since $Z = N_{OG} \times H_{OG}$

$$\frac{mG_m}{L_m} = \frac{26 * 0.048 \text{ kmol/s}}{1.64 \text{ kmol/s}} = 0.8$$

$$Z = 7 \times \left[0.35\, Z^{0.33} + 0.8 \times 0.53 Z^{0.15}\right]$$

Solving for $Z = 9.25$ by rounding off the packing height to $Z = 10$ m.

ONDA'S METHOD

The wetted area a_w is calculated from a correlation developed by Onda et al. [11].

$$a_w = a_P\left\{1 - \exp\left[(-1.45)\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{L}{a_P\,\mu_L}\right)^{0.1}\left(\frac{L^2 a_P}{\rho_L^2 g}\right)^{-0.05}\left(\frac{L^2}{\rho_L\,\sigma\,a_P}\right)^{0.2}\right]\right\}[=]\frac{\text{m}^2}{\text{m}^3}$$

where the value of σ_c is 61 dyne/cm for ceramic packing, 75 dyne/cm for steel packing, and 33 dyne/cm for plastic packing where σ_L is the water surface tension, N/m; a_P is the total packing surface area per packed-bed volume, m^2/m^3; L, G represent the superficial mass velocity of liquid and gas, kg/m^2 s; μ_L is the liquid-phase viscosity, kg/m s; ρ_L is the liquid-phase density, kg/m^3; $R = 0.08314$ bar m^3/kmol K; σ_L is the surface tension of liquid, for water at 20°C; $\sigma_L = 70 \times 10^{-3}$ N/m(70 dyne/cm); $= g = 9.81$ m/s^2; and d_p is the particle diameter 38×10^{-3} m.

From Table 7.2 for 38 mm Intalox saddles

$$a_p = 194 \text{m}^2/\text{m}^3$$

$$\sigma_C \text{ for ceramics} = 61 \times 10^{-3} \text{ N/m (61 dyne/cm)}$$

$$a_w = a_P\left\{1 - \exp\left[(-1.45)\left(\frac{\sigma_c}{\sigma}\right)^{0.75}\left(\frac{L}{a_P\,\mu_L}\right)^{0.1}\left(\frac{L^2 a_P}{\rho_L^2 g}\right)^{-0.05}\left(\frac{L^2}{\rho_L\,\sigma\,a_P}\right)^{0.2}\right]\right\}[=]\frac{1}{m}$$

Substituting values in the above equation:

$$a_w = a_p\left\{1 - \exp\left[-1.45\left(\frac{61 \times 10^{-3}}{70 \times 10^{-3}}\right)^{0.75}\left(\frac{16.7}{194 \times 10^{-3}}\right)^{0.1}\left(\frac{16.7^2 \times 194}{1000^2 \times 9.81}\right)^{-0.05}\right.\right.$$

$$\left.\left.\left(\frac{17.6^2}{1000 \times 70 \times 10^{-3} \times 194}\right)^{0.2}\right]\right\}$$

$$a_w = 194 \times 0.71 = 138 \text{ m}^2/\text{m}^3$$

The value of k_L is determined using the following equation:

$$k_L\left(\frac{\rho_L}{g\mu_L}\right)^{1/3} = 0.0051\left(\frac{L}{a_w\mu_L}\right)^{2/3}\left(\frac{\mu_L}{\rho_L D_L}\right)^{-1/2}\left(a_P d_P\right)^{0.4}$$

Substituting values:

$$k_L\left(\frac{10^3}{9.81\times 10^{-3}}\right)^{1/3} = 0.0051\left(\frac{16.7}{138\times 0^{-3}}\right)^{2/3}\left(\frac{10^{-3}}{10^3\times 1.7\times 10^{-9}}\right)^{-1/2}$$
$$\times\left(194\times 38\times 10^{-3}\right)^{0.4}$$
$$k_L = 2.5\times 10^{-4}\ \text{m/s}$$

The gas mass velocity (G_f) based on actual column diameter = (G/A = (1.39/1.77) = 0.79 kg/m^2 s

$$k_G\left(\frac{RT}{a_P D_G}\right) = 5.23\left(\frac{G_f}{a_P\mu_G}\right)^{0.70}\left(\frac{\mu_G}{\rho_G D_G}\right)^{1/3}\left(a_P d_P\right)^{-2}$$

Substituting values:

$$k_G\left(\frac{0.08314\times 293}{194\times 1.45\times 10^{-5}}\right) = 5.23\left(\frac{0.79}{194\times 0.018\times 10^{-3}}\right)^{0.7}\left(\frac{0.018\times 10^{-3}}{1.21\times 1.45\times 10^{-5}}\right)^{1/3}$$
$$\times\left(194\times 38\times 10^{-3}\right)^{-2}$$
$$k_G = 5.0\times 10^{-4}\ \text{kmol/sm}^2\ \text{bar}$$

The molar gas velocity

$$G_m = \frac{G_f}{M_W} = \frac{0.79\ \text{kg/m}^2\ \text{s}}{29\ \text{kg/kmol}} = 0.027\ \text{kmol/m}^2\ \text{s}$$

The molar liquid velocity

$$L_m = \frac{L}{M_W} = \frac{16.7\ \text{kg/m}^2\ \text{s}}{18\ \text{kg/kmol}} = 0.93\ \text{kmol/m}^2\ \text{s}$$

The gas HTUs

$$H_G = \frac{G_m}{k_G\times a_p\times P} = \frac{0.027}{5.0\times 10^{-4}\times 138\times 1.013} = 0.39\ \text{m}$$

C_T is the total liquid concentration water = $(\rho_L/M_{W,L})(1000/18)$ = 55.6 kmol/m^3

$$H_L = \frac{L_m}{k_L \times a_p \times C_T} = \frac{0.93}{2.5 \times 10^{-4} \times 138 \times 55.6} = 0.49\ \text{m}$$

$$H_{OG} = H_G + \frac{mG_m}{L_m} \times H_L$$

Substituting the required values in the above equation,

$$H_{OG} = 0.39 + \frac{26 \times 0.027}{0.93} \times 0.49 = 0.8\ \text{m}$$

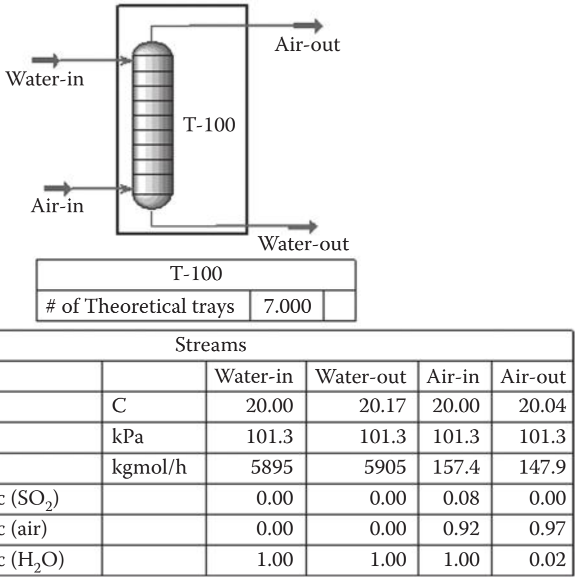
The packed-bed height

$$Z = N_{OG}{}^{*}\ H_{OG} = 7 \times 0.8 = 5.6\ \text{m}$$

The higher value is considered as the packed-column height. The estimated Z using Cornell's method is considered. Round up the packed-bed height to 10 m.

HYSYS/UNISIM SIMULATION

The absorber from object palette is used for this purpose. Inlet air stream is connected to the bottom of the column while liquid stream is connected to the top of the column. Gas stream released from the column is connected to top of the column and liquid stream released from the bottom of the column. Feed streams are fully specified. The required number of trays is set so that the exit SO_2 mole fraction is 0.003 as required. In this example, the number of theoretical plates needed to achieve 0.003 mole fraction of SO_2 in the exit air is greater than 4 and less than 5 since the mole fraction in the air-out stream is 0.0038 (Figure 7.35). The



T-100		
# of Theoretical trays	7.000	

Streams					
		Water-in	Water-out	Air-in	Air-out
Temperature	C	20.00	20.17	20.00	20.04
Pressure	kPa	101.3	101.3	101.3	101.3
Molar flow	kgmol/h	5895	5905	157.4	147.9
Comp mole frac (SO_2)		0.00	0.00	0.08	0.00
Comp mole frac (air)		0.00	0.00	0.92	0.97
Comp mole frac (H_2O)		1.00	1.00	1.00	0.02

FIGURE 7.35
Absorber process flow sheet and stream summary generated with Hysys.

Hysys theoretical number of trays is close to the number of trays obtained with hand calculations.

For tray sizing follow the following steps:

Tools >> Utilities >> Tray sizing >> Add Utilities

Then click on Tray sizing 1 >> Select TS >> TS-1 >> Auto section >> Packed

Select the type of packing material; in this example, the packing material is:

Intalox Ceramic Saddles 1.5 in Random Packing

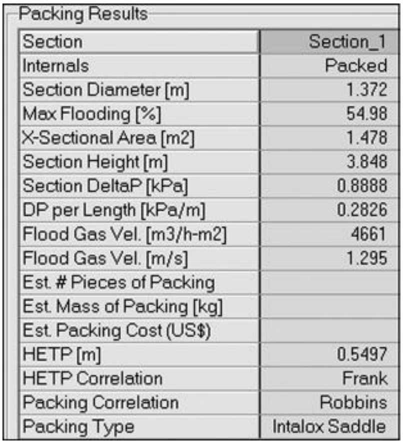
Click on the *Performance* tab to view the results shown in Figure 7.36.

PRO/II SIMULATION

Following the same procedure in previous examples, the process flow sheet and stream summary is shown in Figure 7.37. The column packed height and the inside diameter is shown in Figure 7.38.

ASPENPLUS SIMULATION

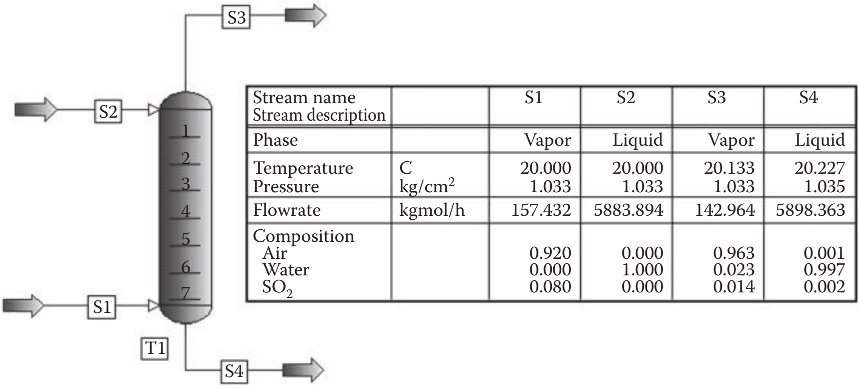
In this example, the number of theoretical stages required to achieve 0.004 mole fraction of sulfur dioxide in the exit stream is set to 7 trays. Block Absbr2 in Aspen is used for this purpose. Absrb2 can be found under the column subdirectory by pressing down arrow to the right of the *RateFrac* icon. Air inlet stream and liquid inlet streams are fully specified (i.e., Temperature, pressure, flow rate, and compositions to be entered). NRTL was used for the property method. In the block setup options, the number of trays is 7, no condenser or reboiler is needed for the absorber. The pressure of the column was set to 1 atm. After supplying all necessary information, and running the system, the stream summary is shown in Figure 7.39.



Packing Results

Section	Section_1
Internals	Packed
Section Diameter [m]	1.372
Max Flooding [%]	54.98
X-Sectional Area [m2]	1.478
Section Height [m]	3.848
Section DeltaP [kPa]	0.8888
DP per Length [kPa/m]	0.2826
Flood Gas Vel. [m3/h-m2]	4661
Flood Gas Vel. [m/s]	1.295
Est. # Pieces of Packing	
Est. Mass of Packing [kg]	
Est. Packing Cost (US$)	
HETP [m]	0.5497
HETP Correlation	Frank
Packing Correlation	Robbins
Packing Type	Intalox Saddle

FIGURE 7.36
Packing results.



Stream name Stream description		S1	S2	S3	S4
Phase		Vapor	Liquid	Vapor	Liquid
Temperature	C	20.000	20.000	20.133	20.227
Pressure	kg/cm^2	1.033	1.033	1.033	1.035
Flowrate	kgmol/h	157.432	5883.894	142.964	5898.363
Composition					
Air		0.920	0.000	0.963	0.001
Water		0.000	1.000	0.023	0.997
SO_2		0.080	0.000	0.014	0.002

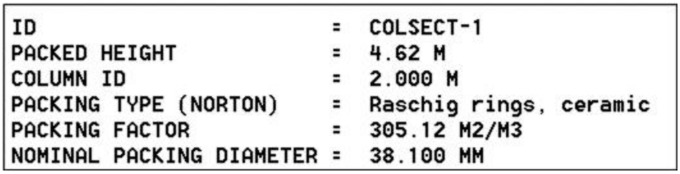
FIGURE 7.37
Process flow sheet and stream summary.

The streams were entered as shown in Figures 7.40 and 7.41. The inlet air should be entered below stage 7.

Using the spreadsheet option to measure the height required to achieve sulfur dioxide concentration in stream 3 as 0.004. The design specification page is shown in Figure 7.42.

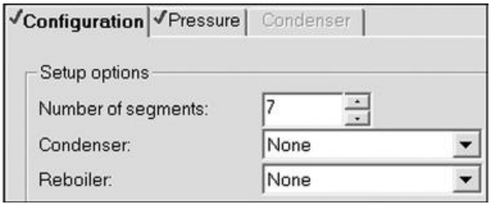
The manipulated variable which is the height of the packed tower is shown in Figure 7.43.

The converged value of the diameter is 1.92 m (Figure 7.44).



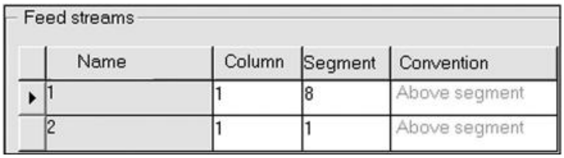
```
ID                          =  COLSECT-1
PACKED HEIGHT               =  4.62 M
COLUMN ID                   =  2.000 M
PACKING TYPE (NORTON)       =  Raschig rings, ceramic
PACKING FACTOR              =  305.12 M2/M3
NOMINAL PACKING DIAMETER =  38.100 MM
```

FIGURE 7.38
Column packed height and inside diameter.



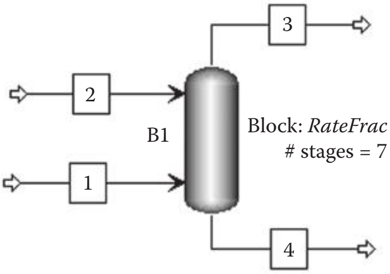
Number of segments: 7
Condenser: None
Reboiler: None

FIGURE 7.39
Block setup configuration.



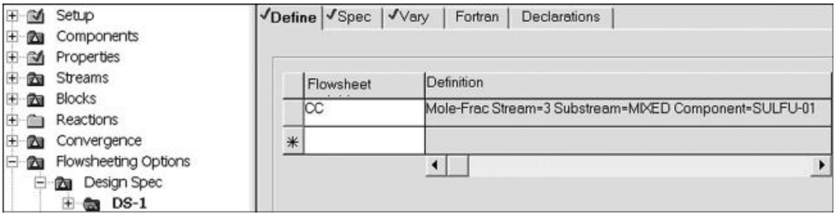
	Name	Column	Segment	Convention
▸	1	1	8	Above segment
	2	1	1	Above segment

FIGURE 7.40
Feed and product stream inlet stages.



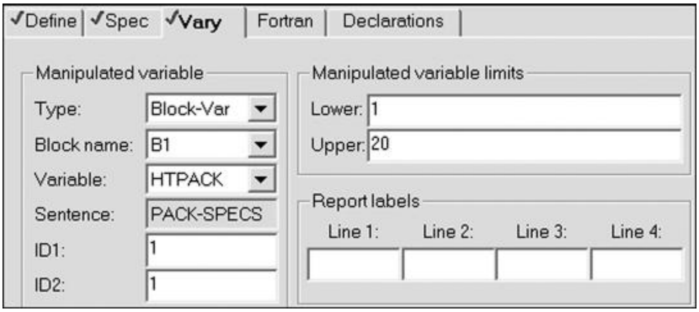
Example 7.7					
Stream ID		1	2	3	4
Temperature	K	293.1	293.1	293.2	293.5
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		1.000	0.000	1.000	0.000
Mole flow	kmol/h	157.432	5894.996	141.439	5910.989
Mass flow	kg/h	5000.000	106200.000	4079.906	107120.094
Volume flow	l/min	63116.610	1772.975	56717.843	1785.705
Enthalpy	MMBtu/h	−3.566	−1598.154	−0.925	−1600.795
Mole frac					
Sulfu-01		0.080		0.004	0.002
Air		0.920		0.973	0.001
Water			1.000	0.023	0.997

FIGURE 7.41
Process flow sheet and stream summary ($N = 7$).



Flowsheet	Definition
CC	Mole-Frac Stream=3 Substream=MIXED Component=SULFU-01

FIGURE 7.42
Design specification of packed-bed height.



Manipulated variable

Type: Block-Var

Block name: B1

Variable: HTPACK

Sentence: PACK-SPECS

ID1: 1

ID2: 1

Manipulated variable limits

Lower: 1

Upper: 20

Report labels

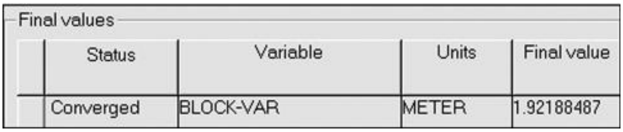
Line 1:

Line 2:

Line 3:

Line 4:

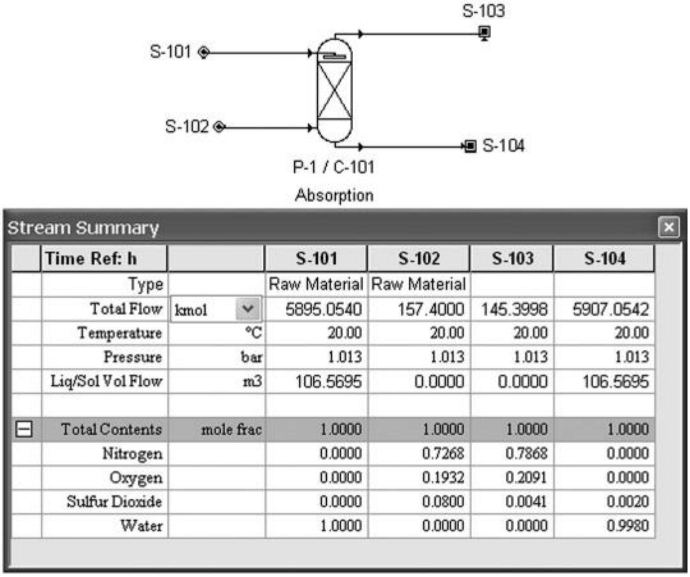
FIGURE 7.43
Limits of the manipulated variable.



Final values

Status	Variable	Units	Final value
Converged	BLOCK-VAR	METER	1.92188487

FIGURE 7.44
Diameter of the packed tower.



Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	kmol	5895.0540	157.4000	145.3998	5907.0542
Temperature	°C	20.00	20.00	20.00	20.00
Pressure	bar	1.013	1.013	1.013	1.013
Liq/Sol Vol Flow	m3	106.5695	0.0000	0.0000	106.5695
Total Contents	mole frac	1.0000	1.0000	1.0000	1.0000
Nitrogen		0.0000	0.7268	0.7868	0.0000
Oxygen		0.0000	0.1932	0.2091	0.0000
Sulfur Dioxide		0.0000	0.0800	0.0041	0.0020
Water		1.0000	0.0000	0.0000	0.9980

FIGURE 7.45
Process flow sheet and stream summary.

SUPERPRO DESIGNER SIMULATION

Following the same procedure in the previous examples, the absorber is selected. Inlet streams are fully specified. The inlet conditions are as shown in Figure 7.45.

The packed-material data are shown in Figure 7.46. The dimensionless packing constant (C_f) is taken from Treybal [10], the resultant diameter and height are shown in Figure 7.47.

Example 7.7: Removal of CO_2 from Natural Gas

CO_2 is absorbed into propylene carbonate in a packed column. The inlet gas stream is 20 mol% CO_2 and 80 mol% methane. The gas stream flows at a rate of 7200 m^3/h and the column operates at 60°C and 60 atm. The inlet solvent flow is 2000 kmol/h. Use available software simulators to determine the concentration of CO_2 (mol%) in the exit gas stream, the column height (m), and the column diameter (m). Compare simulating results to verify hand calculations. The column consists of 1 1/2 in. ceramic Intalox saddles packing material. The carbon dioxide in the exit stream should not exceed 0.4 mol%. Assume 60% flooding.

$$\text{Equilibrium data}: y = 27.341x$$

SOLUTION

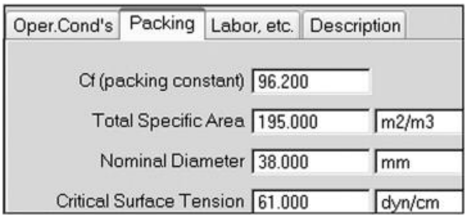
HAND CALCULATIONS

In this section the NTUs, packed-bed diameter, and packing height are calculated.

NUMBER OF TRANSFER UNITS

The NTUs are calculated using the following equation:

$$\text{NTU} = \frac{\ln\left[\left(y_1 - mx_2/y_2 - mx_2\right)\left(1 - (1/\text{AF})\right) + 1/\text{AF}\right]}{1 - (1/\text{AF})}$$



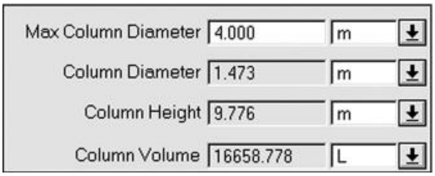
Cf (packing constant) 96.200

Total Specific Area 195.000 m2/m3

Nominal Diameter 38.000 mm

Critical Surface Tension 61.000 dyn/cm

FIGURE 7.46
Packing material specification.



Max Column Diameter 4.000 m

Column Diameter 1.473 m

Column Height 9.776 m

Column Volume 16658.778 L

FIGURE 7.47
Packed-tower height and diameter.

The absorption factor

$$AF = \frac{L_m}{mG_m} = \frac{2000\ \text{kmol/h}}{27.34 \times 304.5\ \text{kmol/h}} = 0.24$$

Substituting values to calculate the NTUs:

$$NTU = \frac{\ln\left[\left(0.2 - 0/0.04 - 0\right)\left(1 - (1/0.24)\right) + 1/0.24\right]}{1 - (1/0.24)} = 5.12$$

The NTUs is rounded off to six stages.

Packing Diameter

The diameter of the column is calculated using the following correlation and Figure 7.1

$$X_{\text{axis}} = \left(\frac{L(\text{kg/h})}{G(\text{kg/h})}\right)\sqrt{\frac{\rho_G}{\rho_L}}$$

Substituting liquid and gas mass flow rate at the bottom of the absorber with corresponding densities into the above equation:

$$X_{\text{axis}} = \left(\frac{207{,}300\ \text{kg/h}}{6588\ \text{kg/h}}\right)\sqrt{\frac{52.64\ \text{kg/m}^3}{1166\ \text{kg/m}^3}} = 6.66$$

From Figure 7.1 or using the following correlation:

$$Y_{\text{axis}} = 10 \wedge \left[-1.668 - 1.085(\log 6.66) - 0.297\left(\log 6.66\right)^2\right] = 0.00176$$

The gas mass flow rate per cross-sectional area of the bed:

$$G_f = \left[\frac{\rho_L \rho_G\, g_c (Y_{\text{axis}})}{F_p \psi (\mu_L)^{0.2}}\right]^{0.5}$$

For packing use, *Raschig* ring (ceramic, random)-2 in.

$$G_f = \left[\frac{(72.78\ \text{lb/ft}^3)(5.92\ \text{lb/ft}^3)(32.2\ \text{ft/s}^2)(0.00176)}{(65)(72.78/62.4)(2.16\ \text{lb/ft h} / (2.42\ \text{lb/ft h})/1\,\text{cp})^{0.2}}\right]^{0.5}$$

$$= 0.574\ \text{lb/ft}^2\,\text{s}$$

The bed cross-sectional area:

$$A = \frac{G}{G_f} = \frac{4.03\ \text{lb/s}}{0.574\ \text{lb/ft}^2\ \text{s}} = 7\ \text{ft}^2$$

The column diameter is determined from the area:

$$D = \sqrt{\frac{4A}{\pi}} = \sqrt{\frac{4 \times 7\,\text{ft}^2}{\pi}} = 3.0\ \text{ft}(0.97\ \text{m})$$

PACKING HEIGHT

The operating liquid mass flow rate per cross-sectional area of the tower:

$$L_f = \frac{456600\ \text{lb/h}\dfrac{\text{h}}{3600\,\text{s}}}{8.33\ \text{ft}^2} = 15\ \text{lb/ft}^2\,\text{s}$$

The height of the gas transfer units:

$$H_G = \frac{0.011 \times \psi_h\,(\text{Sc})_G^{0.5}\,(2.3)\left(\dfrac{Z}{3.05}\right)^{0.33}}{(Lf_1f_2f_3)^{0.5}}$$

$$f_1 = \left(\frac{\mu_L}{\mu_W}\right)^{0.16} = \left(\frac{2.16\ \text{lb/ft h}}{2.4\ (\text{lb/ft h})}\right)^{0.16} = 1.0$$

$$f_2 = \left(\frac{\rho_w}{\rho_L}\right)^{1.25} = \left(\frac{62.4\ \text{lb/ft}^3}{72.78\ \text{lb/ft}^3}\right)^{1.25} = 0.83$$

Assume $f_3 = 1$.
Substituting the necessary values into the above equation

$$\text{Sc}_G = \frac{\mu_G}{\rho_G D_G} = \frac{0.044\ \text{lb/ft h}}{(0.07\ \text{lb/ft}^3)(0.914\ \text{ft}^2/\text{h})} = 0.69$$

$$H_G = \frac{0.011 \times 80 \times 0.69^{0.5}\,(2.3)\left(\dfrac{Z}{3.05}\right)^{0.33}}{(15\ \text{lb/ft}^2\,\text{s} \times 0.83)^{0.5}} = 0.33\,Z^{0.33}$$

The height of the liquid transfer units

$$H_L = 0.305 \times \phi_h (\mathrm{Sc})_L^{0.5} \times K_3 \left(\frac{Z}{3.05}\right)^{0.15}$$

The Schmidt number

$$\mathrm{Sc}_L = \frac{\mu_L}{\rho_L D_L} = \frac{2.16\ \mathrm{lb/ft\ h}}{\left(\frac{72.78\ \mathrm{lb}}{\mathrm{ft}^3}\right)\left(1.07 \times 10^{-5}\ \mathrm{cm^2/s}\right)\left(\frac{1\ \mathrm{ft}}{30.48\ \mathrm{cm}}\right)^2 \left(\frac{3600\ \mathrm{s}}{\mathrm{h}}\right)} = 23.5$$

The liquid mass velocity

$$L_f = 15\ \mathrm{lb/ft^2\ s} \left|\frac{0.454\ \mathrm{kg}}{1\ \mathrm{lb}}\right| \frac{1\ \mathrm{ft}^2}{(0.3048\ \mathrm{m})^2} = 74\ \mathrm{kg/m^2\ s}$$

At $L_f = 74\ \mathrm{kg/m^2\ s}$, $\phi_h = 0.11$
At 60% flooding, $K_3 = 0.85$

$$H_L = 0.305 \times 0.11 \times (23.5)^{0.5} \times 0.85 \left(\frac{Z}{3.05}\right)^{0.15} = 0.12 Z^{0.15}$$

The liquid HTUs:

$$H_L = 0.12\ Z^{0.15}$$

The absorption factor:

$$\mathrm{AF} = \frac{L_m}{mG_m} = \frac{2000\ \mathrm{kmol/h}}{27.341 \times 304.5\ \mathrm{kmol/h}} = 0.24$$

The total HTUs:

$$Z = N_{OG} \times \left(H_G + \frac{1}{\mathrm{AF}} H_L\right) = 6 \times \left(0.33\ Z^{0.33} + \frac{1}{0.24} \times 0.12\ Z^{0.15}\right)$$

Solving for Z

$$Z = 8\ \mathrm{ft}\ (2.4\ \mathrm{m})$$

HYSYS/UNISIM SIMULATION

Using Hysys absorber:

- Fluid package: Sour PR
- Number of trays: 6
- Packing material: Random, ceramic *Raschig* ring, 2 in.

A feed stream condition is as shown in Figure 7.48, packed-column diameter and height is shown in Figure 7.49.

PRO/II SIMULATION

The absorber is selected and the number of stages is set to six stages. The PR equation of state is selected for property measurements. Running the system leads to the process flow sheet and streams material balance shown in Figure 7.50. The estimated packed height and column inside diameter are shown in Figure 7.51.

ASPENPLUS SIMULATION

The following are used to simulate packed-bed absorber in Aspen Plus:

- Absorber type: *RateFrac* block/ absorber
- Fluid package: SRK
- Number of trays: 6
- Packing material: Random, ceramic *Raschig* ring, 2 in.

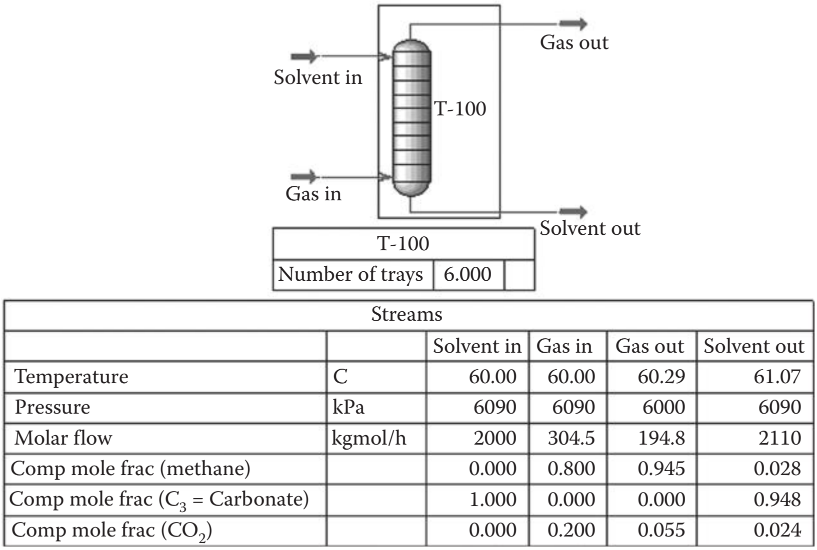
Feed streams conditions are shown in Figure 7.52.

The packed height is calculated by selecting *Flow sheeting options* and then *Design specification* as shown in Figures 7.53 through 7.55. The simulated column diameter is shown in Figure 7.56.

SUPERPRO DESIGNER SIMULATION

The absorber column is used and the following data are supplied:

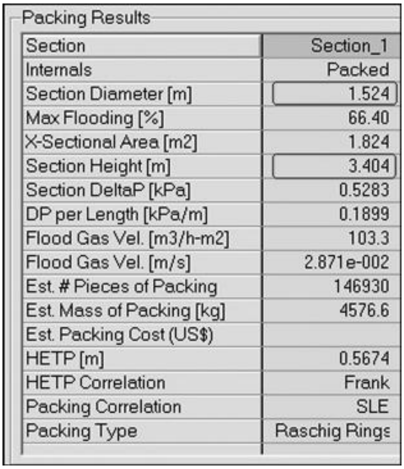
Henry's law constant, $H = 2.95 \times 10^{-2}$ atm m^3/mol
Solute diffusivity in the gas phase = 0.233 cm^2/s



T-100		
Number of trays	6.000	

Streams					
		Solvent in	Gas in	Gas out	Solvent out
Temperature	C	60.00	60.00	60.29	61.07
Pressure	kPa	6090	6090	6000	6090
Molar flow	kgmol/h	2000	304.5	194.8	2110
Comp mole frac (methane)		0.000	0.800	0.945	0.028
Comp mole frac (C_3 = Carbonate)		1.000	0.000	0.000	0.948
Comp mole frac (CO_2)		0.000	0.200	0.055	0.024

FIGURE 7.48
Process flow sheet and stream summary.



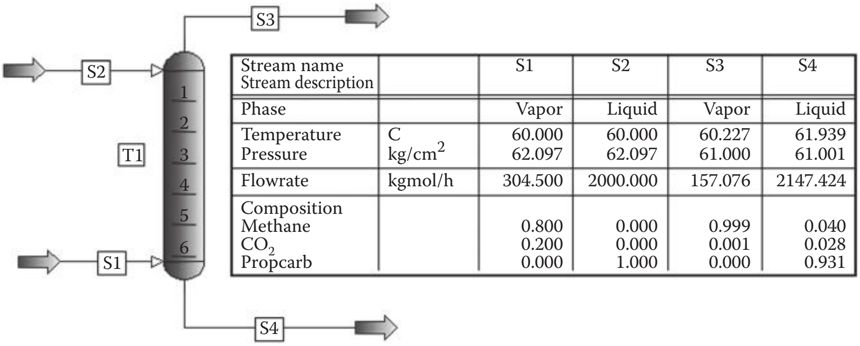
Packing Results

Section	Section_1
Internals	Packed
Section Diameter [m]	1.524
Max Flooding [%]	66.40
X-Sectional Area [m2]	1.824
Section Height [m]	3.404
Section DeltaP [kPa]	0.5283
DP per Length [kPa/m]	0.1899
Flood Gas Vel. [m3/h-m2]	103.3
Flood Gas Vel. [m/s]	2.871e-002
Est. # Pieces of Packing	146930
Est. Mass of Packing [kg]	4576.6
Est. Packing Cost (US$)	
HETP [m]	0.5674
HETP Correlation	Frank
Packing Correlation	SLE
Packing Type	Raschig Rings

FIGURE 7.49
Packing results.

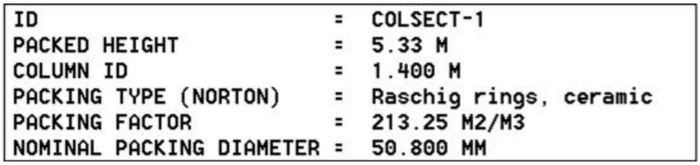
Solute diffusivity in the liquid phase = 1.07×10^{-5} cm²/s
Solute diffusivity gas = 0.015 cP
Liquid-phase viscosity = 1 cP
Percent carbon dioxide removal = 83%
Liquid surface tension = 52.3 dyne/cm

Packing material: *Raschig* ring ceramic, random packing, 2 in. ($Cf = 65$, $a_p = 92$ m²/m³). The process flow sheet and stream summary are shown in Figure 7.57. Packed-bed specifications; HTU, and NTUs are shown in Figure 7.58. The packed-bed height and diameter are shown in Figure 7.59.



Stream name Stream description		S1	S2	S3	S4
Phase		Vapor	Liquid	Vapor	Liquid
Temperature	C	60.000	60.000	60.227	61.939
Pressure	kg/cm^2	62.097	62.097	61.000	61.001
Flowrate	kgmol/h	304.500	2000.000	157.076	2147.424
Composition					
Methane		0.800	0.000	0.999	0.040
CO_2		0.200	0.000	0.001	0.028
Propcarb		0.000	1.000	0.000	0.931

FIGURE 7.50
Stream summaries.



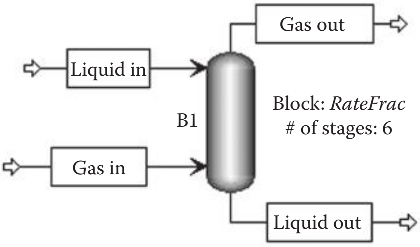
```
ID                        =  COLSECT-1
PACKED HEIGHT             =  5.33 M
COLUMN ID                 =  1.400 M
PACKING TYPE (NORTON)     =  Raschig rings, ceramic
PACKING FACTOR            =  213.25 M2/M3
NOMINAL PACKING DIAMETER =  50.800 MM
```

FIGURE 7.51
Column diameter and height.

7.7 Number of Theoretical Trays

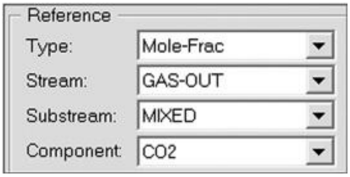
Two methods are the most commonly used to determine the number of ideal trays required for a given removal method. One method used is a graphical technique. The number of ideal plates is obtained by drawing steps on an operating diagram. This procedure is illustrated in Figure 7.60.

The second method is a simplified one used to estimate the number of plates. This equation can only be used if both the equilibrium and operating



Example 7.8-*RateFrac*					
Stream ID		Gas in	Gas out	Liquid in	Liquid out
Temperature	K	333.1	333.2	333.1	334.6
Pressure	atm	60.10	60.10	60.10	64.54
Vapor frac		1.000	1.000	0.000	0.000
Mole flow	kmol/h	304.000	162.625	2000.000	2141.375
Mass flow	kg/h	6577.395	2790.551	204179.680	207966.524
Volume flow	L/min	2120.556	1160.430	2362.873	2464.631
Enthalpy	MMBtu/h	–39.783	–13.382	–1218.228	–1244.629
Mole frac					
Methane		0.800	0.960		0.041
CO_2		0.200	0.040		0.025
Propy-01			31 ppm	1.000	0.934

FIGURE 7.52
Process flow sheet and stream summary using *RateFrac* block.



Reference

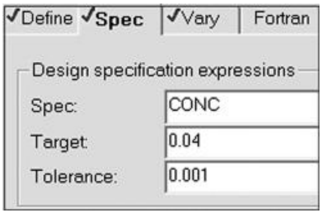
Type: Mole-Frac

Stream: GAS-OUT

Substream: MIXED

Component: CO2

FIGURE 7.53
Variable selections.



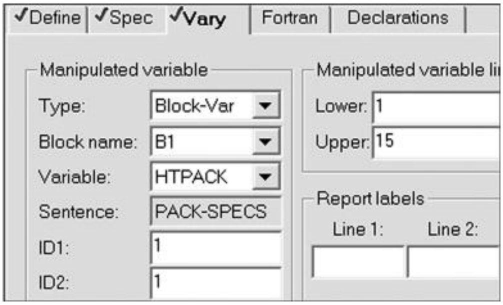
Design specification expressions

Spec: CONC

Target: 0.04

Tolerance: 0.001

FIGURE 7.54
Design specifications.



Manipulated variable

Type: Block-Var

Block name: B1

Variable: HTPACK

Sentence: PACK-SPECS

ID1: 1

ID2: 1

Manipulated variable li

Lower: 1

Upper: 15

Report labels

Line 1:

Line 2:

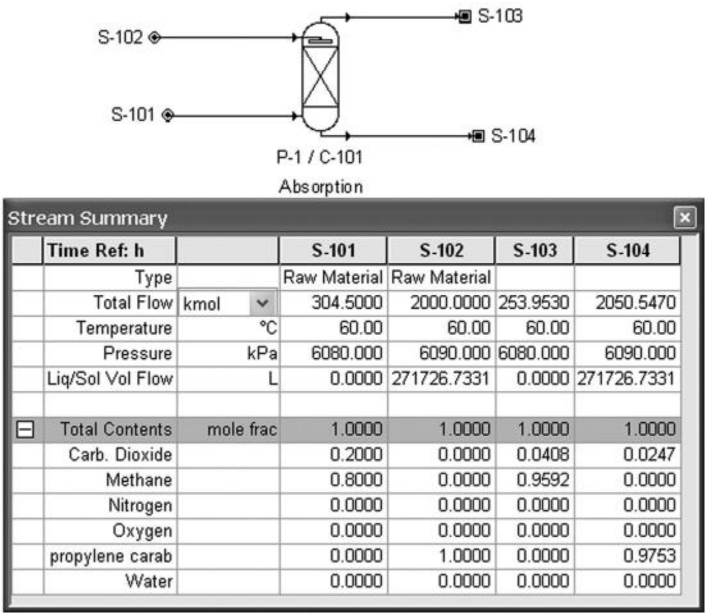
FIGURE 7.55
Manipulating variable, height of packing.

lines for the system are straight. This is a valid assumption for most air pollution control systems [3]. This equation is referred to as the *height equivalent to a theoretical plate*, or HETP instead of HTU in a packed tower. The equation is used to predict the number of theoretical plates required to achieve a given removal efficiency. The operating conditions for a theoretical plate assume

Final values

Status	Units	Final value	Previous value	Error / Tolerance
Converged	METER	1.91430557	1.75110549	-0.168481

FIGURE 7.56
Column heights to achieve 0.04 mole fraction CO_2.



⊟	Time Ref: h		S-101	S-102	S-103	S-104
	Type		Raw Material	Raw Material		
	Total Flow	kmol	304.5000	2000.0000	253.9530	2050.5470
	Temperature	°C	60.00	60.00	60.00	60.00
	Pressure	kPa	6080.000	6090.000	6080.000	6090.000
	Liq/Sol Vol Flow	L	0.0000	271726.7331	0.0000	271726.7331
⊟	Total Contents	mole frac	1.0000	1.0000	1.0000	1.0000
	Carb. Dioxide		0.2000	0.0000	0.0408	0.0247
	Methane		0.8000	0.0000	0.9592	0.0000
	Nitrogen		0.0000	0.0000	0.0000	0.0000
	Oxygen		0.0000	0.0000	0.0000	0.0000
	propylene carab		0.0000	1.0000	0.0000	0.9753
	Water		0.0000	0.0000	0.0000	0.0000

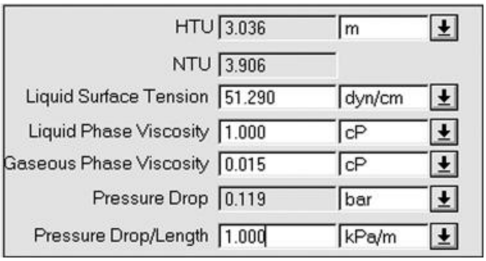
FIGURE 7.57
Process flow sheet and stream summary.

that the gas and liquid streams released from the plate are in equilibrium with each other. Three types of efficiencies are used to describe absorption efficiency for a plate tower; the *overall efficiency* concerns the entire column, *Murphree efficiency* is applicable to a single plate, and *local efficiency* pertains to a specific location on a plate. The overall efficiency is the ratio of the number of theoretical plates to the number of actual plates. The overall tray efficiencies of absorbers operating with low-viscosity liquid fall in the range of 65–80% [13]. The height Z of the column is calculated from the height of the transfer unit HTU and the NTUs N_{OG}. The NTUs is given by the Kremser Method for Theoretical Trays (Absorber):

$$N_{OG} = \frac{\ln\left[y_1 - mx_1/y_2 - mx_1\left(1-(1/\mathrm{AF})\right) + (1/\mathrm{AF})\right]}{\log \mathrm{AF}} \tag{7.36}$$

AF is the absorption factor, $L_m/\mathrm{m}\,G_m$;

L_m, G_m is the liquid and gas molar flow rate, kmol/h; m is the slope of equilibrium curve; y_1, y_2 is the molar fraction of entering and exiting gas; and



HTU 3.036 m

NTU 3.906

Liquid Surface Tension 51.290 dyn/cm

Liquid Phase Viscosity 1.000 cP

Gaseous Phase Viscosity 0.015 cP

Pressure Drop 0.119 bar

Pressure Drop/Length 1.000 kPa/m

FIGURE 7.58
Specification of the packed bed.

x_1, x_2 is the mole fraction of exiting and entering liquid; Kremser method for theoretical trays (Stripper):

$$N = \frac{\log\left[\left(\frac{x_0 - (y_{N+1}/m)}{x_N - (y_{N+1}/m)}\right)\left(1 - (1/S)\right) + \frac{1}{S}\right]}{\log S} \tag{7.37}$$

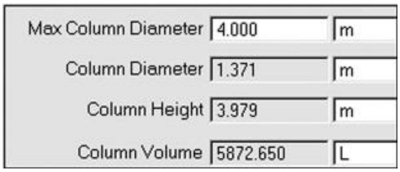
where $S = m\,G/L$.

7.8 Sizing a Plate Tower Absorber

Another absorber used extensively for gas absorption is a plate tower. Here, absorption occurs on each plate, or stage.

7.8.1 Plate Tower Diameter

The minimum diameter of a single plate tower is determined by using the gas velocity through the tower. If the gas velocity is too fast, liquid droplets are entrained causing priming that causes liquid on one tray to foam and then rise to the tray above. Priming reduces absorber efficiency by inhibiting gas and liquid contact. Priming in a plate tower is analogous to the



Max Column Diameter 4.000 m

Column Diameter 1.371 m

Column Height 3.979 m

Column Volume 5872.650 L

FIGURE 7.59
Diameter and height of the packed tower.

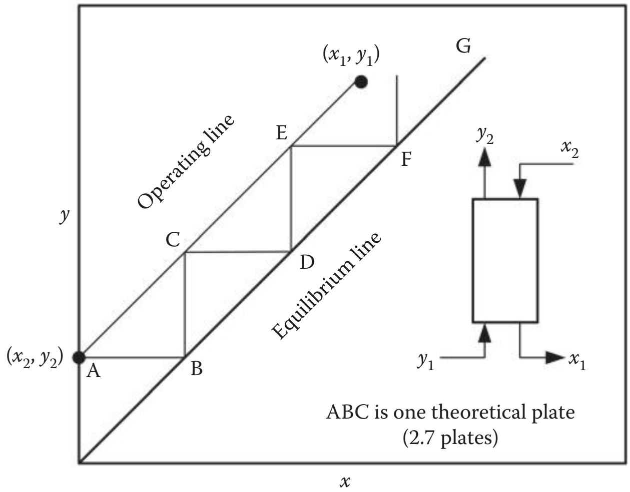


FIGURE 7.60
Graphic determination of the number of theoretical plates.

flooding point in a packed tower. The smallest allowable diameter for a palette tower is

$$d_t = \psi\left(Q_G\sqrt{\rho_g}\right)^{0.5} \tag{7.38}$$

where:
Q_G is the volumetric gas flow rate m^3/h;
ψ is the empirical correlation, $m^{0.25}\ h^{0.5}/kg^{0.25}$; and
ρ_g is the gas density, kg/m^3.

The empirical constant, ψ, for different types of trays are shown in Table 7.5.

Example 7.8: Design of the Plate Tower

Gas absorber is used to remove SO_2 from a gas stream with pure water in a tray tower. The gas stream inlet molar flow rate is 206 kmol/h (3% SO_2, 97% air) and the water inlet molar flow rate is 12,240 kmol/h. The temperature is 293 K and the pressure is 101.32 kPa. The column tray type is bubble cap. The concentration of SO_2 in the exit air should be less than 500 ppm. Determine the number of bubble cap trays and tower diameter.

TABLE 7.5

Empirical Constant (ψ)

Tray	ψ (Metric units)	ψ (English Units)
Bubble cap	0.0162	0.1386
Sieve	0.0140	0.1198
Valve	0.0125	0.1069

Source: Data from Calvert, S. et al. 1972. *Wet Scrubber System Study*, Vol. 1, *Scrubber Handbook*, EPA-R2-72-118a, U.S. Environmental Protection Agency, Washington, DC.

SOLUTION

HAND CALCULATIONS

The minimum acceptable diameter of the plate tower is determined using the following equation:

$$d_t = \psi\left(Q_G\sqrt{\rho_g}\right)^{0.5} = 0.0162\frac{\mathrm{m}^{0.25}\,\mathrm{h}^{0.25}}{\mathrm{kg}^{0.25}}\left[\left(85\frac{\mathrm{m}^3}{\mathrm{min}}\left|\frac{60\,\mathrm{min}}{\mathrm{h}}\right.\right)\times\sqrt{1.17\frac{\mathrm{kg}}{\mathrm{m}^3}}\right]^{0.5}$$

$$= 1.2\,\mathrm{m}$$

The absorption factor

$$\mathrm{AF} = \frac{L_m}{mG_m} = \frac{12{,}240\,\mathrm{kmol/h}}{42.7\times 206\,\mathrm{kmol/h}} = 1.4$$

Number of theoretical trays:

$$N_{OG} = \frac{\ln\left[0.03 - 0/0.0005 - 0\left(1-(1/1.4)\right) + \dfrac{1}{1.4}\right]}{\ln 1.4} = 8.6$$

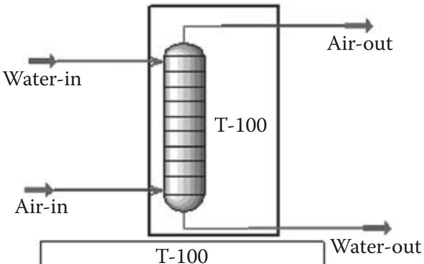
Number of trays is rounded off to nine trays.
The height of the tower: $Z = 9{*}0.6096 = 5.5$ m.

HYSYS/UNISIM SIMULATION

In this example, the packed material of Example 7.3 is replaced by bubble cap trays using tray utilities. The stream summary is shown in Figure 7.61 and the column performance is shown in Figure 7.62.

PRO/II SIMULATION

Selection of the suitable thermodynamic fluid package is very important to get the correct answer. NRTL was selected as the property estimation system using

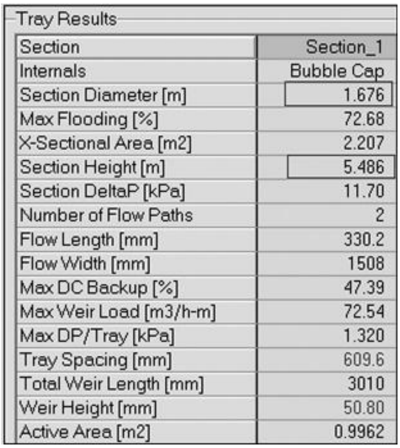


T-100		
Number of trays	9.000	

Streams					
		Water-in	Water-out	Air-in	Air-out
Temperature	C	20.00	19.90	20.00	20.01
Pressure	kPa	101.3	101.3	101.3	101.3
Molar flow	kgmol/h	12239.73	12243.32	205.98	202.38
Comp mole frac (SO_2)		0.0000	0.0005	0.0300	0.0000
Comp mole frac (Air)		0.0000	0.0002	0.9700	0.9769
Comp mole frac (H_2O)		1.0000	0.9993	0.0000	0.0231

FIGURE 7.61
Process flow sheet and stream summary of the bubble cap tray column.

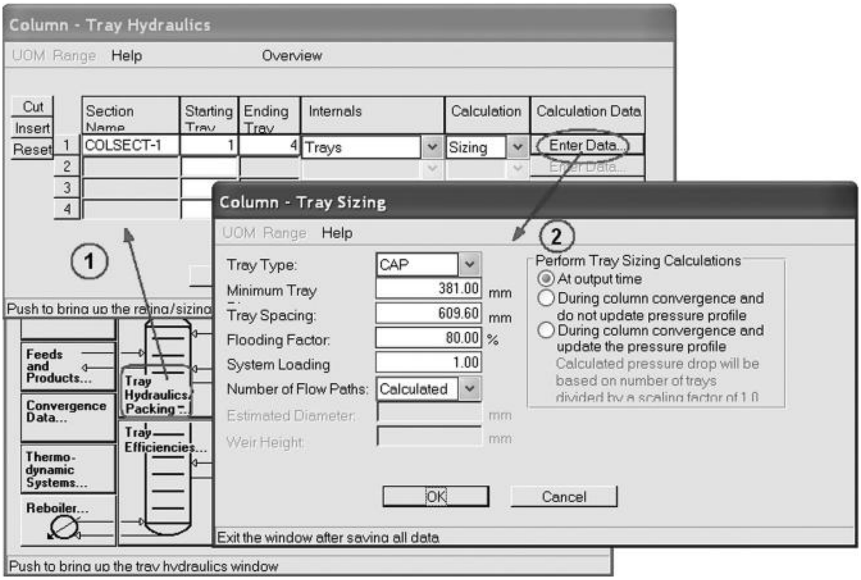
Henry's law constant as shown in Figure 7.63. The process flow sheet and the stream summary are shown in Figure 7.64. It can be observed that nine bubble cap trays are required to achieve the desired separation and the exit mole fraction of SO_2 in the exit stream is 323 ppm. The bubble cap tray tower diameter and height are extracted from the output generated text report (Figure 7.65).



Tray Results

Section	Section_1
Internals	Bubble Cap
Section Diameter [m]	1.676
Max Flooding [%]	72.68
X-Sectional Area [m2]	2.207
Section Height [m]	5.486
Section DeltaP [kPa]	11.70
Number of Flow Paths	2
Flow Length [mm]	330.2
Flow Width [mm]	1508
Max DC Backup [%]	47.39
Max Weir Load [m3/h-m]	72.54
Max DP/Tray [kPa]	1.320
Tray Spacing [mm]	609.6
Total Weir Length [mm]	3010
Weir Height [mm]	50.80
Active Area [m2]	0.9962

FIGURE 7.62
Bubble cap tray column.



	Section Name	Starting Tray	Ending Tray	Internals	Calculation	Calculation Data
1	COLSECT-1	1	4	Trays	Sizing	Enter Data...
2						Enter Data...
3						
4						

Push to bring up the rating/sizing

Push to bring up the tray hydraulics window

Tray Type: CAP
Minimum Tray: 381.00 mm
Tray Spacing: 609.60 mm
Flooding Factor: 80.00 %
System Loading: 1.00
Number of Flow Paths: Calculated
Estimated Diameter: mm
Weir Height: mm

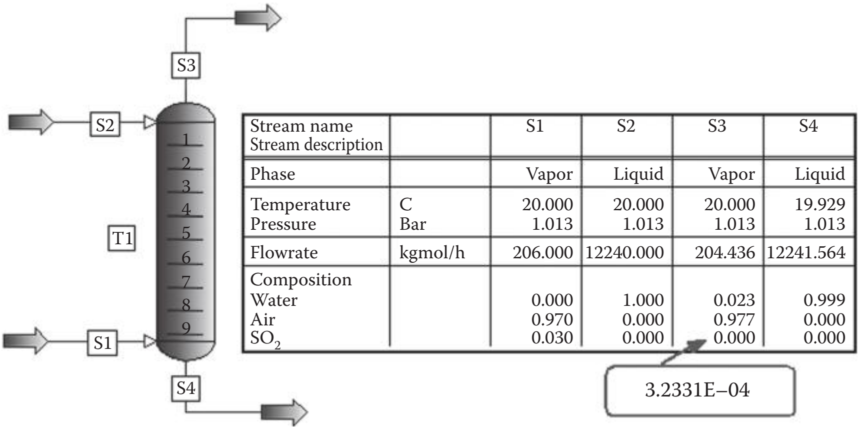
Perform Tray Sizing Calculations
● At output time
○ During column convergence and do not update pressure profile
○ During column convergence and update the pressure profile
Calculated pressure drop will be based on number of trays divided by a scaling factor of 1.0

Exit the window after saving all data

FIGURE 7.63
Selection of bubble cap trays.

ASPEN SIMULATION

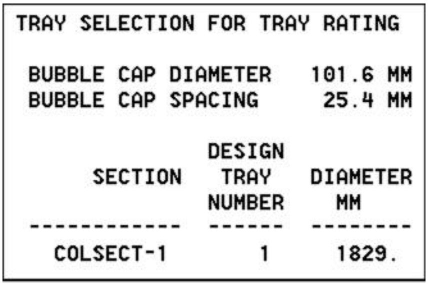
Using the converged AspenPlus file developed for Example 7.3, in this case the packing is replaced by bubble cap trays. The stream summary result is shown in Figure 7.66. The tray tower diameter using the spread options is shown in Figure 7.67.



Stream name Stream description		S1	S2	S3	S4
Phase		Vapor	Liquid	Vapor	Liquid
Temperature	C	20.000	20.000	20.000	19.929
Pressure	Bar	1.013	1.013	1.013	1.013
Flowrate	kgmol/h	206.000	12240.000	204.436	12241.564
Composition					
Water		0.000	1.000	0.023	0.999
Air		0.970	0.000	0.977	0.000
SO_2		0.030	0.000	0.000	0.000

3.2331E−04

FIGURE 7.64
Process flow sheet and stream summary.



```
TRAY SELECTION FOR TRAY RATING

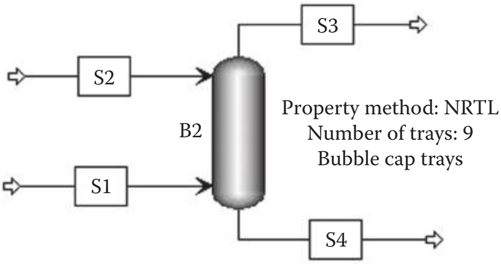
 BUBBLE CAP DIAMETER   101.6 MM
 BUBBLE CAP SPACING     25.4 MM

                   DESIGN
      SECTION       TRAY    DIAMETER
                   NUMBER     MM
 ------------      ------   --------
   COLSECT-1          1       1829.
```

FIGURE 7.65
Calculated diameter of the tray tower.

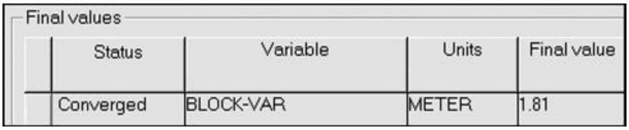
SuperPro Designer

In SuperPro designer there is no tray option. Changing the percent SO_2 removal in Example 7.3 to 99% leads to exit SO_2 concentration as 310 ppm which is within the accepted range. The process flow sheet and stream summary are shown in Figure 7.68.



Example 7.3					
Stream ID		S1	S2	S3	S4
Temperature	K	293.0	293.0	293.0	292.9
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		1.000	0.000	1.000	0.000
Mole flow	kmol/h	206.000	12240.000	188.168	12257.832
Mass flow	kg/h	6180.809	220507.027	5400.523	221287.313
Volume flow	l/min	82545.657	3680.764	75402.972	3694.252
Enthalpy	MMBtu/h	–1.768	–3318.427	–1.012	–3319.182
Mole frac					
Sulfu-01		0.030		12 ppb	504 ppm
Air		0.970		0.977	0.001
Water			1.000	0.023	0.998

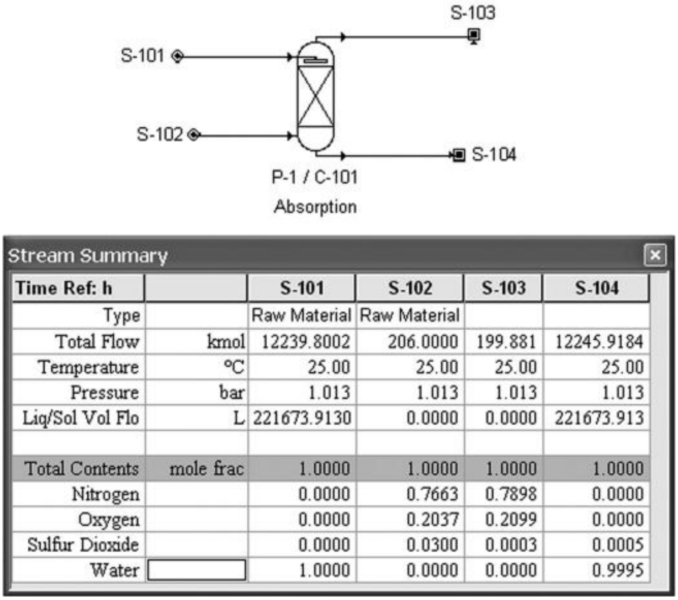
FIGURE 7.66
Process flow sheet and stream summary of tray towers.



Final values

	Status	Variable	Units	Final value
	Converged	BLOCK-VAR	METER	1.81

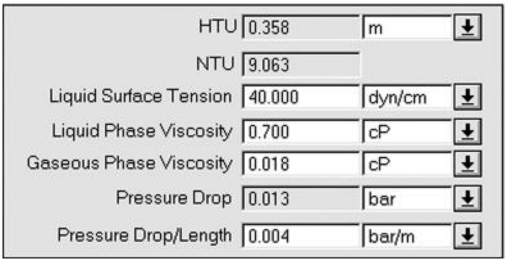
FIGURE 7.67
Tray column diameters.



Stream Summary

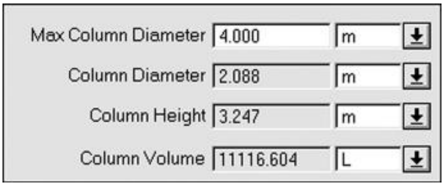
Time Ref: h		S-101	S-102	S-103	S-104
Type		Raw Material	Raw Material		
Total Flow	kmol	12239.8002	206.0000	199.881	12245.9184
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Liq/Sol Vol Flo	L	221673.9130	0.0000	0.0000	221673.913
Total Contents	mole frac	1.0000	1.0000	1.0000	1.0000
Nitrogen		0.0000	0.7663	0.7898	0.0000
Oxygen		0.0000	0.2037	0.2099	0.0000
Sulfur Dioxide		0.0000	0.0300	0.0003	0.0005
Water		1.0000	0.0000	0.0000	0.9995

FIGURE 7.68
Column diameter and height.



HTU	0.358	m
NTU	9.063	
Liquid Surface Tension	40.000	dyn/cm
Liquid Phase Viscosity	0.700	cP
Gaseous Phase Viscosity	0.018	cP
Pressure Drop	0.013	bar
Pressure Drop/Length	0.004	bar/m

FIGURE 7.69
Estimated NTUs.



Max Column Diameter 4.000 m

Column Diameter 2.088 m

Column Height 3.247 m

Column Volume 11116.604 L

FIGURE 7.70
Column diameter.

The calculated NTUs is 9 that are close to those previously found using Hysys, PRO/II, and Aspen Plus (Figure 7.69).

The column diameter and the height of the packed-bed absorber estimated by PRO/II are shown in Figure 7.70.

CONCLUSION

The tray tower diameters obtained with four software packages were around 2 m, which is above the minimum required diameter estimated with hand calculation (1.2 m) which is acceptable.

SUMMARY OF DESIGN PROCEDURE

The following steps can be followed in the design of gas absorbers:

- Henry's law constant is to be determined from the slope of the equilibrium line $y - x$ diagram.
- The minimum liquid-to-gas ratio is determined from the operating line equation.
- Determine the actual liquid flow rate by multiplying the ratio with a predefined factor.
- Determine the mass flow rate of the gas per unit cross-sectional area of the tower using the generalized flooding correlation.
- The required cross-sectional area and diameter of the absorption tower are determined at the gas operating point velocity (50–75% of the flooding velocity).
- The tower height is calculated from the NTU times the HTUs.
- The tower height strongly depends on the pollutant gas concentration in the inlet gas and on the removal efficiency.
- The tower height also depends on the size of the packing material.

PROBLEMS

7.1 Absorption of Ammonia in a Packed Tower

Ammonia NH_3 is absorbed by water in a packed column. The inlet polluted air stream is 20,000 ppm NH_3. The air stream flow at a rate of 7 ft^3/min and the column operates at 70°F and 1 atm. The inlet water is pure flowing at a rate of 500 mL/min. The concentration of ammonia in the exit air should not exceed 250 ppm. The packing consists of ceramic *Raschig* rings, length 3/8 in., width 3/8 in., wall thickness 1/16 in., weight 15 lbs/cubic foot, equivalent spherical diameter is 0.35 in., 0.68 void fraction. The packed column consists of a 4 in. ID × 36 in.-long section of borosilicate pipe. Determine the NTUs, column diameter, and column height, and then verify your answer with simulation results obtained from Hysys, PRO/II, Aspen, and SuperPro designer software packages.

7.2 Absorption of Acetone from Air Using Water

Acetone is being absorbed from air by pure water in a packed column designed for 80% of flooding velocity at 293 K and 1 atm. The inlet air contains 2.6 mol% acetone and outlet 0.5 mol% acetone. The total gas inlet flow rate is 14.0 kmol/h. The pure water inlet flow is 45.36 kmol/h. The column is randomly packed with ceramic *Raschig* rings, 1.5 in. nominal diameter. Calculate the packed-column height and verify your answer using Hysys/Unisim, PRO/II, Aspen, and SuperPro designer.

7.3 Stripping of Ethane from a Hydrocarbon Mixture

A measure of 100 kgmol/h of feed gas at 17 atm and 100°C, containing 3% ethane, 20% propane, 37% *n*-butane, 35% *n*-pentane, 5% *n*-hexane, is to be separated such that 100% ethane, 95% propane, and 1.35% *n*-butane of the feed stream are to be recovered in the overhead stream. Use stripper to find the molar flow rates and compositions of the bottom stream.

7.4 Absorption of CO_2 from Gas Stream in a Fermentation Process

Ethanol is absorbed from a gas stream in a fermentation process. The gas stream contains 2 mol% ethanol and remaining CO_2. All streams enter at 30°C and the process is isobaric at 1 atm. Entering gas flow rate is 1000 kgmol/h. Water flow rate is 2000 kgmol/h with no ethanol. Use 60% Murphree Tray efficiencies. Determine the number of stages required to absorb 95% of the ethanol from the air stream using water as the absorption media.

7.5 Absorption of CO_2 from a Gas Stream Using Methanol

A gas stream is flowing at a rate of 100 kmol/h at 100°C and 6000 kPa pressure enters a gas absorber. The primary objective of the CO_2 absorber is to absorb CO_2 contained in the feed stream by contacting countercurrently with methanol solvent in an absorber. The gas stream contains 0.35 CO, 0.002 H_2O, 0.274 CO_2, 0.37 H_2, 0.002 CH_4, and 0.002 N_2. Methanol at 30°C and 6000 kPa is used as an absorbent solvent. The molar flow rate of methanol liquid is 330 kmol/h. Determine the number of theoretical trays required to achieve 0.06 mol fraction of CO_2 in the exit stream, column diameter, and height.

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8

Liquid–Liquid Extraction

At the end of this chapter you should be able to

1. Understand the principles of liquid–liquid extraction (LLE).
2. Plot ternary equilibrium diagram and find the equilibrium number of stages.
3. Find exit flow rate and compositions of extract and raffinate streams by hand calculations.
4. Verify hand calculations using four software packages; Hysys, Pro/II, Aspen Plus, and SuperPro Designer.
5. Compare hand calculations with software simulation results.

8.1 Introduction

Liquid–liquid extraction (LLE) is an important unit operation that allows one to separate fluids based on solubility differences of solutes in different solvents. In liquid extraction, separation of liquid solution occurred as a result of contact with another insoluble liquid. If the components of the original solution are distributed differently between the two liquids, separation will result (Figure 8.1). Extraction is driven by chemical differences and it can be used in situations when distillation is impractical, such as separation of compounds with similar boiling points in which distillation is not viable, or mixtures containing temperature-sensitive components. The solution to be extracted is called the *feed*, and the liquid used in contacting is the *solvent*. The enriched solvent product is the *extract* and the depleted feed is called the *Raffinate* [1]. In the design of liquid–liquid extraction column, there are two primary calculations:

1. The number of stages needed to make a separation.
2. The amount of solvent needed to make a separation.

Since liquid–liquid equilibrium is seldom available in algebraic form, the calculations tend to be iterative or graphical. A modified McCabe–Thiele approach can be used if y data versus x data are available. The coordinates for the diagram are the mass fraction of solute in the extract phase and the

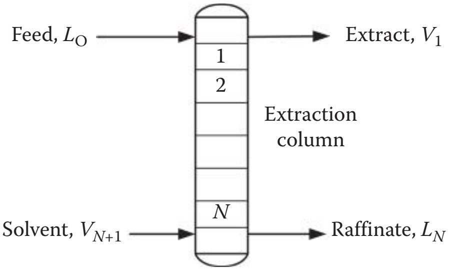


FIGURE 8.1
Schematic diagram of a multistage countercurrent liquid–liquid extraction column.

mass fraction in the raffinate for the other. When one has a convenient equilateral triangle diagram (Figure 8.2), construction can be done directly on the triangle. Some authors refer to this as the Hunter–Nash method [2].

8.2 Material Balance

The feed stream containing the solute *A* to be extracted enters at one end of the process and the solvent stream enters at the other end. The extract and

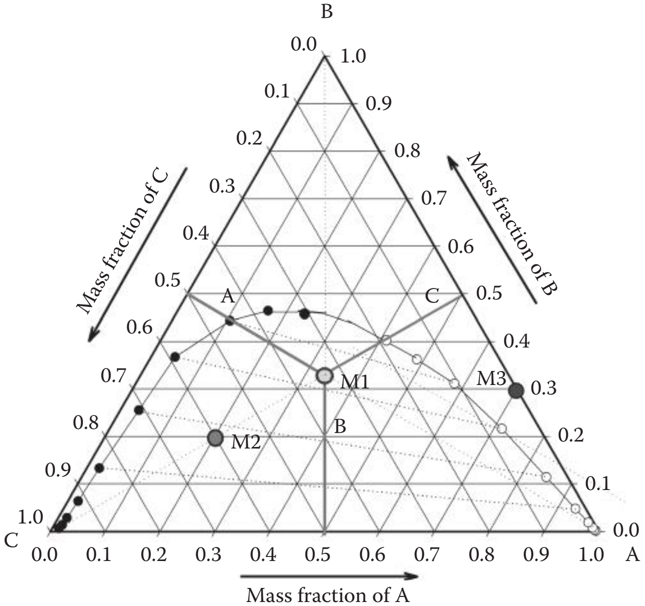


FIGURE 8.2
Triangular phase diagram.

raffinate streams flow countercurrently from stage to stage, and the final products are the extracted stream V_1 leaving stage 1 and the raffinate stream L_N leaving stage N. The overall material balance on the column [3,5]:

$$L_o + V_{N+1} = L_N + V_1 = M \tag{8.1}$$

where M represents total mass flow rate and is constant, L_o the inlet feed mass flow rate, V_{N+1} the inlet solvent mass flow rate, V_1 the exit extract stream, and L_N the exit raffinate stream. Mass flow rates in kg/h or lb/h.

Making an overall component balance on component C:

$$L_o x_{C0} + V_{N+1} y_{CN+1} = L_N x_{CN} + V_1 y_{C1} = M x_{CM} \tag{8.2}$$

Dividing Equation 8.2 by Equation 8.1 and rearranging:

$$\frac{L_o x_{C0} + V_{N+1} y_{CN+1}}{L_o + V_{N+1}} = \frac{L_N x_{CN} + V_1 y_{C1}}{L_N + V_1} = \frac{M x_{CM}}{M} = x_{CM} \tag{8.3}$$

Component balance on component A:

$$L_o x_{A0} + V_{N+1} y_{AN+1} = L_N x_{AN} + V_1 y_{A1} = M x_{AM} \tag{8.4}$$

Dividing Equation 8.4 by Equation 8.1:

$$\frac{L_o x_{A0} + V_{N+1} y_{AN+1}}{L_o + V_{N+1}} = \frac{L_N x_{AN} + V_1 y_{A1}}{L_N + V_1} = \frac{M x_{AM}}{M} = x_{AM} \tag{8.5}$$

$$x_{CM} = \frac{L_o x_{C0} + V_{N+1} y_{CN+1}}{L_o + V_{N+1}} \tag{8.6}$$

$$x_{AM} = \frac{L_o x_{A0} + V_{N+1} y_{AN+1}}{L_o + V_{N+1}} \tag{8.7}$$

Equations 8.6 and 8.7 can be used to calculate the coordinates of point M on the phase diagram that ties together the two entering streams L_o and V_{N+1} and the two exit streams V_1 and L_N. Triangular phase diagram is shown in Figure 8.2. Each apex of triangle represents pure component. The mass fraction of components at point M1 are 0.33 A, 0.33 B, and 0.34 C. The mass fraction of components at point M2 are 0.6 C, 0.2 A, and 0.2 B. The mass fraction at point M3 is 0.3 B and 0.7 A. Figure 8.3 shows the operating lines. The intersection of the operating lines is the operating point (P).

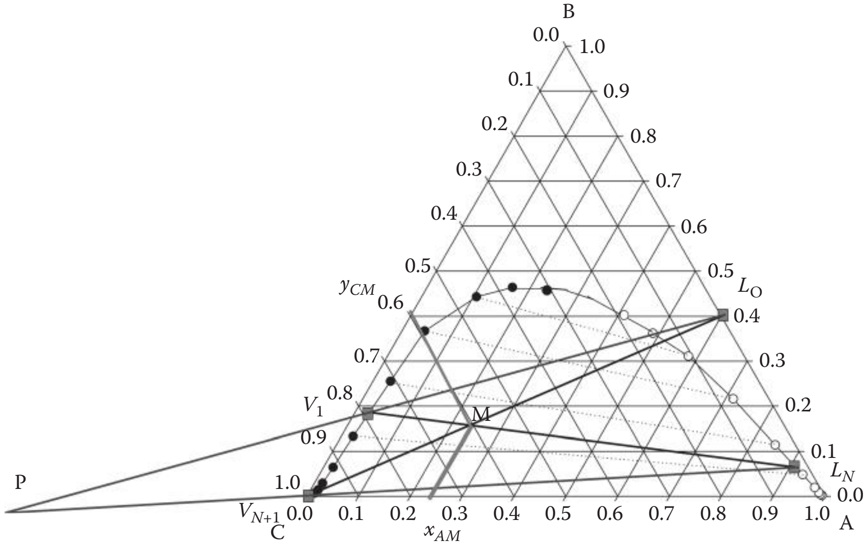


FIGURE 8.3
Equilateral triangle ternary equilibrium diagrams.

Example 8.1: Extraction of Acetone from Water by Methyl Isobutyl Ketone

A countercurrent liquid–liquid extractor is used to remove acetone from a feed that contains 43% acetone (A), 50 wt% water (B), and 7 wt% methyl isobutyl ketone (MIBK) (C). Pure MIBK, at a flow rate of 820 kg/h, is used as the solvent in this separation. A feed flow rate of 1000 kg/h is to be treated. It is desired to have a final raffinate of 4 wt% acetone. The operation takes place at 25°C and 1 atm.

a. Determine the number of stages necessary for the separation as specified.
b. Give the composition of the final extract.

SOLUTION

HAND CALCULATION

Plot the ternary equilateral triangle diagram using the equilibrium data in Table 8.1. The mixing point compositions are calculated using overall material and the component balance,

$$M = L_N + V_1 = V_{N+1} + L_o$$

Component balance for water,

$$Mx_c = L_N x_{CN} + V_1 y_{C1} = V_{N+1} y_{cN+1} + L_o x_{c0}$$

TABLE 8.1

Equilibrium Data for System Acetone–MIBK–Water

Raffinate Layer, Mass Fraction			Extract Layer, Mass Fraction		
Water	**Acetone**	**MIBK**	**Water**	**Acetone**	**MIBK**
0.02	0.02	0.96	0.97	0.01	0.02
0.025	0.06	0.915	0.95	0.03	0.02
0.03	0.10	0.87	0.91	0.06	0.03
0.035	0.16	0.805	0.88	0.09	0.03
0.04	0.20	0.76	0.83	0.13	0.04
0.045	0.25	0.705	0.79	0.17	0.04
0.05	0.30	0.65	0.745	0.20	0.055
0.07	0.36	0.57	0.68	0.26	0.06
0.09	0.40	0.51	0.62	0.30	0.08
0.14	0.48	0.38	0.49	0.40	0.11
0.33	0.49	0.18	0.33	0.49	0.18

Source: Data from Geankoplis, J. C. 1998. *Transport Process and Unit Operations*, 3rd edn, McGraw-Hill, Boston, MA.

Rearranging the above equations,

$$x_{CM} = \frac{y_{cN+1}V_{N+1} + x_{c0}L_o}{V_{N+1} + L_o}$$

From the overall material balance and acetone component balance, the mass fraction of acetone at the mixing point is

$$x_{AM} = \frac{y_{AN+1}V_{N+1} + x_{A0}L_o}{V_{N+1} + L_o} = \frac{0 \times 820 + 0.43 \times 1000}{820 + 1000} = 0.24$$

The mass fraction of MIBK (C) component at the mixing point:

$$x_{CM} = \frac{y_{cN+1}V_{N+1} + x_{c0}L_o}{V_{N+1} + L_o} = \frac{1 \times 820 + 0.07 \times 1000}{820 + 1000} = 0.49$$

To calculate the raffinate and extract streams mass flow rate,

$$M = 1820 = L_N + V_1$$

$$M = 1820 - V_1 = L_N$$

Determine MIBK compositions at extract and raffinate from Figure 8.4.

$$Mx_{CM} = (1820 - V_1)x_{NC} + V_1y_{1C}$$

$$1820 \times 0.49 = (1820 - V_1) \times 0.03 + V_1 \times 0.67$$

$$V_1 = 1308 \text{ kg/h}$$

$$L_N = 512 \text{ kg/h}$$

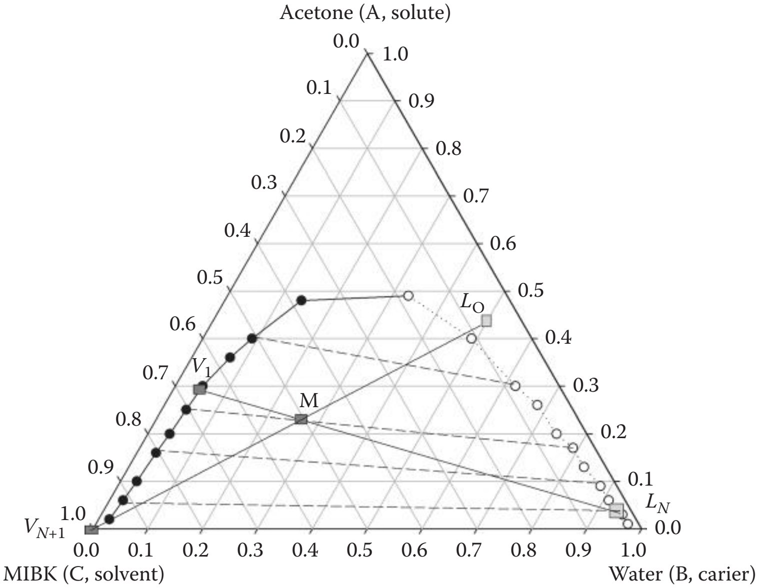


FIGURE 8.4
Ternary equilibrium diagram of Acetone, Water, and MIBK.

Locate the mixing point on the ternary diagram from calculated compositions. Draw a line starting from L_N through the mixing point (M) to the exit equilibrium concentrations of the extract (V_1) (Figure 8.4). There are two operating lines. The first is drawn by connecting the point of L_o and V_1 and extending the line to the right. The second operating line is connecting L_N and V_{N+1}, then extend the line until both lines cross each other. The joint of the operating lines is called the operating point (P) as shown in Figure 8.5. From V_1 draw the equilibrium tie line that ends at the raffinate equilibrium line. From the end of the equilibrium raffinate line draw a line to the operating point (P). From the point that crosses the equilibrium extract curve, draw a tie line. Repeat until lines crosses the exit raffinate concentration (L_N). Figure 8.6 shows that seven equilibrium stages are necessary to reach a raffinate concentration of 4% acetone.

THE FINAL EXTRACT COMPOSITION

The extract composition is the composition at V_N.
$y_C = 0.67$, $y_A = 0.29$ and $y_B = 0.04$.

HYSYS CALCULATION

In Hysys one has to specify number of equilibrium stages, and then Hysys will calculate exit flow rates and components mass fractions.

1. Start a new case in Hysys, Select Acetone, Water, and MIBK for the components. Use the NRTL Fluid Package.
2. For LLE cases, the binary coefficients of the components have to be checked. If some of the coefficients are not specified by Hysys, a fatal error will occur,

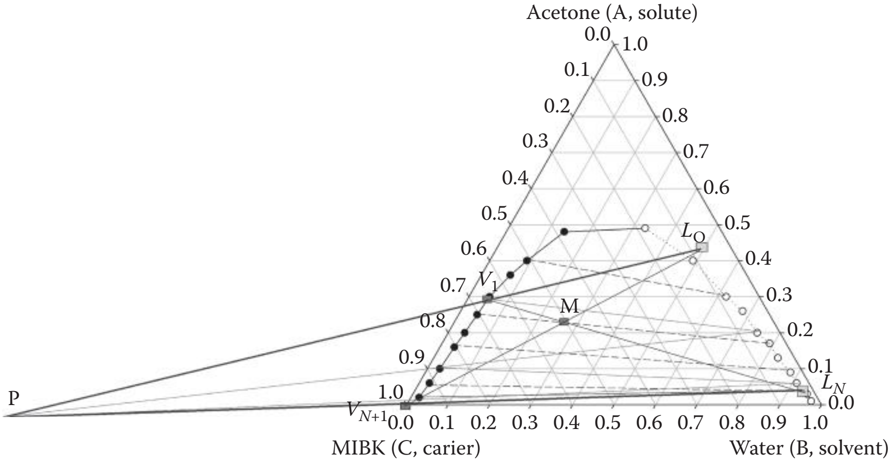
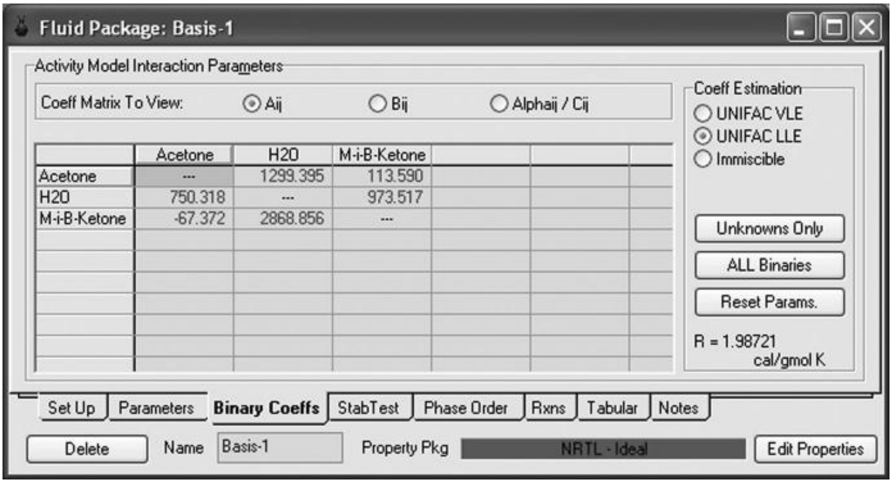


FIGURE 8.5
Equilibrium number of equilibrium stages of Example 8.1 (2.5 stages).

and the process cannot be simulated. Simply click on the *Binary Coeffs* tab. If some of the coefficients are not specified, select UNIFAC LLE, click on *Unknowns only*.

3. Close and return to simulation environment. From the object palette select *Liquid–Liquid Extraction* icon; double click and in the connection page; name the streams as Feed, Solvent, Extract, and Raffinate, then click on *Next* to continue.
4. Specify a constant pressure of 1 atm by entering it in the pressure columns.



Coeff Matrix To View: ● Aij ○ Bij ○ Alphaij / Cij

	Acetone	H2O	M-i-B-Ketone
Acetone	---	1299.395	113.590
H2O	750.318	---	973.517
M-i-B-Ketone	-67.372	2868.856	---

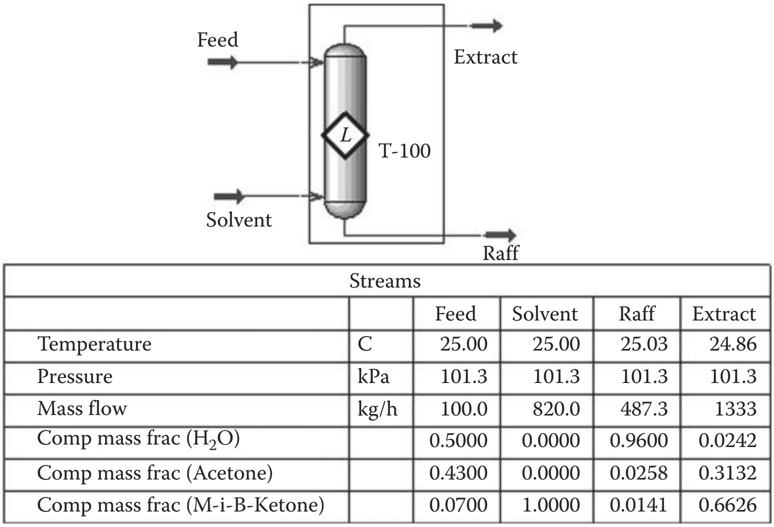
○ UNIFAC VLE
● UNIFAC LLE
○ Immiscible

R = 1.98721 cal/gmol K

Name Basis-1

Property Pkg NRTL - Ideal

FIGURE 8.6
Activity model interaction parameters of components involved in Example 8.1.



Streams					
		Feed	Solvent	Raff	Extract
Temperature	C	25.00	25.00	25.03	24.86
Pressure	kPa	101.3	101.3	101.3	101.3
Mass flow	kg/h	100.0	820.0	487.3	1333
Comp mass frac (H_2O)		0.5000	0.0000	0.9600	0.0242
Comp mass frac (Acetone)		0.4300	0.0000	0.0258	0.3132
Comp mass frac (M-i-B-Ketone)		0.0700	1.0000	0.0141	0.6626

FIGURE 8.7
Hysys simulation of Example 8.1.

5. The optional temperature estimates for the top and bottom stages can be ignored. Click on *Done* to complete this section.
6. Specify number of trays as three trays, the same as those obtained by hand calculation.
7. Double click on the Feed stream. Make an entry of the desired feed properties; a temperature of 25°C, a pressure of 1 atm, a flow rate of 1000 kg/h, and a feed mass fraction of 0.43 acetone, 0.5 water, and 0.07 MIBK.
8. The solvent stream is pure MIBK, at a flow rate of 820 kg/h, at 25°C, 1 atm.
9. Double click on the column and click on *Run*. Close the window and see that the Extracted Product and Raffinate streams have turned from light to dark blue, signifying that Hysys has successfully solved for those streams of unknown properties. After this stage, if any of the specifications on the Liquid–Liquid Extraction column are changed, the *Reset* option must be selected, and then the *Run* button clicked on again to rerun the column with the new specifications (Figure 8.7).

PRO/II CALCULATIONS

Open a new case in PRO/II, and select distillation column from the object palette. No condenser or reboiler is needed. Specify the number of stages as 3 to verify the hand calculation results. The number of stages is close to the value obtained using hand calculations (2.5 stages). Click on *Streams*, and then add two feed streams and two product streams.

Click on the *Component Selection* icon (the benzene ring) in the toolbar, then select Acetone, Water, and MIBK, and then click on *OK* to close the window.

Click on *Thermodynamic Data*, under *Category* select *liquid activity*, and then NRTL under *Primary Method*. Click on *Add*, then in the pop-up window select

Enable Two Liquid-Phase Calculations. Click on *OK* to close the current window and then on *OK* to close another following window.

Click on Feed stream and specify the total flow rate and compositions. Click on *Flow rate and compositions*, then select *Total Flow Rate*. Specify the total flow rate as 1000 kg/h and specify the compositions as 0.43 acetone, 0.5 for water, and 0.07 mass fractions MIBK, click *OK* to close the window (Figure 8.8). Under *Thermal specification*, select *Temperature* and *Pressure*, specify the temperature as 25°C and pressure as 1 atm. Use *UOM* at the left top corner to change the units when needed Temperatures and Pressures are shown in Figure 8.9.

Double click on solvent feed stream and specify total flow rate as 820 kg/h, for compositions, set mass fraction of MIBK as 1 (pure solvent).

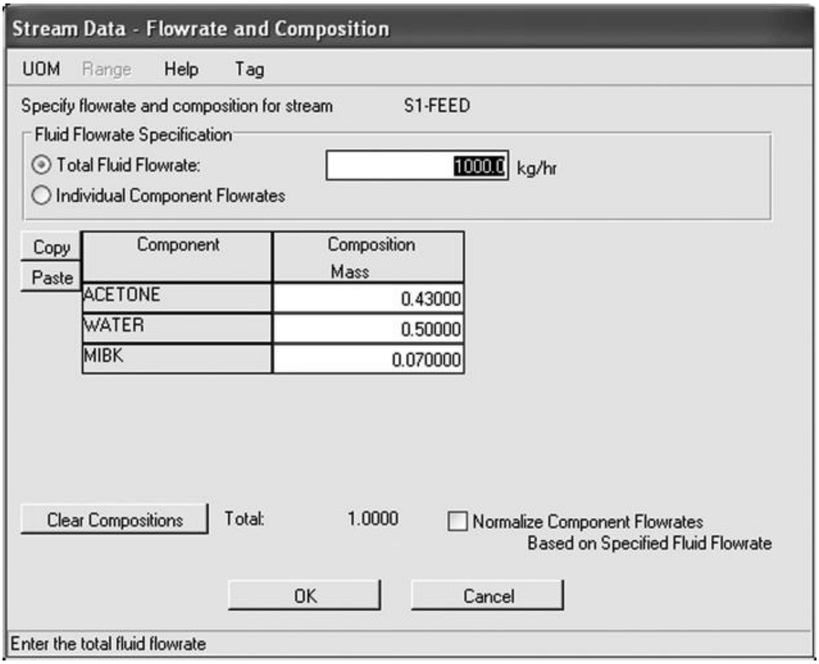
Double click on the *Column* icon, under *Algorithm* and *Calculated Phases*, from the pull-down menu select *Liquid-Liquid*.

Click on *Pressure Profile*. Set the pressure to 1 atm; the pressure drop per tray is 0.0 and then click on *OK*. The red button turns into black (Figure 8.9).

Double click on *Feeds and Products*. Specify the feed and product tray and initial estimate of product stream. Click on *OK*, and then once again, click on *OK* (Figure 8.10). Column required data are completed (Figure 8.11).

Click on *Run* for the column to be converged and the color of the PFD will change to light blue as shown in Figure 8.12.

To generate the results as shown in Figure 8.13, click *Output* in the toolbar, and then click on *Generate report*. The required portion of the report is shown in Figure 8.13.



Specify flowrate and composition for stream S1-FEED

Fluid Flowrate Specification

● Total Fluid Flowrate: 1000.0 kg/hr

○ Individual Component Flowrates

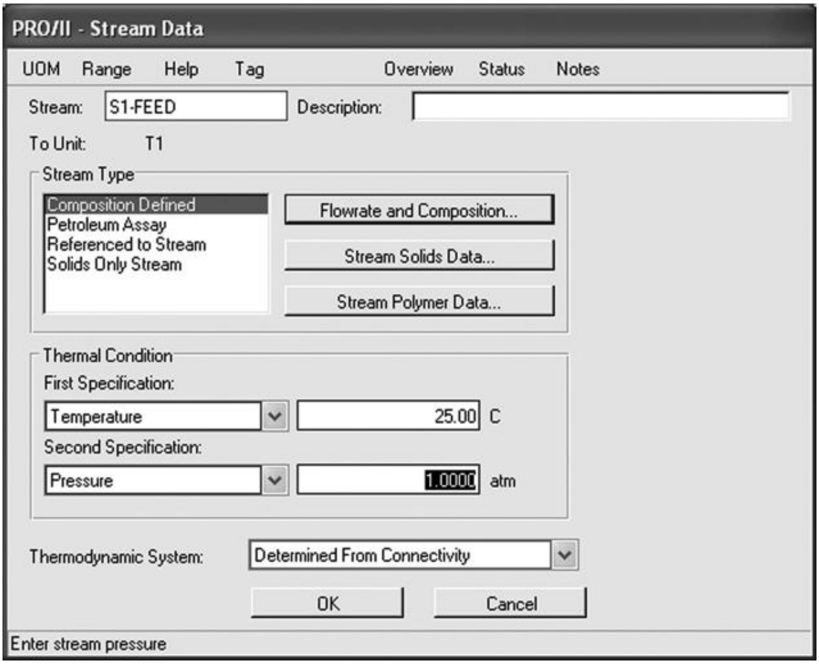
Component	Composition Mass
ACETONE	0.43000
WATER	0.50000
MIBK	0.070000

Total: 1.0000

☐ Normalize Component Flowrates Based on Specified Fluid Flowrate

Enter the total fluid flowrate

FIGURE 8.8
Feed stream flow rate and compositions.



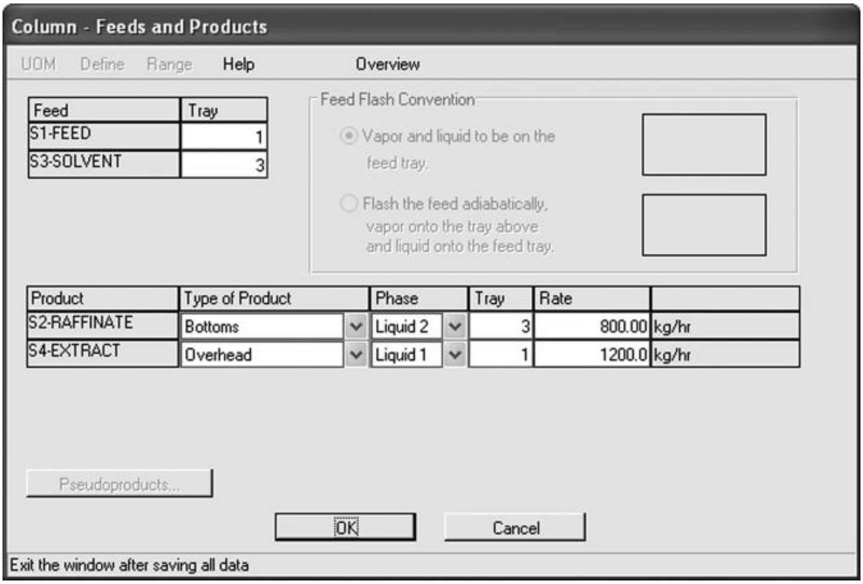
Stream: S1-FEED
Description:
To Unit: T1

Stream Type:
- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

First Specification: Temperature 25.00 C
Second Specification: Pressure 1.0000 atm
Thermodynamic System: Determined From Connectivity

Enter stream pressure

FIGURE 8.9
Thermal conditions menu, temperature, and pressure.



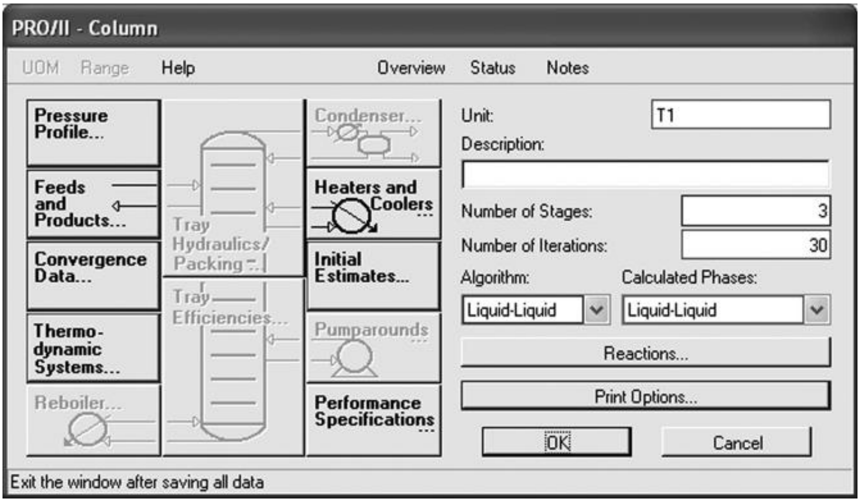
Feed	Tray
S1-FEED	1
S3-SOLVENT	3

● Vapor and liquid to be on the feed tray.
○ Flash the feed adiabatically, vapor onto the tray above and liquid onto the feed tray.

Product	Type of Product	Phase	Tray	Rate	
S2-RAFFINATE	Bottoms	Liquid 2	3	800.00	kg/hr
S4-EXTRACT	Overhead	Liquid 1	1	1200.0	kg/hr

Exit the window after saving all data

FIGURE 8.10
The column menu should appear as shown in Figure 8.11.



Unit: T1

Description:

Number of Stages: 3

Number of Iterations: 30

Algorithm: Liquid-Liquid

Calculated Phases: Liquid-Liquid

Exit the window after saving all data

FIGURE 8.11
Column required specifications.

ASPEN PLUS CALCULATIONS

The following steps are followed in simulating LLE:

1. Start the Aspen program. The Connect to Engine window will appear; you should select the default Server Type (Local PC).
2. Select *Extraction* from the Equipment Model Library and then convert to the flow sheet window.
3. Streams can be added by clicking on the process flow sheet in the place where you want the stream to begin and by clicking one more time on the stream if you want the stream to end.

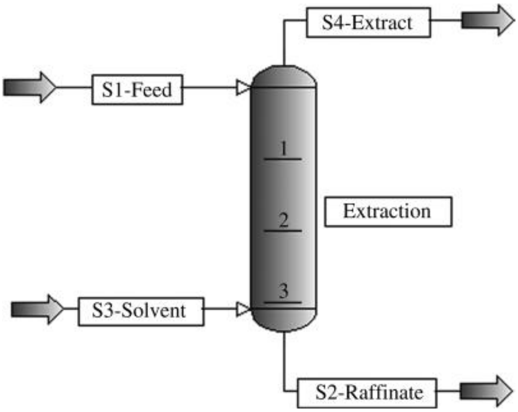
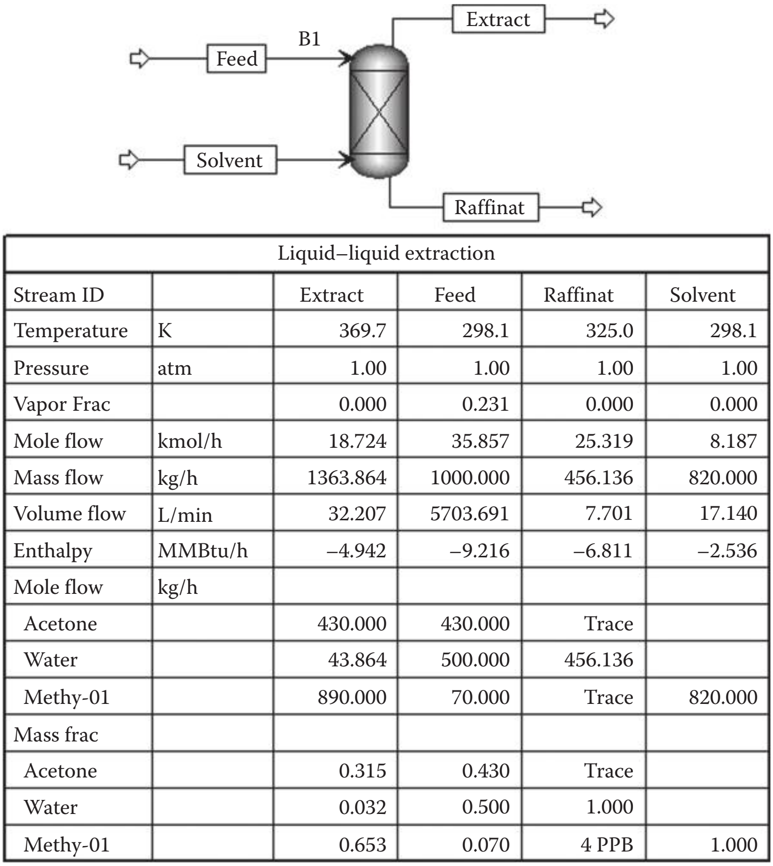


FIGURE 8.12
PFD for Example 8.1.

Stream name Stream description		S1-Feed	S2-Raffinate	S3-Solvent	S4-Extract
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	25.000	25.000	25.000	25.000
Pressure	kg/Cm^2	1.033	1.033	1.033	1.033
Flow rate	kgmol/h	35.857	23.988	8.187	20.055
Composition					
Acetone		0.206	0.001	0.000	0.367
Water		0.774	0.995	0.000	0.194
MIBK		0.019	0.004	1.000	0.438

FIGURE 8.13
Streams flow rate and weight fraction.

4. Under the *Components* tab, input the components that will be used in this simulation.
5. The input under the *Property* tab is probably the most critical input required to run a successful simulation. This key input is the Base Method found under the *Specifications* option. The Base Method is the thermodynamic basis for all simulation calculations.
6. Under the *Streams* tab, enter all of the specifications for each of the feed streams one at a time.
7. To run the simulation, the user could select *Next* in the toolbar which will tell you that all the required inputs are complete and ask if you would like to run the simulation. Or the user can also run the simulation by just selecting the *Run* button in the toolbar (this is the button with a block arrow pointing to the right). Finally, the user can go to *Run* on the menu bar and select *Run*.
8. After the simulation is run and converged, you will notice that the *Results Summary* tab on the *Data Browser* window has a blue check mark. Clicking on that tab will open up the Run Status. If your simulation has really been converged, the run status should state "Calculations were completed normally."
9. Adding stream tables to the process flow sheet is a simple process. On the current screen you will see two of the options for varying the stream table: *Display* and *Format*. Under the *Display* drop-down menu there are two options, *All Streams* or *Streams*. The *Streams* option allows the user to choose which stream they would like to present, one by one. Under the *Format* drop-down menu there are a number of types of stream tables. Each of the options presents the data in a slightly different fashion, depending on the intended application. Use the CHEM_E option. In order to add a stream table, simply click on the *Stream Table* button and a stream table will be added to your process flow sheet (Figure 8.14).
10. There is one other location where the user can modify the appearance and content of stream tables. In the *Data Browser* window, under the *Setup* tab there is an option titled *Report Options*.
11. If some changes would be preferred, first reinitialize the simulation in order to delete the existing results. This can be done by going to *Run/Reinitialize* in the menu bar.



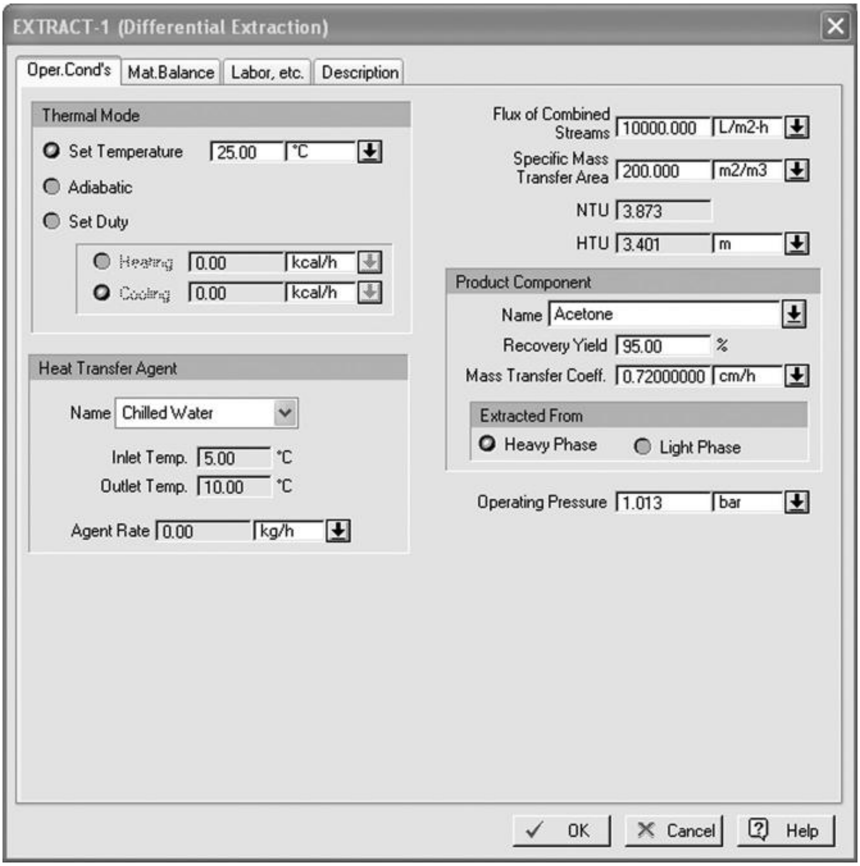
Liquid–liquid extraction					
Stream ID		Extract	Feed	Raffinat	Solvent
Temperature	K	369.7	298.1	325.0	298.1
Pressure	atm	1.00	1.00	1.00	1.00
Vapor Frac		0.000	0.231	0.000	0.000
Mole flow	kmol/h	18.724	35.857	25.319	8.187
Mass flow	kg/h	1363.864	1000.000	456.136	820.000
Volume flow	L/min	32.207	5703.691	7.701	17.140
Enthalpy	MMBtu/h	–4.942	–9.216	–6.811	–2.536
Mole flow	kg/h				
Acetone		430.000	430.000	Trace	
Water		43.864	500.000	456.136	
Methy-01		890.000	70.000	Trace	820.000
Mass frac					
Acetone		0.315	0.430	Trace	
Water		0.032	0.500	1.000	
Methy-01		0.653	0.070	4 PPB	1.000

FIGURE 8.14
Process flow sheet with Stream Table of Example 8.1.

SUPERPRO DESIGNER SIMULATION

SuperPro Designer Pro is different from the previous three softwares, Hysys, Pro/II, and Aspen Plus in a way that Partition coefficient and solubility of the solvent are required in this program. These values are either found from searching the literature or done experimentally. In SuperPro:

1. Under Unit Procedure, go to Extraction then Liquid Extraction, select Differential Extractor (Figure 8.15).
2. Click on *Connection Mode*; add two inlet streams (heavy liquid from the top, usually the feed stream, and light liquid in the bottom, for example, solvent). Now there are two product streams, Extract (top) and Raffinate (bottom). The result is shown in Figure 8.17.
3. Required parameters are shown in Figure 8.16. Partition coefficients of solute should be obtained experimentally or found from the literature. Accurate



Thermal Mode

● Set Temperature 25.00 °C

○ Adiabatic

○ Set Duty

○ Heating 0.00 kcal/h

● Cooling 0.00 kcal/h

Heat Transfer Agent

Name Chilled Water

Inlet Temp. 5.00 °C

Outlet Temp. 10.00 °C

Agent Rate 0.00 kg/h

Flux of Combined Streams 10000.000 L/m2-h

Specific Mass Transfer Area 200.000 m2/m3

NTU 3.873

HTU 3.401 m

Product Component

Name Acetone

Recovery Yield 95.00 %

Mass Transfer Coeff. 0.72000000 cm/h

Extracted From

● Heavy Phase ○ Light Phase

Operating Pressure 1.013 bar

FIGURE 8.15
Process flow sheet and operating conditions window.

values of partition coefficients are necessary to get number of transfer units (NTU).

$$\text{Distribution coefficient}, K = \frac{\text{Mass fraction solute in } E \text{ phase}}{\text{Mass fraction solute } R \text{ phase}}$$

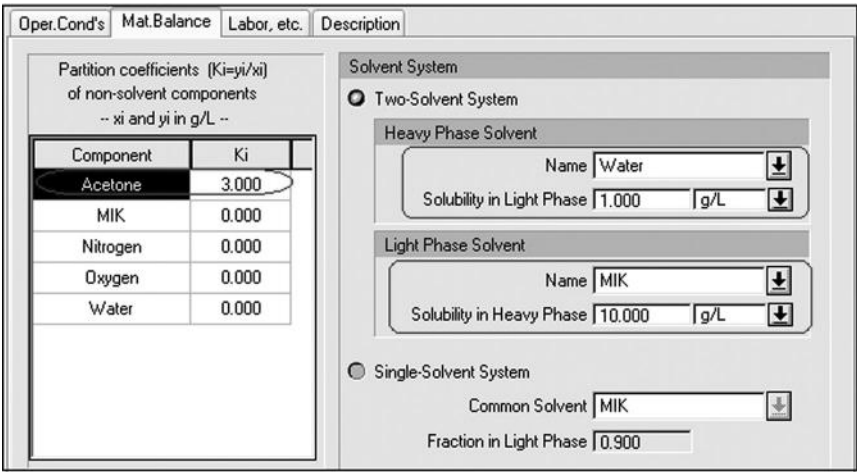
Consider a feed of acetone (solute)/water /chloroform (solvent),

$$\text{Distribution coefficient}, K = \frac{\text{mass fraction acetone in chloroform phase}}{\text{mass fraction solute water phase}}$$

$$\text{Distribution coefficient}, K = \frac{\text{kg acetone/kg chloroform}}{\text{kg acetone/kg water}} = \frac{y}{x} = 1.72$$

This means acetone is preferentially soluble in the chloroform phase.

4. Solubility of heavy phase and light phase solvent should be specified.



Partition coefficients (Ki=yi/xi)
of non-solvent components
-- xi and yi in g/L --

Component	Ki
Acetone	3.000
MIK	0.000
Nitrogen	0.000
Oxygen	0.000
Water	0.000

Solvent System

● Two-Solvent System

Heavy Phase Solvent

Name: Water

Solubility in Light Phase: 1.000 g/L

Light Phase Solvent

Name: MIK

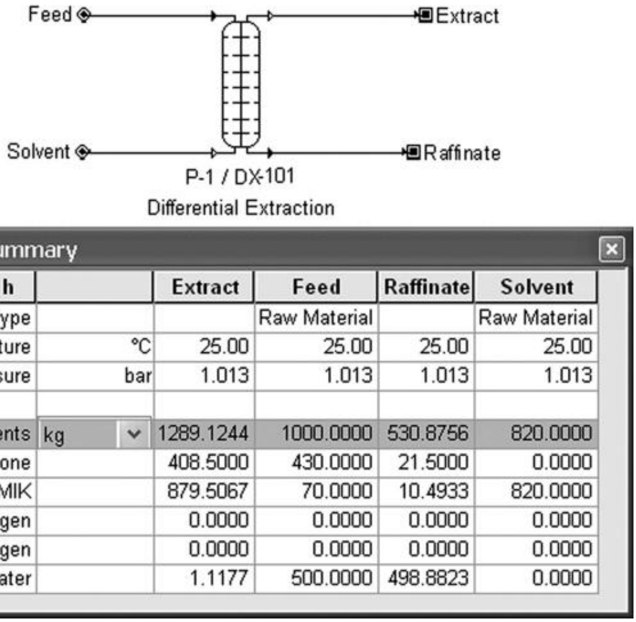
Solubility in Heavy Phase: 10.000 g/L

○ Single-Solvent System

Common Solvent: MIK

Fraction in Light Phase: 0.900

FIGURE 8.16
Required parameters for simulation for Example 8.1.



Time Ref: h		Extract	Feed	Raffinate	Solvent
Type			Raw Material		Raw Material
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	1289.1244	1000.0000	530.8756	820.0000
Acetone		408.5000	430.0000	21.5000	0.0000
MIK		879.5067	70.0000	10.4933	820.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		1.1177	500.0000	498.8823	0.0000

FIGURE 8.17
Stream details.

TABLE 8.2

Results of Example 8.1

	Hand Calculations	Hysys	PRO/II	Aspen Plus	SuperPro Designer
Feed (kg/h)	1000	1000	1000	1000	1000
Solvent (kg/h)	820	820	820	820	820
Extract (kg/h)	1308	1333	1378	1327	1289
Raffinate (kg/h)	512	487	441	429	531

CONCLUSIONS

The results of hand calculations and the four simulation softwares are shown in Table 8.2. Results reveal that hand calculations and those obtained from the software packages were in good agreement.

Example 8.2: Extraction of Acetone Using Pure Trichloroethane

In a continuous countercurrent extraction column, 100 kg/h of a 40-wt% acetone, 60-wt% water solution is to be reduced to 10 wt% acetone by extraction with pure 1,1,2 trichloroethane (TCE) at 25°C and 1 atm; determine (see Table 8.3)

1. The minimum solvent rate.
2. At 1.8 times the minimum solvent/feed rate, find the number of mixer settlers required.

SOLUTION

HAND CALCULATION

Plot the ternary equilibrium diagram and locate inlet and outlet stream compositions as shown in Figure 8.18. To calculate the minimum amount of solvent, one needs to connect the feed stream location to equilibrium point on the extract line employing equilibrium tie line. The line crosses the extract equilibrium line

TABLE 8.3

Equilibrium Data of Ternary Mixture, Acetone–Water–TCE

Water Phase (Mass Fraction)			Water Phase (Mass Fraction)		
Water	Acetone	$C_2H_3Cl_3$	Water	Acetone	$C_2H_3Cl_3$
0.822	0.170	0.007	0.011	0.251	0.738
0.721	0.269	0.010	0.023	0.385	0.592
0.680	0.309	0.012	0.031	0.430	0.539
0.627	0.357	0.016	0.043	0.482	0.475
0.570	0.409	0.021	0.061	0.540	0.400
0.502	0.461	0.038	0.089	0.574	0.337
0.417	0.518	0.065	0.134	0.603	0.263

Source: Data from McCabe, W. L., J. C., Smith, and P. Harriott, 1993. *Unit Operations of Chemical Engineering*, 5th edn, McGraw-Hill, Boston, MA.

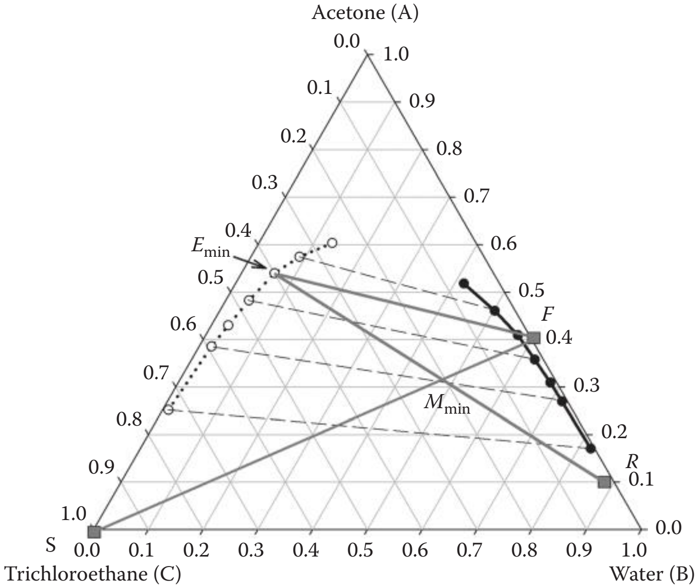


FIGURE 8.18
Location of feed and product stream at minimum solvent feed rate.

at E_{min}. From Figure 8.18 the mass fraction of water at minimum solvent feed rate, $x_{B@}M_{\text{min}}$

$$x_{B@M_{\text{min}}} = \frac{x_B F + x_B S_{\text{min}}}{F + S_{\text{min}}} = \frac{0.6 \times 100\ \text{kg/h} + 0}{100 + S_{\text{min}}} = 0.48$$

The minimum solvent flow rate

$$S_{\text{min}} = \frac{(60 - 48)}{0.48} = 25\ \text{kg/h}$$

Actual inlet solvent is

$$S = 1.8 \times S_{\text{min}} = 1.8 \times 25\ \text{kg/h} = 45\ \text{kg/h}$$

To locate the mixing point on the ternary equilibrium diagram, the water (B) mass fraction at mixing point,

$$x_{B,M} = \frac{x_B F + x_B S}{F + S} = \frac{0.6 \times 100\ \text{kg/h} + 0}{100 + 45} = 0.41$$

The mass fraction of acetone (A) at the mixing point,

$$x_{A,M} = \frac{x_A F + x_A S}{F + S} = \frac{0.4 \times 100\ \text{kg/h} + 0}{100 + 45} = \frac{40}{145} = 0.276$$

To calculate product streams flow rate and compositions (Extract and Raffinate streams), locate the calculated mixing point compositions point (M_{min}) on the ternary diagram as shown in Figure 8.19. Connect E_{min} with M_{min}, and then extend the line to cross the raffinate equilibrium line to point R.

Overall material balance:

$$R + E = F + S = M = 145$$

Acetone component balance:

$$0.1R + 0.42E = 0.276M = 0.276(145)$$

Substitute $R = 145–E$:

$$0.1(145 - E) + 0.42E = 0.276M = 0.276(145)$$

Rearranging:

$$14.5 - 0.1E + 0.42E = 0.276(145) = 39.15$$

$$14.5 - 0.1E + 0.42E = 0.276(145) = 40.0$$

$$0.32E = 25.5 \rightarrow E = 77.75 \text{ kg/h}, \quad R = 145 - E \quad R = 67.25 \text{ kg/h}$$

From Figure 8.20, the equilibrium number of stages is around 3.

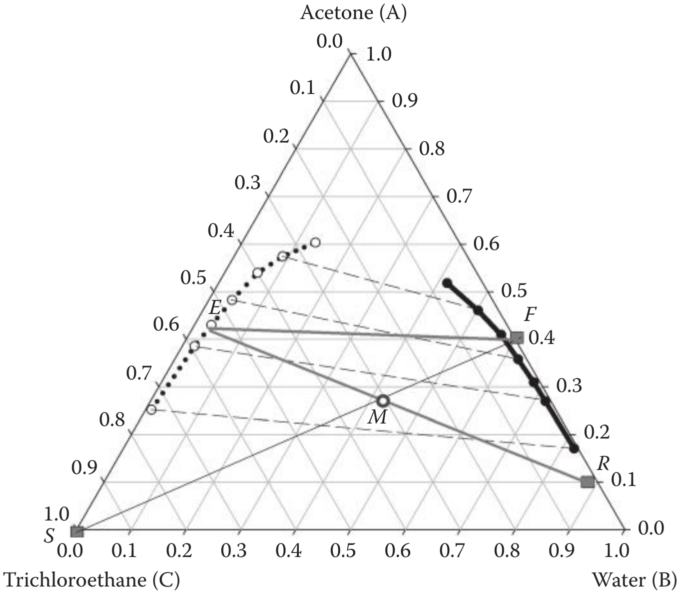


FIGURE 8.19
Feed and product streams at solvent rate is 1.8 minimum solvent rate.

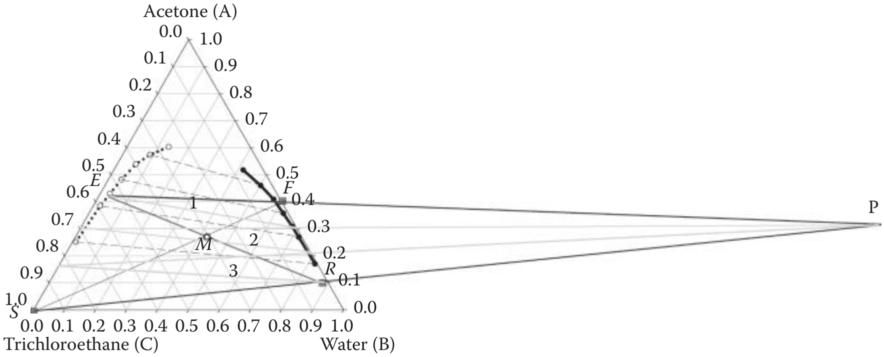


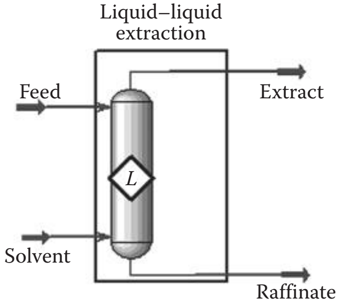
FIGURE 8.20
Equilibrium numbers of stages of Example 8.2.

Hysys Simulation

Select the component, use UNIQUAQ for fluid package (note that NRTL did not work for this example). Make sure that the binary coefficients exist, otherwise use UNIQUAQ LLE to calculate unknown values. The results are shown in Figure 8.21.

PRO/II Calculations

After component and thermodynamic package were selected, select distillation column, uncheck the condenser and reboiler since both are not needed. Set the number of equilibrium stages to three stages. The PFD is shown in Figure 8.22.



Streams					
		Feed	Solvent	Raffinate	Extract
Temperature	C	25.00	25.00	25.05	25.21
Pressure	kPa	101.3	101.3	101.3	101.3
Mass flow	kg/h	100.0	45.00	53.42	91.58
Comp mass frac (H_2O)		0.6000	0.0000	0.9669	0.0912
Comp mass frac (Acetone)		0.4000	0.0000	0.0267	0.4212
Comp mass frac (112-ClC_2)		0.0000	1.0000	0.0064	0.4876

FIGURE 8.21
Hysys simulation of Example 8.2.

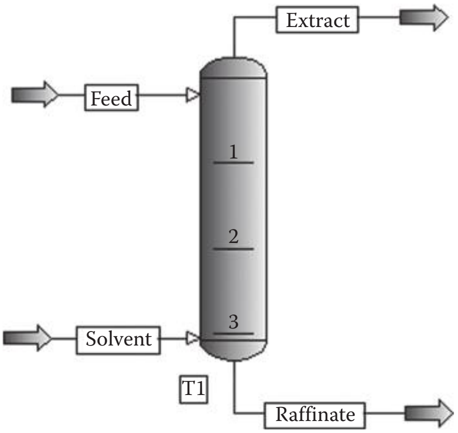
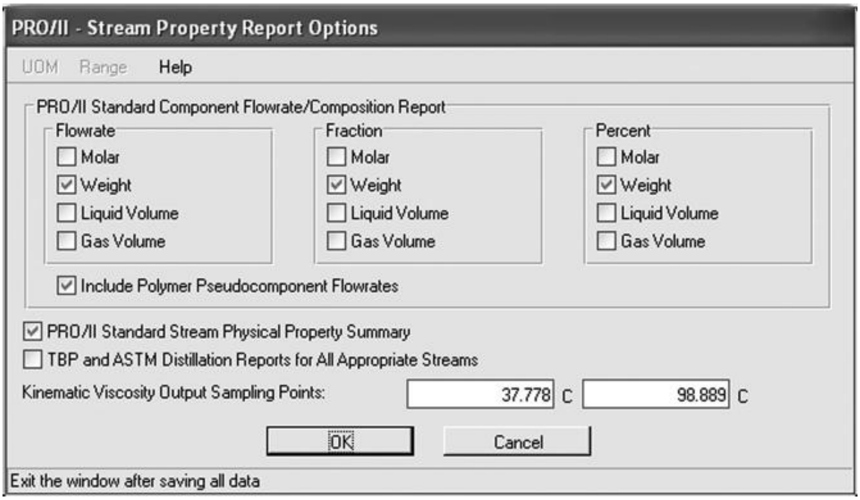


FIGURE 8.22
The PFD of Example 8.2.

Note: to display streams in weight fraction, click on *Output* in the tool bar, then *report format, stream properties* (Figure 8.23). Stream component flow rate and composition report. The result is shown in Figure 8.24.

ASPEN PLUS RESULTS

Using Aspen Plus the process flow sheet and stream table compositions are shown in Figure 8.25, as a base model NRTL was used. The extraction column consists of three equilibrium stages.



PRO/II Standard Component Flowrate/Composition Report

Flowrate
☐ Molar
☑ Weight
☐ Liquid Volume
☐ Gas Volume

Fraction
☐ Molar
☑ Weight
☐ Liquid Volume
☐ Gas Volume

Percent
☐ Molar
☑ Weight
☐ Liquid Volume
☐ Gas Volume

☑ Include Polymer Pseudocomponent Flowrates

☑ PRO/II Standard Stream Physical Property Summary
☐ TBP and ASTM Distillation Reports for All Appropriate Streams

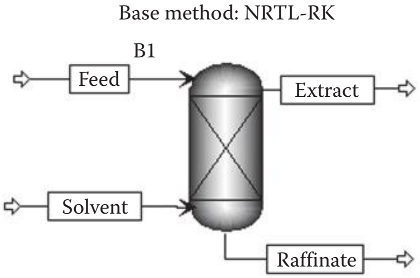
Kinematic Viscosity Output Sampling Points: 37.778 C 98.889 C

Exit the window after saving all data

FIGURE 8.23
Component flow rate and composition in weight.

Stream name Stream description		Extract	Feed	Raffinate	Solvent
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	25.000	25.000	25.000	25.000
Pressure	kg/Cm^2	1.033	1.033	1.033	1.033
Flow rate	kgmol/h	1.113	4.019	3.243	0.337
Composition					
Acetone		0.560	0.171	0.020	0.000
Water		0.139	0.829	0.979	0.000
112TCLET		0.301	0.000	0.001	1.000

FIGURE 8.24
PRO/II results of Example 8.2.



Liquid–Liquid extraction

Stream ID		Extract	Feed	Raffinate	Solvent
Temperature	K	295.8	298.1	289.9	298.1
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	kmol/h	1.003	4.019	3.354	0.337
Mass flow	kg/h	75.982	100.000	69.018	45.000
Volume flow	L/min	1.130	1.858	1.193	0.485
Enthalpy	MMBtu/h	–0.222	–1.068	–0.904	–0.058
Mass flow	kg/h				
Acetone		28.642	40.000	11.358	
Water		3.219	60.000	56.781	
1,1,2–01		44.121		0.879	45.000
Mass frac					
Acetone		0.377	0.400	0.165	
Water		0.042	0.600	0.823	
1,1,2–01		0.581		0.013	1.000

FIGURE 8.25
Process flow sheet with Stream Table of Example 8.2 using Aspen Plus.

SuperPro Designer Simulation

In SuperPro Designer, the partition factor of the solvent should be specified along with the solubility of light- and heavy-phase solvents as previously shown in Example 8.1. A process flow sheet and streams components mass flow rates are shown in Figure 8.26.

Conclusion

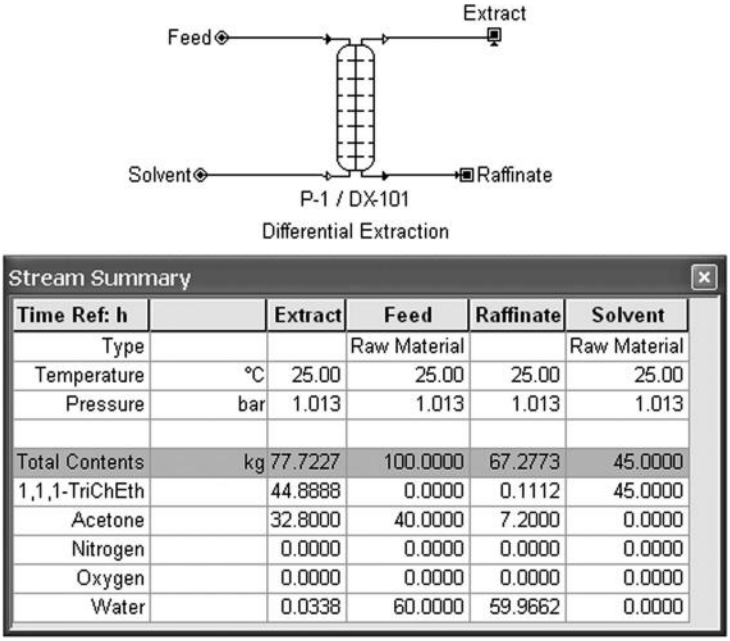
The results of hand calculations and the four simulation software are shown in Table 8.4. Results reveal that hand calculations and those obtained from the software packages were in good agreement. The result obtained by PRO/II is close to hand calculations; in contrast, the Hysys results were far from hand calculations.

Example 8.3: Extraction of Acetone from Water Using MIBK

A countercurrent extraction plant (Figure 8.27) is used to extract acetone from 100 kg/h of feed mixture. The feed consists of 40 wt% acetone (A) and 60 wt% water (w) by means of MIBK at a temperature of 25°C and 1 atm100 kg/h of pure solvent (MIBK) is used as the extracting liquid [3].

How many ideal stages are required to extract 99% of the acetone fed?

What are the extract and raffinate mass flow rates and compositions?



Stream Summary

Time Ref: h		Extract	Feed	Raffinate	Solvent
Type			Raw Material		Raw Material
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	77.7227	100.0000	67.2773	45.0000
1,1,1-TriChEth		44.8888	0.0000	0.1112	45.0000
Acetone		32.8000	40.0000	7.2000	0.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		0.0338	60.0000	59.9662	0.0000

FIGURE 8.26
Process flow sheet with Stream Table of Example 8.2 using SuperPro Designer.

TABLE 8.4

Results of Example 8.2

	Hand Calculations	Hysys	PRO/II	Aspen Plus	SuperPro Designer
Feed (kg/h)	100	100	100	100	100
Solvent (kg/h)	45	45	45	45	45
Extract (kg/h)	77.75	91.58	83.66	76	77.7
Raffinate (kg/h)	67.25	53.42	61.34	69	67.3

SOLUTION

HAND CALCULATION

The composition and flow rate of inlet streams (Feed and Solvent) are given:

Feed: 100 kg/h, 0.4 mass fraction acetone, and 0.6 mass fraction water.
Solvent: 100 kg/h of pure MIBK.

First, determine stream compositions:

Assume that mass flow rate of water in the extract stream = w.
Mass flow rate of MIBK in the raffinate stream = m.
Since 99% of the acetone is recovered in the extract
$0.99\ (0.4*100) = 39.6$ kg/h.
Mass flow rate of acetone in the raffinate = $40 - 39.6 = 0.4$ kg/h.

Stream flow rates:
$L_o = 100$ kg/h, $V_{N+1} = 100$ kg/h
$V_N = 39.6 + (100 - m) + w$

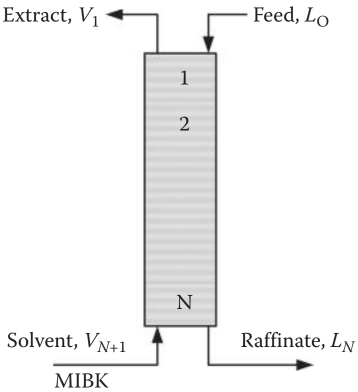


FIGURE 8.27
Process flow chart of Example 8.3.

$L_N = 0.4 + (60 - w) + m = 60.4 + m - w$
As first assumption neglect the amount of w and m,

$$V_N = 140 \text{ kg/h.}$$

The mass fraction of acetone in the exit extract stream

$$y_{A,N} = \frac{39.6}{140} = 0.283$$

The corresponding mass fraction of water from the equilibrium diagram is

$$y_{W,N} = 0.049$$

$$w = \frac{0.049}{1 - 0.049}\left(39.6 + 100 - m\right)$$

The amount of m is very small and can be neglected as in the first trial:

$$w = 7.2 \text{ kg/h}$$

The mass fraction of acetone in the exit raffinate stream

$$x_{A,N} = \frac{0.4}{60} = 0.007$$

The corresponding mass fraction of MIBK from the equilibrium diagram is

$$x_{M,N} = 0.02$$

The amount of MIBK:

$$m = \frac{0.02}{1 - 0.02}\left(0.4 + 60 - w\right)$$
$$m = \frac{0.02}{1 - 0.02}\left(0.4 + 60 - 7.2\right) = 1.1 \text{kg/h}$$

The revised value of water

$$w = \frac{0.049}{1 - 0.049}\left(39.6 + 100 - 1.1\right) = 7.1 \text{kg/h}$$

SUMMARY

$$L_o = 100 \text{ kg/h}$$

$$x_{A,o} = 0.4, \ x_{w,o} = 0.6$$

$$V_{N+1} = 100 \text{ kg/h}$$

$$y_{A,N+1} = 0, \quad y_{M,N+1} = 1.0$$

$$L_N = 0.4 + (60 - w) + m = 60.4 + m - w = 60.4 + 1.1 - 7.1 = 54.4 \text{ kg/h}$$

$$x_{A,N} = \frac{0.4}{54.4} = 0.0074$$

$$V_N = 39.6 + (100 - m) + w = 139.6 - 1.1 + 7.1 = 145.6 \text{ kg/h}$$

$$y_{A,N} = \frac{39.6}{145.6} = 0.272$$

RESULTS

The inlet and exit streams compositions are located in the ternary diagram shown in Figure 8.28. Performing stage-by-stage calculations reveals that four equilibrium stages are required.

$$L_o = 100 \text{ kg/h}, \; V_{N+1} = 100 \text{ kg/h}, \; L_N = 54.4 \text{ kg/h}, \; V_{N+1} = 145.6 \text{ kg/h}$$

HYSYS CALCULATIONS

Start a new case in Hysys, Select Acetone, Water, and MIBK for the components. Use the UNIQUAQ Fluid Package. Check the binary coefficients; simply click the *Binary Coeffs* tab. To specify the undefined values; in LLE processes, select UNIFAC LLE, and click on *Unknowns Only* (Figure 8.29).

1. Close and return to simulation environment. Name the streams: Feed, Solvent, Extract, and Raffinate, then click on *Next*. Specify a constant pressure of 1 atm by typing it in to the pressure columns. Click on *Done* to complete the Liquid–Liquid Extractor Input screen.
2. Specify number of stages as four stages to compare with hand calculation.
3. Double click on the Feed stream. Enter the desired feed properties; a temperature of 25°C, a pressure of 1 atm, a flow rate of 100 kg/h, and a feed with a 40-wt% acetone and 60 wt% water.

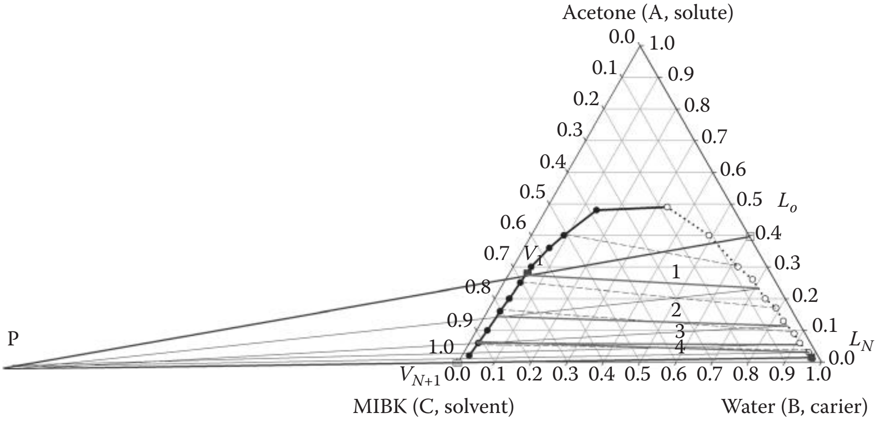
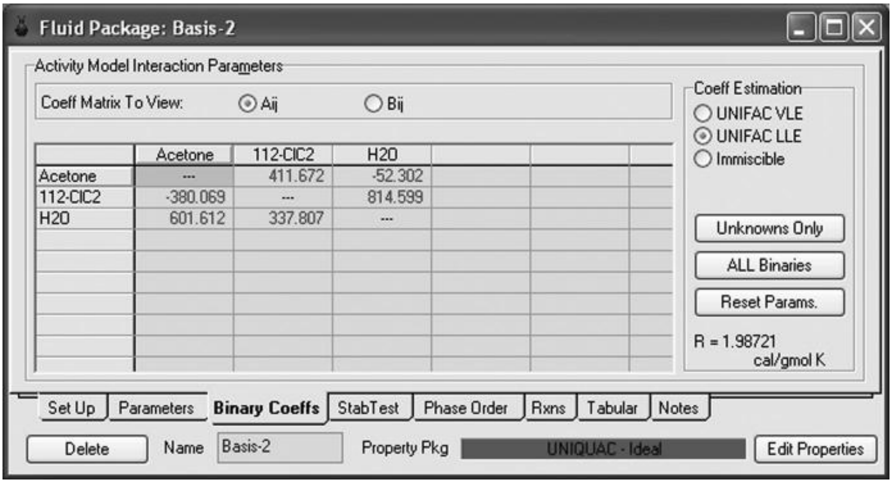


FIGURE 8.28
Equilibrium stages of Example 8.3.



Coeff Matrix To View: ● Aij ○ Bij

	Acetone	112-ClC2	H2O
Acetone	---	411.672	-52.302
112-ClC2	-380.069	---	814.599
H2O	601.612	337.807	---

Coeff Estimation
○ UNIFAC VLE
● UNIFAC LLE
○ Immiscible

R = 1.98721 cal/gmol K

Name: Basis-2

Property Pkg: UNIQUAC - Ideal

FIGURE 8.29
Activity model interaction parameters.

4. The solvent stream contains pure MIBK entering at 25°C, 1 atm and flowing at 100 kg/h.
5. Double click on the column and click on *Run*. Close the window and see that the Extracted Product and Raffinate streams have turned light to dark blue, signifying that Hysys has successfully solved for those streams of unknown properties. After this stage, if any of the specifications on the liquid–liquid extraction column are changed, the *Reset* button must be pressed, and then the *Run* button pressed again to rerun the distillation simulation with the new specifications (Figure 8.30).

PRO/II CALCULATIONS

Select Acetone, Water, and MIBK from the components menu. Use the UNIQUAQ Fluid Package. Select distillation column from object palette, uncheck the reboiler and condenser, specify the number of stages as four equilibrium stages. Repeat the PRO/II procedure used in Example 8.1. The process flow sheet is shown in Figure 8.31.

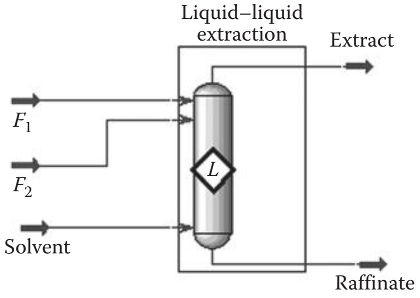
The generated output report is shown in Figure 8.32.

ASPEN PLUS RESULTS

Use SRK for fluid package to measure fluid property; the first liquid-phase key components are acetone and water. The second liquid-phase key component is MIBK (Figure 8.33).

SUPERPRO DESIGNER SIMULATION

Using SuperPro Designer the result is shown in Figure 8.34; as previously mentioned, the partition coefficient of solute should be specified either by trial and error to achieve certain separation or by using experimental values.



Streams						
		F_1	F_2	Solvent	Extract	Raffinate
Temperature	C	25.00	25.00	25.00	25.20	25.00
Pressure	kPa	101.3	101.3	101.3	101.3	101.3
Mass flow	kg/h	7500.0	7500.00	5000.00	11679.46	8320.54
Comp mass frac (H_2O)		0.500	0.750	0.000	0.105	0.979
Comp mass frac (Acetone)		0.500	0.250	0.000	0.471	0.015
Comp mass frac (112-ClC_2)		0.000	0.000	1.000	0.424	0.006

FIGURE 8.30
Hysys results of Example 8.3.

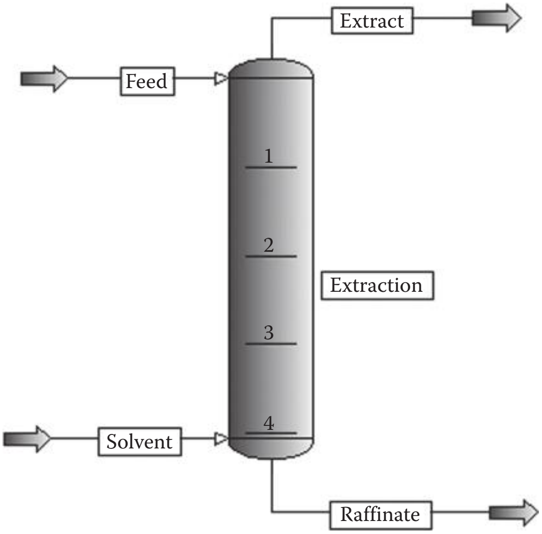
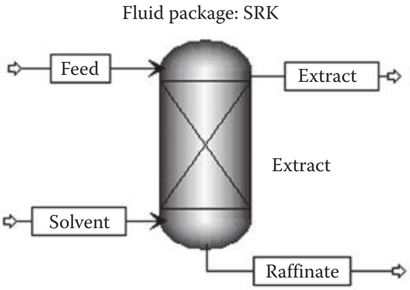


FIGURE 8.31
PFD of Example 8.3.

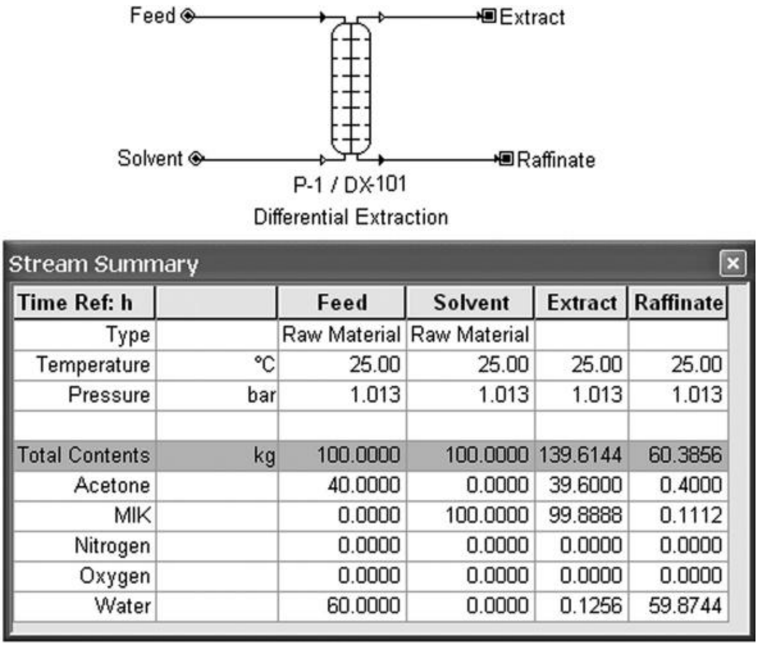
Stream name Stream description		Extract	Feed	Raffinate	Solvent
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	25.000	25.000	25.000	25.000
Pressure	kg/Cm^2	1.055	1.033	1.055	1.033
Flow rate	kgmol/h	1.958	4.019	3.060	0.998
Composition					
Acetone		0.351	0.171	0.001	0.000
Water		0.145	0.829	0.996	0.000
MIBK		0.505	0.000	0.003	1.000

FIGURE 8.32
PRO/II results of Example 8.3.



Example 8.3					
Stream ID		Extract	Feed	Raffinate	Solvent
Temperature	K	364.6	298.1	319.3	298.1
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		0.000	0.175	0.000	0.000
Mole flow	kmol/h	3.241	4.019	1.777	0.998
Mass flow	kg/h	58.404	100.000	141.596	100.000
Volume flow	L/min	1.010	486.213	3.088	2.090
Enthalpy	MMBtu/h	–0.863	–1.043	–0.489	–0.309
Mass flow	kg/h				
Acetone		0.021	40.000	39.979	
Water		58.382	60.000	1.618	
Methy-01		Trace		100.000	100.000
Mass frac					
Acetone		362 ppm	0.400	0.282	
Water		1.000	0.600	0.011	
Methy-01		Trace		0.706	1.000

FIGURE 8.33
Process flow sheet with Stream Table of Example 8.3 using Aspen Plus.



Time Ref: h		Feed	Solvent	Extract	Raffinate
Type		Raw Material	Raw Material		
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	100.0000	100.0000	139.6144	60.3856
Acetone		40.0000	0.0000	39.6000	0.4000
MIK		0.0000	100.0000	99.8888	0.1112
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		60.0000	0.0000	0.1256	59.8744

FIGURE 8.34
Process flow sheet with Stream Table of Example 8.3 using SuperPro Designer.

CONCLUSIONS

The results of hand calculations and the four simulation softwares are shown in Table 8.5. Results reveal that hand calculations and those obtained from the software packages were in good agreement. The result obtained by PRO/II is close to hand calculations, in contrast, the results obtained using SuperPro Designer were far from hand calculations and other software packages, accurate values of partition coefficients may give better results.

Example 8.4: Extraction of Acetone from Water Using 1,1,2-Trichloroethane

A countercurrent extraction column is used to extract acetone from water in a two feed streams using 5000 kg/h of 1,1,2-trichloroethane to give a raffinate containing 10 wt% acetone. The feed stream F_1 is at a rate 7500 kg/h, containing 50% acetone, 50 wt% water. Second feed, F_2 is at a rate 7500 kg/h containing 25 wt% acetone and 75 wt% water. The column is operating at 25°C and 1 atm [3]. Calculate the required equilibrium number of stages and the stage to which feed streams should be introduced.

Note: Use equilibrium data of Example 8.2.

SOLUTION

Hand Calculations

Draw the ternary diagram and locate feed streams (F_1, F_2, and S). Find the mixing point compositions (Figure 8.35).

Mixing point compositions,

$$F_1 + F_2 + V_{N+1} = L_N + V_1 = \mathrm{M}$$

$$7500 + 7500 + 5000 = L_N = V_1 = \mathrm{M}$$

$$M = 20{,}000\ \mathrm{kg/h}$$

Component balance of acetone (A),

$$0.5 \times 7500 + 0.25 \times 7500 + 0 \times 5000 = L_N = V_1 = x_{AM} \times 20{,}000$$

$$x_{AM} = 0.28$$

Component balance of 1,1,2 trichloroethane (C),

$$0.0 \times 7500 + 0.0 \times 7500 + 1 \times 5000 = x_{CM} \times 20{,}000$$

$$x_{CM} = 0.25$$

The raffinate (L_N) and extract (V_1) mass flow rate,

$$L_N + V_1 = M = 20{,}000$$

Component balance (acetone),

$$0.1 \times L_N + 0.47 \times V_1 = 0.28 \times 20{,}000$$

Substituting total balance,

$$0.1 \times (20{,}000 - V_1\ ) + 0.47 \times V_1 = 0.28 \times 20{,}000$$

$$V_1 = 9729\ \mathrm{kg/h}$$

$$L_N = 10{,}271\ \mathrm{kg/h}$$

TABLE 8.5

Results of Example 8.3

	Hand Calculations	Hysys	PRO/II	Aspen Plus	SuperPro Designer
Feed (kg/h)	100	100	100	100	100
Solvent (kg/h)	100	100	100	100	100
Extract (kg/h)	54.4	58.6	56.1	58.4	60.4
Raffinate (kg/h)	145.6	141.8	143.92	141.6	139.6

HYSYS SIMULATION

To verify the hand calculations using Hysys, open a new case in Hysys, select the components (water, acetone, 1,1,2 trichloroethane). Select UNIQUAQ as the fluid package. Make sure that the binary coefficients exist, otherwise estimate unknown values, and set number of stages to 5. The Hysys process flow sheet and the result of exit stream are shown in Figure 8.36.

PRO/II SOLUTION

Select distillation column from object palette, no condenser or reboiler is required, so uncheck reboiler and condenser radio button. Set equilibrium number of stages to five; enter first feed at stage 1 and the second feed at stage 3. Add components (water, acetone, TCE); select UNIQUAQ for fluid package under the *Liquid Activity* menu. The converged PRO/II PFD is shown in Figure 8.37. The generated report is shown in Figure 8.38. The report shows the streams flow rate and composition.

ASPEN PLUS CALCULATIONS

Using UNIQUAQ for fluid property measurement, the Aspen Plus process flow sheet and stream table compositions is shown in Figure 8.39.

SUPERPRO DESIGNER SIMULATION

The process flow sheet and stream table simulation results are shown in Figure 8.40.

CONCLUSIONS

The results of hand calculations and the four simulation softwares are shown in Table 8.6. Results reveal that hand calculations and those obtained from the

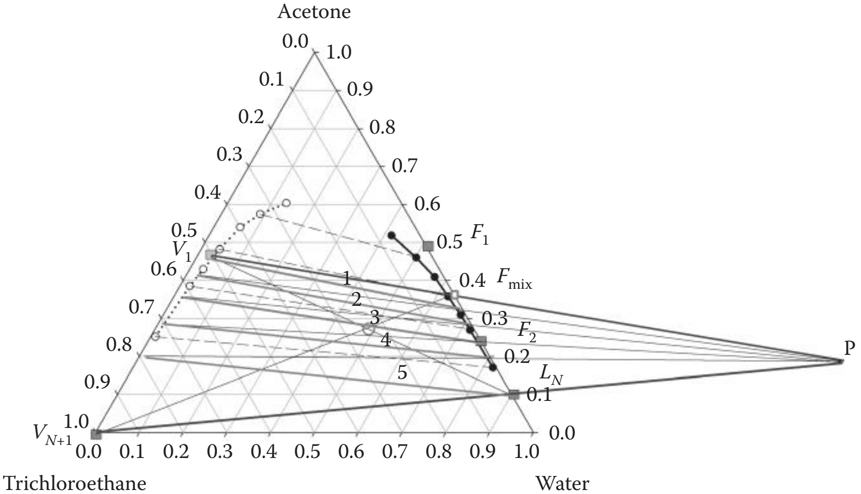
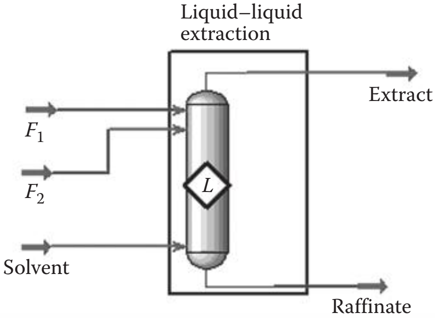


FIGURE 8.35
Ternary diagram of Example 8.4 (5 stages).



Streams						
		Solvent	Extract	Raffinate	F_1	F_2
Temperature	C	25.00	25.01	25.01	25.00	25.00
Pressure	kPa	101.3	101.3	101.3	101.3	101.3
Mass flow	kg/h	5000	11677	8323	7500	7500
Comp mass frac (H_2O)		0.000	0.105	0.979	0.500	0.750
Comp mass frac (Acetone)		0.000	0.471	0.015	0.500	0.250
Comp mass frac (112-ClC_2)		1.000	0.424	0.006	0.000	0.000

FIGURE 8.36
Hysys results of Example 8.4.

software packages were in good agreement. The result obtained by PRO/II is closer to hand calculations than others; in contrast, the results obtained using Hysys were far from hand calculations and other software packages; trying other fluid packages from Hysys will give better results.

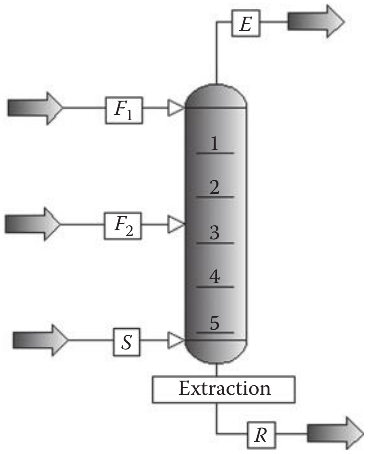
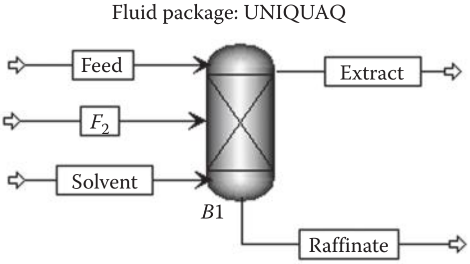


FIGURE 8.37
PFD of Example 8.4.

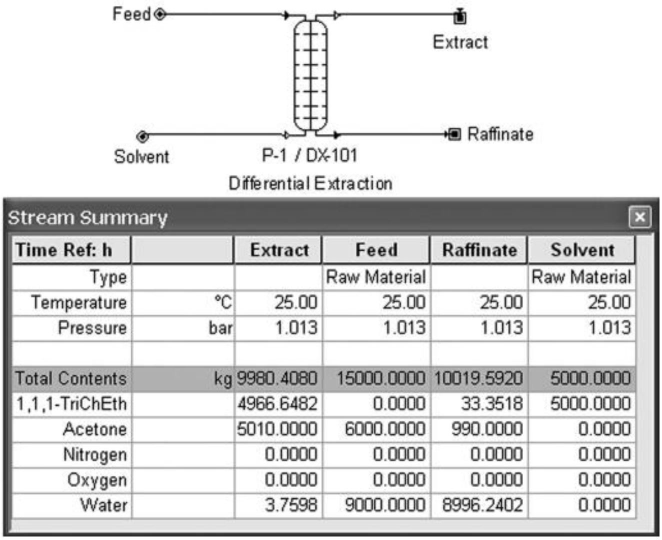
Stream name Stream description		E	F_1	F_2	R	S
Phase		Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	F	77.000	77.000	77.000	77.000	77.000
Pressure	psia	14.696	14.696	14.696	14.696	14.696
Flow rate	lb-mol/h	331.071	601.251	759.533	1112.343	82.630
Composition						
Acetone		0.584	0.237	0.094	0.018	0.000
Water		0.169	0.763	0.906	0.981	0.000
112TCLET		0.247	0.000	0.000	0.001	1.000

FIGURE 8.38
Stream weight component fractions of Example 8.4.



Example 8.4						
Stream ID		Extract	F_2	Feed	Raffinate	Solvent
Temperature	K	298.1	298.1	298.1	298.2	298.1
Pressure	atm	1.00	1.00	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000	0.000	0.000
Mole flow	kmol/h	315.889	344.518	272.723	338.832	37.480
Mass flow	kg/h	8248.365	7500.000	7500.000	11751.635	5000.000
Volume flow	L/min	155.090	134.259	142.731	178.967	61.315
Enthalpy	MMBtu/h	−83.190	−92.101	−71.475	−86.590	−6.204
Mass flow	kg/h					
Acetone		3706.226	1875.000	3750.000	1918.774	
Water		4541.084	5625.000	3750.000	4833.916	
1, 1, 1–01		1.056			4998.944	5000.000
Mass frac						
Acetone		0.449	0.250	0.500	0.163	
Water		0.551	0.750	0.500	0.411	
1, 1, 1–01		128 ppm			0.425	1.000

FIGURE 8.39
Process flow sheet and Stream Table of Example 8.4 (Aspen Plus).



Time Ref: h		Extract	Feed	Raffinate	Solvent
Type			Raw Material		Raw Material
Temperature	°C	25.00	25.00	25.00	25.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	9980.4080	15000.0000	10019.5920	5000.0000
1,1,1-TriChEth		4966.6482	0.0000	33.3518	5000.0000
Acetone		5010.0000	6000.0000	990.0000	0.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		3.7598	9000.0000	8996.2402	0.0000

FIGURE 8.40
Process flow sheet and Stream Table of Example 8.4 (SuperPro Designer).

Example 8.5: Extraction of Acetic Acid Using Isopropyl Ether [4]

A mixture of 15 kg/h of acetic acid and water containing 30 wt% acid is to be extracted by 45 kg/h of pure isopropyl ether at 20°C and 1 atm. Calculate the number of equilibrium stages required to achieve a concentration of 2 wt% acetic acid in the product raffinate stream (Table 8.7)

SOLUTION

HAND CALCULATIONS

The schematic diagram of a process flow sheet is shown in Figure 8.41. The ternary equilibrium diagram is shown in Figure 8.42.

The mixing point of the second stage is determined as follows:

$$S_1 + L_o = V_1 + L_N = M_1 = 60 \text{ kg/h}$$

TABLE 8.6
Results of Example 8.4

		Hand Calculations	Hysys	PRO/II	Aspen Plus	SuperPro Designer
Feed (kg/h)	F_1	7500	7500	7500	7500	7500
	F_2	7500	7500	7500	7500	7500
Solvent (kg/h)		5000	5000	5000	5000	5000
Extract (kg/h)		9729	11679	10500	11752	10020
Raffinate (kg/h)		10271	8321	9500	8248	9980

TABLE 8.7

Equilibrium Data at 20°C for the Acetic Acid–WaterIsopropyl Ether

Water Layer (Mass Fraction)			Isopropyl Ether Layer (Mass Fraction)		
Water	**Acetic Acid**	**Isopropyl Ether**	**Water**	**Acetic Acid**	**Isopropyl Ether**
0.981	0.007	0.012	0.005	0.002	0.993
0.971	0.014	0.015	0.007	0.004	0.989
0.955	0.029	0.016	0.008	0.008	0.984
0.917	0.064	0.019	0.010	0.019	0.971
0.844	0.133	0.023	0.019	0.048	0.933
0.711	0.255	0.034	0.039	0.114	0.847
0.589	0.367	0.044	0.069	0.216	0.715
0.451	0.443	0.106	0.108	0.311	0.581
0.371	0.464	0.165	0.151	0.362	0.487

Source: Data from Geankoplis, J. C. 1998. *Transport Process and Unit Operations,* 3rd edn, McGraw-Hill, Boston, MA.

The mass fraction of isopropyl ether (C) at the mixing point

$$x_{CM} = \frac{y_{C1}S_1 + x_{C0}L_o}{S_1 + L_o} = \frac{1 \times 45 + 0 \times 15}{45 + 15} = 0.75$$

The mass fraction of acetic acid at the mixing point

$$x_{AM} = \frac{y_{A1}S_1 + x_{A0}L_o}{S_1 + L_o} = \frac{0 \times 45 + 0.3 \times 15}{45 + 15} = 0.075$$

Locate the mixing point on the ternary diagram; the mass fraction of the extract stream leaving stage 1, V_1 is

$$x_{A1} = 0.1, \quad x_{B1} = 0.02, \quad x_{C1} = 0.88$$

The amount of L_N can be calculated such that

$$L_N + V_1 = 60 \ \rightarrow \ V_1 = 60 - L_N$$

Component balance (isopropyl ether, C):

$$0.02 \times L_N + 0.88(60 - L_N) = 0.75 \times 60$$

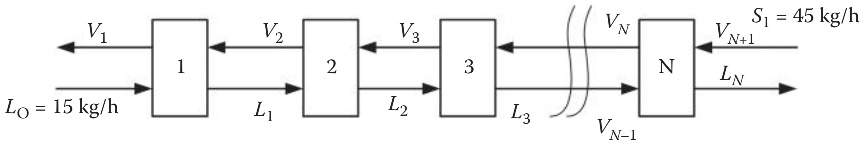


FIGURE 8.41

Schematic diagram of three stages countercurrent extraction.

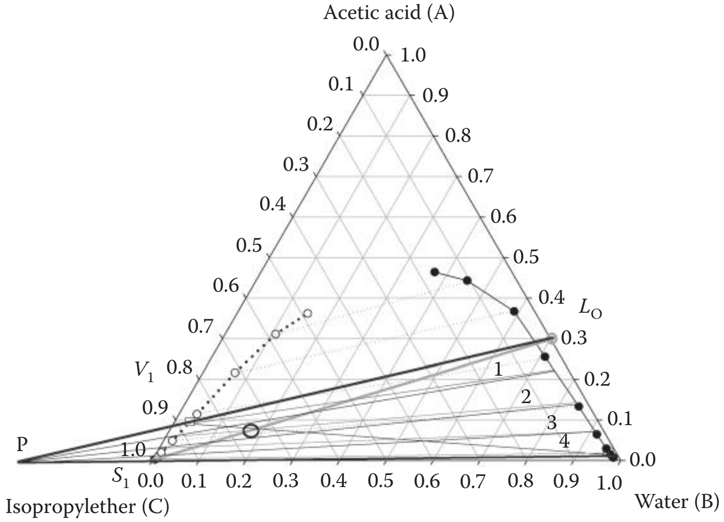


FIGURE 8.42
Ternary equilibrium diagram of Example 8.5.

Mass flow rate of streams leaving unit:

$$L_N = 9.1 \text{ kg/h}, \quad V_1 = 50.9 \text{ kg/h}$$

HYSYS SIMULATIONS

The fluid package used in the simulation is NRTL and the binary coefficients were calculated using UNIFAC LLE. Built-in default values of binary coefficients with NRTL fluid package did not give reasonable results (Figure 8.43).

PRO/II SIMULATIONS

The Pro/II process flow sheet is shown in Figure 8.44, and the simulation result is shown in Figure 8.45.

ASPEN PLUS CALCULATIONS

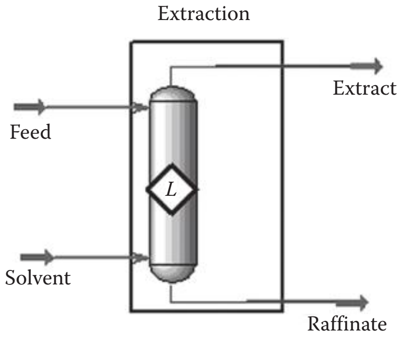
The Aspen Plus process flow sheet, stream table weight, and mass fractions are shown in Figure 8.46.

SUPERPRO DESIGNER SIMULATION

The SuperPro Designer flow sheet and stream table with weight and mass fractions included in it can be seen in Figure 8.47.

CONCLUSIONS

The results of hand calculations and the four simulation softwares are shown in Table 8.8. The table reveals that the results obtained from the four software packages were very close to each other while there is also discrepancy in that obtained



Streams					
		Feed	Solvent	Extract	Raffinate
Temperature	C	20.00	20.00	19.98	20.00
Pressure	kPa	101.3	101.3	101.3	101.3
Mass flow	kg/h	15.00	45.00	49.78	10.22
Comp flow frac (Acetic acid)		0.3000	0.0000	0.0884	0.0099
Comp flow frac (di-i-P-ether)		0.0000	1.0000	0.9037	0.0012
Comp flow frac (H_2O)		0.7000	0.0000	0.0079	0.9890

FIGURE 8.43
Hysys process flow sheet and Stream Table of Example 8.5.

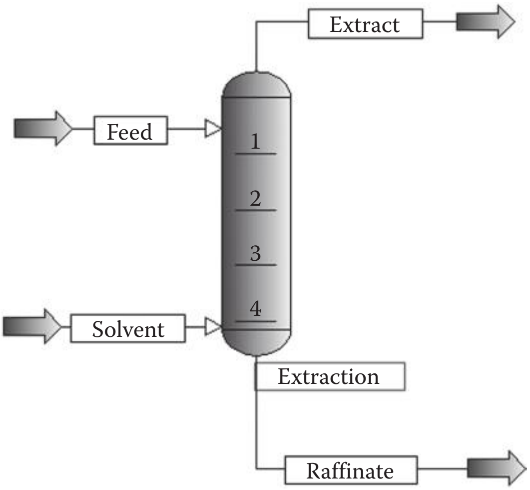
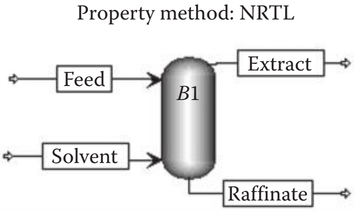


FIGURE 8.44
Process flow sheet of Example 8.5.

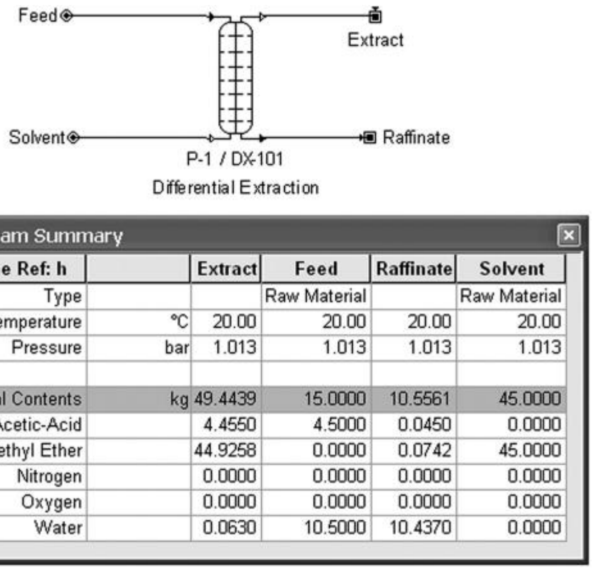
Stream name Stream description		Extract	Feed	Raffinate	Solvent
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	22.521	20.000	24.823	25.000
Pressure	kg/cm^2	1.055	1.033	1.055	1.033
Flow rate	kgmol/h	0.528	0.658	0.570	0.440
Composition					
Water		0.070	0.886	0.958	0.000
Acetic		0.100	0.114	0.039	0.000
DIPE		0.831	0.000	0.003	1.000

FIGURE 8.45
Stream weight component fractions of Example 8.5.



Example 8.5					
Stream ID		Extract	Feed	Raffinate	Solvent
Temperature	K	292.4	293.1	292.4	293.1
Pressure	atm	1.00	1.00	1.00	1.00
Vapor frac		0.000	0.000	0.000	0.000
Mole flow	kmol/h	0.544	0.658	0.555	0.440
Mass flow	kg/h	49.236	15.000	10.764	45.000
Volume flow	L/min	1.071	0.253	0.181	1.033
Enthalpy	MMBtu/h	–0.185	–0.190	–0.153	–0.147
Mass flow	kg/h				
ACETI-01		3.640	4.500	0.860	
Water		0.804	10.500	9.696	
DIISO-01		44.792		0.208	45.000
Mass frac					
ACETI-01		0.074	0.300	0.080	
Water		0.016	0.700	0.901	
DIISO-01		0.910		0.019	1.000

FIGURE 8.46
Process flow sheet and Stream Table for Example 8.5 (Aspen Plus).



Time Ref: h		Extract	Feed	Raffinate	Solvent
Type			Raw Material		Raw Material
Temperature	°C	20.00	20.00	20.00	20.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	49.4439	15.0000	10.5561	45.0000
Acetic-Acid		4.4550	4.5000	0.0450	0.0000
Diethyl Ether		44.9258	0.0000	0.0742	45.0000
Nitrogen		0.0000	0.0000	0.0000	0.0000
Oxygen		0.0000	0.0000	0.0000	0.0000
Water		0.0630	10.5000	10.4370	0.0000

FIGURE 8.47
Process flow sheet and Stream Table for Example 8.5 (SuperPro Designer).

by hand calculations due to the accuracy in drawing of the equilibrium tie lines in the equilibrium ternary diagram.

PROBLEMS

8.1 Extraction of Acetone from Water by MIBK

A countercurrent liquid–liquid extractor is used to remove acetone from a feed that contains 50% acetone (A), 50 wt% water (B). Pure MIBK, at a flow rate of 80 kg/h, is used as the solvent in this separation. A feed flow rate of 100 kg/h is to be treated. It is desired to have a final raffinate of 4 wt% acetone. The operation takes place at 25°C and 1 atm. Determine the number of stages necessary for the separation as specified.

TABLE 8.8
Results of Example 8.5

	Hand Calculations	Hysys	PRO/II	Aspen Plus	SuperPro Designer
Feed (kg/h)	15	15	15	15	15
Solvent (kg/h)	45	45	45	45	45
Extract (kg/h)	50.9	49.8	48.6	49.2	49.4
Raffinate (kg/h)	9.1	10.2	11.4	10.8	10.6

8.2 Extraction of Acetone Using Pure TCE

In a continuous countercurrent extraction column, 100 kg/h of a 30 wt% acetone, 70 wt% water solution is to be reduced to 10 wt% acetone by extraction with 100 kg/h of pure 1,1,2 trichloroethane (TCE) at 25°C and 1 atm, find: Find the number of mixer settlers required.

8.3 Extraction of Acetone from Water Using MIBK

A countercurrent extraction plant is used to extract acetone from 100 kg/h of feed mixture. The feed consists of 20 wt% acetone (A) and 80 wt% water (w) by means of MIBK at a temperature of 25°C and 1 atm. 100 kg/h of pure solvent MIBK is used as the extracting liquid. How many ideal stages are required to extract 90% of the acetone fed? What are the extract and raffinate mass flow rates and what are the compositions?

8.4 Extraction of Acetone from Water Using 1,1,2 Trichloroethane

A countercurrent extraction column is used to extract acetone from water in a two-feed stream using 50 kg/h of 1,1,2 trichloroethane to give a raffinate containing 10 wt% acetone. The feed stream F_1 is at a rate 75 kg/h, containing 50% acetone, 50 wt% water. The second feed, F_2 is at a rate 75 kg/h containing 25 wt% acetone and 75 wt% water. The column is operating at 25°C and 1 atm. Calculate the required equilibrium number of stages and the stage to which feed streams should be introduced.

8.5 Extraction of Acetic Acid from Water Using Isopropyl Ether

A mixture of 100 kg of an acetic acid and water containing 30 wt% acid is to be extracted in a three-stage extractor with isopropyl ether at 20°C using 40 kg of pure solvent. A fresh solvent at 40 kg/h of pure solvent is added to the second stage.

Determine the composition and quantities of the raffinate and extract streams (Figure 8.48).

8.6 Extraction of Acetone in Two Stages

A mixture mass flow rate 100 kg/h contains 0.24 mass fraction acetone and 0.78 water is to be extracted by 50 kg/h of MIBK in two stages using a countercurrent continuous extractor. Determine the amount and composition of the extract and raffinate phases.

8.7 Three-Stage Extractor Continuous Extractor

A three-stage countercurrent extractor is used to extract acetic acid from water by isopropyl ether. A solution of 40 kg/h of containing 35 wt% acetic acid in water is contacted with 40 kg/h of pure isopropyl ether. Calculate the amount and composition of the extract and raffinate layers.

8.8 Extraction of Acetic Acid with Pure Isopropyl Ether

An aqueous feed solution of acetic acid contains 30 wt% acetic acid and 70 wt% water is to be extracted in a continuous countercurrent extractor

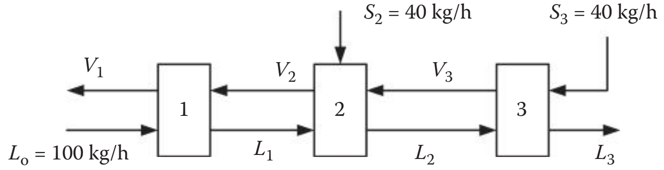


FIGURE 8.48
Process flow sheet of Problem 8.3.5.

with pure isopropyl ether to reduce the acetic acid concentration to 5 wt% in the final raffinate. If 2500 kg/h of pure isopropyl ether is used [1], determine the number of theoretical stages required.

8.9 Extraction of Acetic Acid with Pure Isopropyl Ether

An aqueous feed solution of acetic acid contains 30 wt% acetic acid and 70 wt% water is to be extracted in a continuous countercurrent extractor with pure isopropyl ether to reduce the acetic acid concentration to 5 wt% in the final raffinate. If 1000 kg/h of pure isopropyl ether is used, determine the number of theoretical stages required. Compare the number of theoretical stages with Example 8.3.8 and the effect of the amount of solvent on required number of theoretical stages.

8.10 Extraction of Acetic Acid with Nonpure Isopropyl Ether

An aqueous feed solution of acetic acid contains 30 wt% acetic acid and 70 wt% water is to be extracted in a continuous countercurrent extractor with pure isopropyl ether to reduce the acetic acid concentration to 5 wt% in the final raffinate. If 1000 kg/h of 90 wt% isopropyl ether and 10 wt% acetic acid is used, determine the number of theoretical stages required. Compare the number of theoretical stages with example 8.3.9 and the effect of the amount of solvent on required number of theoretical stages.

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1. Geankoplis, J. C., 1998. *Transport Processes and Unit Operations*, 3rd edn, McGraw-Hill, Boston, MA.
2. McCabe, W. L., J. C. Smith, and P. Harriott, 1993. *Unit Operations of Chemical Engineering*, 5th edn, McGraw-Hill, Boston, MA.
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9

Process Simulation

At the end of this chapter you should be able to

1. Apply the knowledge gained from previous chapters together.
2. Select appropriate process units.
3. Build the process flow diagram.
4. Simulate an entire process using Hysys, PRO/II, Aspen Plus, and SuperPro software packages.

9.1 Introduction

Industrial processes rarely involve one process unit. Keeping track of material flow for overall processes and material flow of all individual units requires simulating the overall plant [1]. A chemical plant is an industrial process plant that manufactures chemicals usually on a large scale. The general objective of a chemical plant is to create new material [2]. Computer simulation softwares are the key to know and control the full-scale industrial plant used in the chemical, oil, gas, and electrical power industries [3]. Simulation software is used widely to design equipment so that the final product will be as close to design specifications as possible without further expenses in process modification. Simulation software gives useful training experience without panic of a catastrophic outcome. Process simulation is used for the design, development, analysis, and optimization of technical processes and is mainly applied to chemical plants and chemical processes. Process simulation is a model-based representation of chemical, physical, biological, and other technical processes and unit operations in software. The necessary fundamentals are a thorough knowledge of chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models which in combination allow the calculation of a process in computers. Process simulation software describes processes in flow diagrams where unit operations are positioned and connected by product or inlet streams. The software has to solve the mass and energy balance to find a stable operating point [4]. In this chapter, the knowledge gained from the previous chapters together is employed for simulating an entire process.

Example 9.1

Ethyl chloride is produced by the gas-phase reaction of HCl with ethylene over a copper chloride catalyst supported on silica. The feed stream is composed of 50% HCl, 48 mol% C_2H_4, and 2 mol% N_2 at 100 kmol/h, 25°C, and 1 atm. Since the reaction achieves only 90 mol% conversion, the ethyl chloride product is separated from the unreacted reagents, and the latter is recycled. The separation is achieved using a distillation column. To prevent accumulation of inerts in the system, a portion of the distillate is withdrawn in a purge stream. Design a process for this purpose using Hysys, PRO/II, Aspen Plus, and SuperPro software packages.

METHODOLOGY

The reaction of ethylene (C_2H_4) and hydrogen chloride (HCl) over a copper chloride catalyst supported on silica to produce of ethylene chloride (C_2H_5Cl) is a highly exothermic reaction. In this example, the reaction is assumed to take place in an isothermal conversion reactor. The heat evolved from the reaction is removed from the reactor to keep the reaction at constant temperature. The reactor effluent stream is compressed, cooled, and then separated in a flash unit followed by a distillation column. The flash and distillation top products are collected and then recycled to the reactor after a portion of the stream is purged to avoid accumulation of an inert component (N_2). The recycled stream is depressurized and heated to the fresh feed stream conditions. The liquid from the bottom of the flash enters a distillation column where ethyl chloride is separated from unreacted HCl and ethylene. The entire process is simulated using Hysys/Unisim, PRO/II, Aspen, and SuperPro Designer software packages.

HYSYS/UNISIM SIMULATION

Aspen Hysys is a process simulator used mainly in the oil and gas industry. Hysys is a highly interactive process flow diagram for building and navigating through large simulations. In this section the entire process is simulated using Hysys. The shortcut method is used for the separation of ethylene chloride from unreacted gases. Start a new case in Hysys and add all components involved in the process (ethylene, hydrogen chloride, ethyl chloride, and nitrogen). The Peng–Robinson EOS was chosen as the base property package. While in the simulation environment, select *Mixer* from the object palette and place it on the PFD. The same procedure is followed for a conversion reactor, compressor, cooler, flash, distillation column, mixer, tee, recycle, throttling valve, and heater as shown in Figure 9.1.

The second step is to utilize the knowledge gained from previous chapters and define each unit operation. Defining reaction, from Flowsheet/*Reaction Package*, then click *Add Rxn*, and choose *Conversion*. Add the three components involved in the reaction and set the stoichiometric coefficient accordingly. Click Basis page, and type 90 for Co as percent conversion, where ethylene is the basis component. Close the reaction page and create new set suppose named *conversion set* and then send the conversion set to available reaction sets. Double click the conversion reactor, click *Reaction* tab, and then choose conversion set from the pull-down menu. Double click on the compressor and set exit pressure to 20 atm and then cool the stream to 20°C to liberate unreacted components nitrogen, hydrogen chloride, and ethylene. The bottom of the flash unit is separated in a distillation

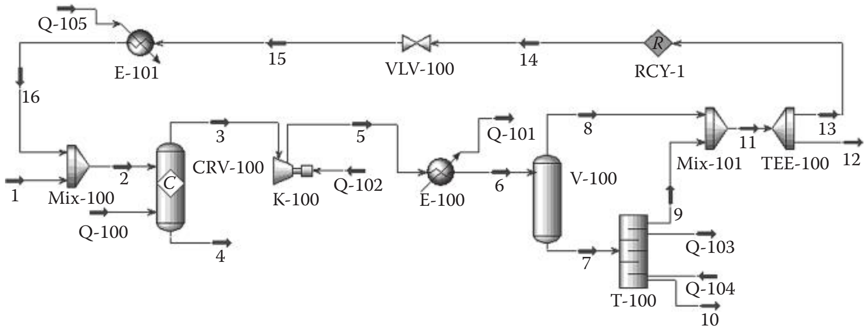


FIGURE 9.1
Process flow sheet for the production of ethylene chloride.

column where almost pure ethylene chloride is collected in the bottom and unreacted compounds with negligible amount of ethylene chloride are recycled. The shortcut method is employed for this purpose. The *Light Key in the Bottom* is HCl, its mole fraction is 0.001, and the *Heavy Key in Distillate* is C_2H_5Cl with mole fraction 0.001. The *External Reflux Ratio* is 2. The top product from the flash unit and distillate from the separation column were collected using a mixer. The exit of the mixer is recycled after a portion is purged (10%). The recycled streams are throttled to 1 atm and heated to 25°C (the fresh feed conditions). The process flow sheet and stream summary table is shown in Figure 9.2. The stream summary table is generated using the *Workbook* from the toolbar.

In the second case the shortcut column is replaced with a distillation column as shown in Figure 9.3. The stream summary result is shown in Figure 9.4. The

		Streams							
		1	2	3	4	5	6	7	8
Temperature	C	25.00	24.99	25.00	25.00	255.4	20.00	20.00	20.00
Pressure	kPa	101.3	101.3	101.3	101.3	2026	2026	2026	2026
Molar flow	kgmol/h	100.0	144.5	97.09	0.0000	97.09	97.09	61.42	35.68
Comp mole frac (Ethylene)		0.4800	0.3647	0.0543	0.0029	0.0543	0.0543	0.0314	0.0937
Comp mole frac (HCl)		0.5000	0.4905	0.2416	0.0214	0.2416	0.2416	0.1881	0.3337
Comp mole frac (ClC_2)		0.0000	0.0162	0.5128	0.9750	0.5128	0.5128	0.7681	0.0734
Comp mole frac (Nitrogen)		0.0200	0.1285	0.1913	0.0007	0.1913	0.1913	0.0124	0.4993
		9	10	11	12	13	14	15	16
Temperature	C	−178.5	126.5	−35.79	−35.79	−35.79	−35.81	−92.27	25.00
Pressure	kPa	2026	2026	2026	2026	2026	2026	101.3	101.3
Molar flow	kgmol/h	14.21	47.20	49.89	4.989	44.90	44.53	44.53	44.53
Comp mole frac (Ethylene)		0.1356	0.0000	0.1057	0.1057	0.1057	0.1058	0.1058	0.1058
Comp mole frac (HCl)		0.8096	0.0010	0.4692	0.4692	0.4692	0.4693	0.4693	0.4693
Comp mole frac (ClC_2)		0.0010	0.9990	0.0528	0.0528	0.0528	0.0527	0.0527	0.0527
Comp mole frac (Nitrogen)		0.0538	0.0000	0.3724	0.3724	0.3724	0.3722	0.3722	0.3722

FIGURE 9.2
Stream summaries; conditions and compositions.

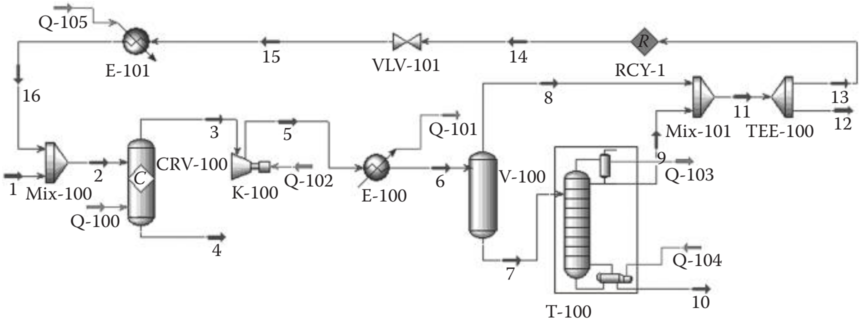


FIGURE 9.3
Process flow sheet diagram using the distillation column.

distillation column required providing the condenser and reboiler pressure as 20 atm, the reflux ratio is 2, and the initial estimate of distillate molar flow rate is 10 kmol/h; the data can be found using the shortcut method.

PRO/II SIMULATION

PRO/II has the power and flexibility to simulate a wide range of processes at steady state; it provides robust and accurate results based on industry standard thermodynamic methods and physical property data. PRO/II is a valuable tool allowing engineers and management to enhance the bottom line of their process or plant. Example 9.1 is prepared in PRO/II by building the process flow sheet shown in Figure 9.5 using the PFD palette. Connect each process component with the following streams. The process components are connected by the streams by

Streams									
		1	2	3	4	5	6	7	8
Temperature	C	25.00	24.99	25.00	25.00	248.2	20.00	20.00	20.00
Pressure	kPa	101.3	101.3	101.3	101.3	2026	2026	2026	2026
Molar flow	kgmol/h	100.0	138.2	90.77	0.0000	90.77	90.77	58.22	32.55
Comp mole frac (Ethylene)		0.4800	0.3815	0.0581	0.0029	0.0581	0.0581	0.0339	0.1013
Comp mole frac (HCl)		0.5000	0.4618	0.1804	0.0151	0.1804	0.1804	0.1413	0.2503
Comp mole frac (ClC_2)		0.0000	0.0161	0.5473	0.9813	0.5473	0.5473	0.8107	0.0763
Comp mole frac (Nitrogen)		0.0200	0.1406	0.2142	0.0007	0.2142	0.2142	0.0141	0.5721
		9	10	11	12	13	14	15	16
Temperature	C	−180.5	120.4	−35.67	−35.67	−35.67	−35.69	−87.62	25.00
Pressure	kPa	2026	2026	2026	2026	2026	2026	101.3	101.3
Molar flow	kgmol/h	9.997	48.23	42.55	4.255	38.29	38.23	38.23	38.23
Comp mole frac (Ethylene)		0.1965	0.0002	0.1237	0.1237	0.1237	0.1237	0.1237	0.1237
Comp mole frac (HCl)		0.7215	0.0210	0.3610	0.3610	0.3610	0.3618	0.3618	0.3618
Comp mole frac (ClC_2)		0.0000	0.9787	0.0583	0.0583	0.0583	0.0583	0.0583	0.0583
Comp mole frac (Nitrogen)		0.0820	0.0000	0.4569	0.4569	0.4569	0.4562	0.4562	0.4562

FIGURE 9.4
Stream Summaries using the distillation column.

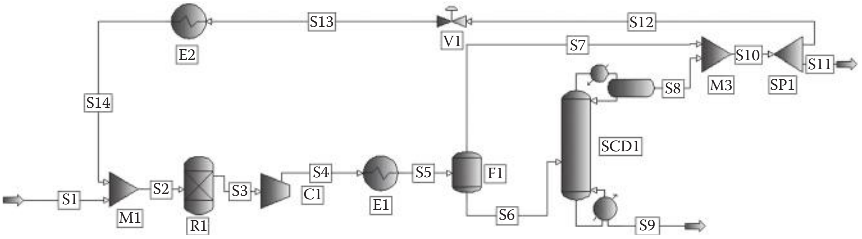


FIGURE 9.5
Process flow sheet using the shortcut column for separation.

first clicking on the *Streams* icon on the PFD palette, then by dragging the other end of the stream to the next process component. The following components are selected: a mixer, conversion reactor, compressor, cooler, shortcut column, mixer, splitter, pressure release valve, and simple heater; all are selected from the PFD palette and placed on the screen. Click on the first mixer and set the pressure drop to zero. Click the *Conversion Reactor* and then select the *Conversion* in the Reaction Set Name. Click on the *Extent of Reaction* and *Pressure* and then input the contents for each component. Under *Thermal Specification* select fixed temperature and set the temperature as 25°C. Pressure drop is zero; the extent of reaction for the ethylene component is 0.9. Click on the compressor and enter the outlet pressure 20 bar. Click on the *Simple HX* (heat exchanger) and set the pressure drop to zero. Click on the *Specification* tab and select the exit temperature and type in value 20°C. Click on the flash column and type the pressure drop and heat duty as zero. Click on the Shortcut distillation and then click on the specification button and set the mole fraction of HCl in the distillate to 0.7 and the mole fraction of ethyl chloride to 0.99 at the bottom. Click on *Products* and the initial estimate sets the molar flow rate of the top stream to 10 kmol/h. After the splitter, the recycled stream is connected to a pressure release valve followed by heat to bring the recycle stream to feed stream conditions. Construct a table to insert on the process screen, click on *stream properties* in the PFD palette, and place a table on the process screen. Double click on the table. A window will open. Select *Stream Summary* and click on *Add All* then click on *OK* (Figure 9.6).

In the second method the shortcut column is replaced by a distillation column (Figure 9.7). Click on the distillation column; the number of trays is 10 and the feed tray is the fifth tray. Click on *Feed and Products* and set the initial estimate of the bottom stream flow rate as 10 kmol/h. In the performance specifications, the reflux ratio is specified as 2 and the molar fraction of ethyl chloride in the bottom stream is 0.99. The stream summary is shown in Figure 9.8.

Aspen Plus Simulation

Aspen Plus includes the world's largest database of pure component and phase-equilibrium data for conventional chemicals, electrolytes, solids, and polymers. In this example the mixer, conversion reactor, compressor, cooler, flash, shortcut column mixer, splitter, throttling valve, and heater are connected as shown in Figure 9.9. In the mixer no information is required. Double click on the reactor and specify the reaction stoichiometry; the fractional conversion of ethylene is 0.9. The reactor product is compressed to 20 bar and then cooled to 20°C before flashed.

Stream name Stream description		S1	S2	S3	S4	S5	S6	S7	S3	S9	S10	S11	S12	S13	S14
Phase		Vapor	Vapor	Vapor	Vapor	Mixed	Liquid	Vapor	Liquid	Liquid	Mixed	Mixed	Mixed	Mixed	Vapor
Temperature	C	25.000	24.990	25.000	370.233	20.000	20.000	20.000	−113.013	124.716	8.685	8.685	8.685	−40.975	25.000
Pressure	kg/cm^2	1.033	1.033	1.033	20.665	20.665	20.665	20.665	20.665	20.665	20.665	20.665	20.665	1.033	1.033
Flowrate	kgmol/h	100.000	525.215	477.222	477.222	477.222	82.991	394.231	34.782	48.208	429.013	0.100	428.913	428.913	428.913
Composition															
Ethylene		0.480	0.102	0.011	0.011	0.011	0.004	0.013	0.010	0.000	0.012	0.012	0.012	0.012	0.012
HCL		0.500	0.413	0.354	0.354	0.354	0.216	0.383	0.501	0.010	0.392	0.392	0.392	0.392	0.392
CLE		0.000	0.033	0.192	0.192	0.192	0.766	0.072	0.456	0.990	0.103	0.103	0.103	0.103	0.103
N_2		0.020	0.402	0.443	0.443	0.443	0.014	0.533	0.032	0.000	0.492	0.492	0.492	0.492	0.492

FIGURE 9.6
Stream summary using shortcut columns for separation.

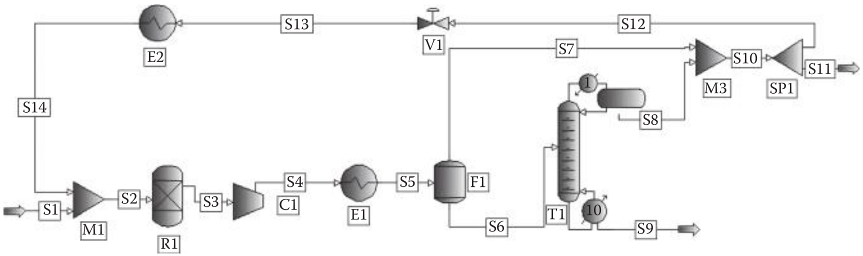


FIGURE 9.7
Process flow sheet using the distillation column for separation.

Stream name Stream description		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14
Phase		Vapor	Vapor	Vapor	Vapor	Mixed	Liquid	Vapor	Liquid	Liquid	Mixed	Mixed	Mixed	Vapor	Vapor
Temperature	C	25.000	24.986	25.000	388.702	20.000	20.000	20.000	−203.079	124.742	11.730	11.730	11.730	−22.050	25.000
Pressure	kg/cm^2	1.033	1.033	1.033	20.665	20.665	20.665	20.665	20.665	20.665	20.665	20.665	20.665	1.033	1.033
Flowrate	kgmol/h	100.000	531.625	483.627	483.627	483.627	62.550	421.077	14.339	48.211	435.416	0.100	435.316	435.316	435.316
Composition															
Ethylene		0.480	0.100	0.011	0.011	0.011	0.004	0.012	0.018	0.000	0.012	0.012	0.012	0.012	0.012
HCL		0.500	0.424	0.367	0.367	0.367	0.219	0.389	0.924	0.010	0.407	0.407	0.407	0.407	0.407
CLE		0.000	0.056	0.161	0.161	0.161	0.763	0.071	0.000	0.990	0.069	0.069	0.069	0.069	0.069
N_2		0.020	0.419	0.461	0.461	0.461	0.013	0.528	0.058	0.000	0.512	0.512	0.512	0.512	0.512

FIGURE 9.8
Stream summary using the distillation column for separation.

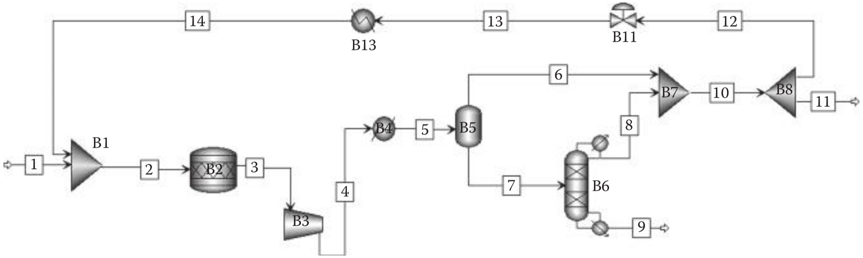


FIGURE 9.9
Process flow sheet with Aspen Plus.

The flash is operating adiabatically at 20 bar. The bottom of the flash is separated in a shortcut column. In the shortcut column, the condensor and reboiler pressure is 20 bar. The light key component in distillate is HCl and its mole fraction in the bottom is set at 0.001. The heavy key is ethyl chloride and its composition in the distillate is very small; in this example it is 0.001. The reflux ratio is 2. The bottom product is mostly pure ethylene chloride. The purge (stream 11) split fraction in the distillate is set at 0.1. The pressure of the recycle stream is reduced to 1 atm using a throttling valve. The exit stream from the valve is heated in a heater to the fresh feed temperature and linked with the fresh feed. The stream conditions and compositions are shown in Figure 9.10.

In the second case the shortcut column is replaced by the distillation column (Figure 9.11). In the distillation column; the number of trays is 10 stages, the distillate rate is 10 kmol/h, the reflux ratio is 2, and the column pressure is 20 atm. The generated table of the stream conditions and compositions is shown in Figure 9.12.

SuperPro Designer Software

SuperPro Designer facilitates modeling, evaluation, and optimization of integrated processes in a wide range of industries. The combination of manufacturing and environmental operation models in the same package enables the user to concurrently design and evaluate manufacturing and end-of-pipe treatment processes and practice waste minimization via pollution prevention as well as pollution control.

In a new case in SuperPro Designer, all involved components are selected. Ethyl chloride is to be added by the user, since this component is not existing in the superPro library. The process units are inserted in the process flow sheet diagram; streams were connected as shown in Figure 9.13. In the PFR conversion reactor, *Reaction taking Place* in vapor phase should be checked. Set the *Exit Temperature* to 25°C and *Extent* to 90% based on reference component *ethylene*. The exit of the reactor is pressurized to 20 bar in a compressor (compressor's efficiency is 70%). The pressurized gases are cooled to 20°C and fed into a shortcut column. The relative volatilities and percent in the distillate of each component are to be provided by the user. The *Light key* is HCl and *Heavy key* is ethyl chloride. In the splitter set 90% to the top stream. The table of stream conditions is shown in Figure 9.14.

PROBLEMS

9.1 Ethyl Chloride Production in an Adiabatic Reactor

Ethyl chloride is produced by the gas-phase reaction of HCl with ethylene over a copper chloride catalyst supported on silica. The feed stream is composed of 50% HCl, 48 mol% C_2H_4, and 2 mol% N_2 at 100 kmol/h, 25°C, and 1 atm. Since the reaction achieves only 80 mol% conversion, the ethyl chloride product is separated from the unreacted reagents, and the latter is recycled. The reaction takes place in an adiabatic reactor. The separation is achieved using a distillation column. To prevent accumulation of inerts in the system, a portion of the distillate is withdrawn in a purge stream. Suggest a process flow sheet for this purpose and simulate the process using accessible software package. Compare results with those obtained from Example 9.1.

Example 9.1															
Stream ID		1	2	3	4	5	6	7	8	9	10	11	12	13	14
Temperature	K	298.0	298.0	827.8	1603.3	293.1	293.2	293.2	262.4	400.8	286.2	286.2	286.2	264.0	298.1
Pressure	atm	1.00	1.00	0.07	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	1.00	1.00
Vapor frac		1.000	1.000	1.000	1.000	0.385	1.000	0.000	1.000	0.000	0.996	0.996	0.996	1.000	1.000
Mole flow	kmol/h	100.000	147.943	100.470	100.470	100.470	38.670	61.800	14.600	47.201	53.270	5.327	47.943	47.943	47.943
Mass flow	kg/h	3225.639	4853.384	4853.384	4853.384	4853.384	1297.154	3556.231	511.457	3044.773	1808.605	180.861	1627.745	1627.745	1627.745
Volume flow	l/min	40507.814	59981.223	1.67163E+6	11073.269	787.139	721.047	66.097	214.345	71.838	945.574	94.563	851.066	17214.737	19472.429
Enthalpy	MMBtu/h	−1.990	−4.008	−4.008	2.645	−8.553	−1.312	−7.241	−0.986	−5.553	−2.297	−0.230	−2.063	−2.063	−2.013
Mole flow	kmol/h														
Ethyl-01		48.000	52.747	5.275	5.275	5.275	3.416	1.859	1.858	<0.001	5.274	0.527	4.747	4.747	4.747
Hydro-0l		50.000	72.641	25.169	25.169	25.169	13.239	11.929	11.917	0.012	25.157	2.516	22.641	22.641	22.641
Ethyl-02			2.555	50.027	50.027	50.027	2.792	47.236	0.047	47.188	2.839	0.284	2.555	2.555	2.555
Nitro-0l		2.000	20.000	20.000	20.000	20.000	19.223	0.777	0.777	trace	20.000	2.000	18.000	18.000	18.000

FIGURE 9.10
Stream summary table using shortcut distillation methods.

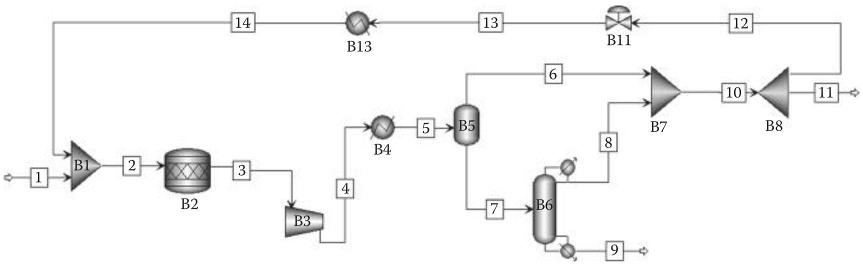


FIGURE 9.11
Process flow sheet diagram using a rigorous distillation method.

Example 9.1															
Stream ID		1	2	3	4	5	6	7	8	9	10	11	12	13	14
Temperature	K	298.0	298.0	877.2	1592.5	253.2	253.2	253.2	105.2	389.4	198.1	198.1	198.1	159.0	298.1
Pressure	atm	1.00	1.00	0.07	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	20.00	1.00	1.00
Vapor frac		1.000	1.000	1.000	1.000	0.283	1.000	0.000	0.000	0.000	0.713	0.713	0.713	0.803	1.000
Mole flow	kmol/h	100.000	130.052	82.629	82.629	82.629	23.391	59.238	10.000	49.238	33.391	3.339	30.052	30.052	30.052
Mass flow	kg/h	3225.639	4138.947	4138.947	4138.947	4138.947	687.125	3451.822	327.665	3124.157	1014.787	101.479	913.308	913.308	913.308
Volume flow	l/min	40507.814	52737.631	1.45668E+6	9048.878	447.766	386.887	60.879	5.419	71.215	299.319	29.932	269.387	5194.777	12226.647
Enthalpy	MMBtu/h	−1.990	−2.407	−2.407	3.207	−7.123	−0.171	−6.952	−0.535	−5.811	−0.706	−0.071	−0.636	−0.636	−0.417
Mole flow	kmol/h														
Ethyl-01		48.000	52.691	5.269	5.269	5.269	1.983	3.287	3.230	0.056	5.213	0.521	4.691	4.691	4.691
Hydro-0l		50.000	57.037	9.614	9.614	9.614	2.207	7.407	5.611	1.796	7.819	0.782	7.037	7.037	7.037
Ethyl-02			0.324	47.746	47.746	47.746	0.360	47.386	<0.001	47.386	0.360	0.036	3.324	0.324	0.344
Nitro-0l		2.000	19.999	19.999	19.999	19.999	18.841	1.158	1.158	trace	19.999	2.000	17.999	17.999	17.999

FIGURE 9.12
Stream summary tables using a rigorous distillation method.

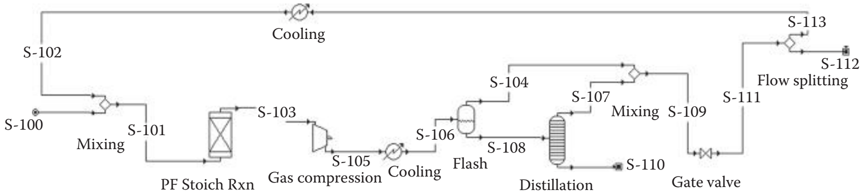


FIGURE 9.13
Process flow sheet using SuperPro Designer.

9.2 Ethylene Production in an Isothermal Reactor

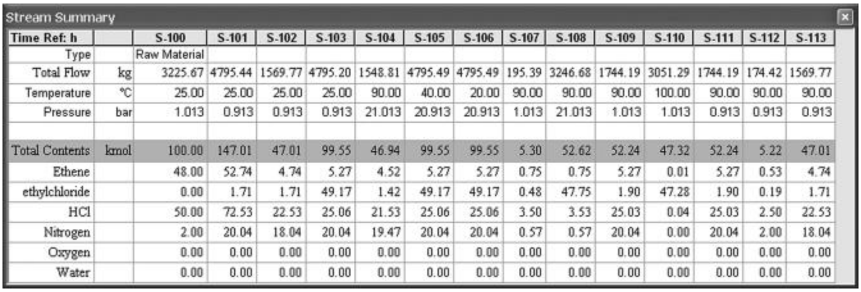
Ethylene is produced using ethane in a steam cracking furnace at 800°C. Assume that the reaction takes place in an isothermal conversion reactor where ethane single-pass conversion is 65%. Develop a process flow sheet for the production of ethylene from pure ethane. Use existing software package in your university to perform the material and energy balance of the entire process.

9.3 Ammonia Synthesis Process in an Adiabatic Reactor

Ammonia is synthesized through the reaction of nitrogen and hydrogen in an adiabatic conversion reactor. The feed stream to the reactor is at 400°C. Nitrogen and hydrogen are fed in stoichiometric proportions. The single-pass fractional conversion is 0.15. The product from the convertor is condensed and ammonia is produced in liquid form. The unreacted gases are recycled. The reactor effluent gas is used to heat the recycle gas from the separator in a combined reactor effluent/recycle heat exchanger. Construct a process flow diagram and use one of the available software packages to simulate the entire process.

9.4 Ammonia Synthesis Process in an Isothermal Reactor

Repeat Problem 9.3; in this case, the reaction takes place at 400°C in an isothermal reactor. Compare the results with Problem 9.3.


Stream Summary

Time Ref: h		S-100	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-109	S-110	S-111	S-112	S-113
Type		Raw Material													
Total Flow	kg	3225.67	4795.44	1569.77	4795.20	1548.81	4795.49	4795.49	195.39	3246.68	1744.19	3051.29	1744.19	174.42	1569.77
Temperature	°C	25.00	25.00	25.00	25.00	90.00	40.00	20.00	90.00	90.00	90.00	100.00	90.00	90.00	90.00
Pressure	bar	1.013	0.913	0.913	0.913	21.013	20.913	20.913	1.013	21.013	1.013	1.013	0.913	0.913	0.913
Total Contents	kmol	100.00	147.01	47.01	99.55	46.94	99.55	99.55	5.30	52.62	52.24	47.32	52.24	5.22	47.01
Ethene		48.00	52.74	4.74	5.27	4.52	5.27	5.27	0.75	0.75	5.27	0.01	5.27	0.53	4.74
ethylchloride		0.00	1.71	1.71	49.17	1.42	49.17	49.17	0.48	47.75	1.90	47.28	1.90	0.19	1.71
HCl		50.00	72.53	22.53	25.06	21.53	25.06	25.06	3.50	3.53	25.03	0.04	25.03	2.50	22.53
Nitrogen		2.00	20.04	18.04	20.04	19.47	20.04	20.04	0.57	0.57	20.04	0.00	20.04	2.00	18.04
Oxygen		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

FIGURE 9.14
Stream summary table.

9.5 Methanol Dehydrogenation

Methanol at 675°C and 1 bar is fed at a rate of 100 kmol/h into an adiabatic reactor where 25% of it is dehydrogenated to formaldehyde (HCHO). Calculate the temperature of the gases leaving the reactor, and separate the component where unreacted methanol is recycled and almost pure formaldehyde is produced.

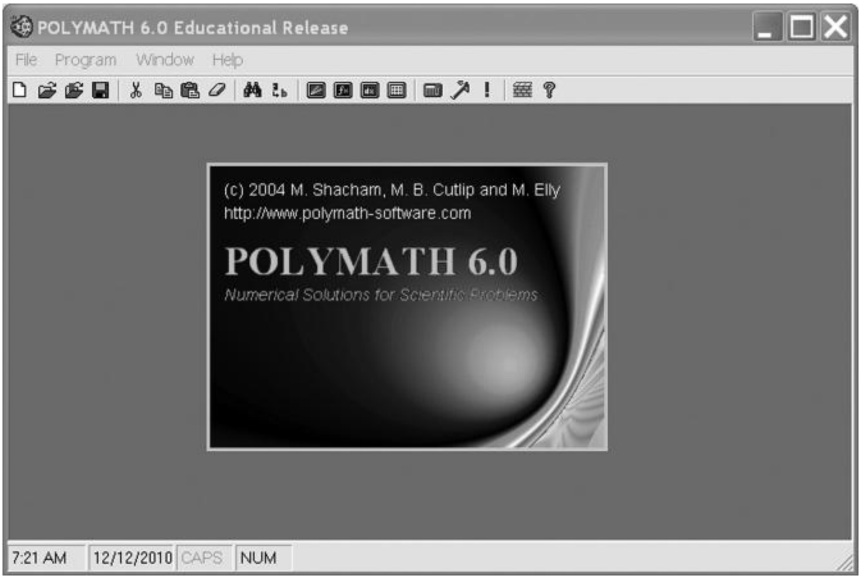
References

1. Ghasem, N. M. and R. Henda. 2009. *Principles of Chemical Engineering Processes*, CRC Press, New York, NY.
2. Douglas, J. M. 1988. *Conceptual Design of Chemical Processes*, McGraw-Hill, New York, NY.
3. Thomas, P. J. 1999. *Simulation of Industrial Processes for Control Engineers*, Butterworth Heinmann, Oxford.
4. Rhodes, C. L. 1996. The process simulation revolution: thermophysical property needs and concerns, *Journal of Chemical Engineering Data*, 41, 947–950.

Appendix A: Polymath Software

Using Polymath software (Figure A.1) you can solve systems consisting of the following forms:

1. Solve linear equations using the LEQ solver.
2. Solve nonlinear equations using the NLE solver.
3. Solve differential equations using the DEQ solver.
4. Fit a set of experimental data using the regression option using the REG option.
    a. Input of a set of data in a table.
    b. Using linear and polynomial regression for fitting the data.
    c. Use multiple linear regressions.
    d. Use nonlinear regression.



(c) 2004 M. Shacham, M. B. Cutlip and M. Elly
http://www.polymath-software.com
POLYMATH 6.0
Numerical Solutions for Scientific Problems

FIGURE A.1
Polymath software packages.

Example A.1: Solving a Set of ODE

Consider the following reaction taking place in a batch reactor:

$$A \xrightarrow{k_1} B$$

$$B \xrightarrow{k_2} C$$

Find the concentrations of A, B, C as a function of time for 3 min, $k_1 = 0.1$, $k_2 = 0.2$

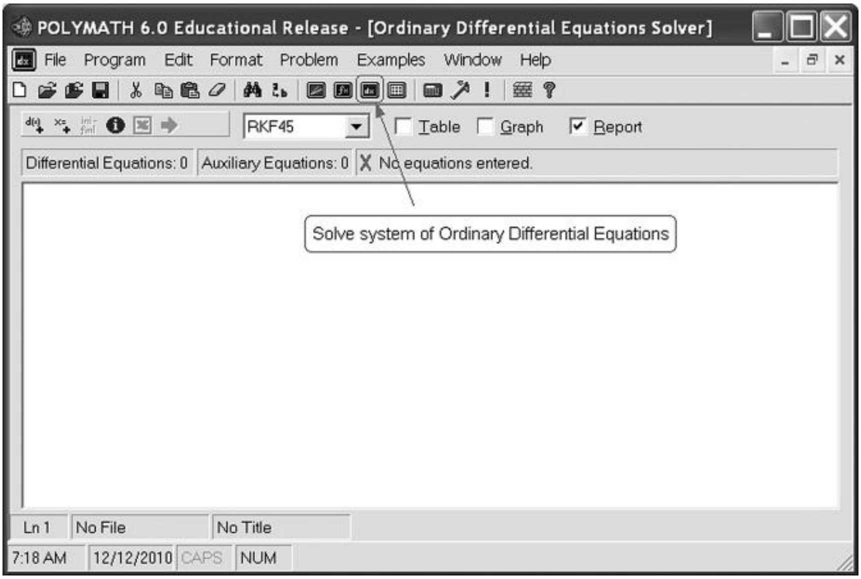
$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = -k_1 C_A$$

$$\frac{\mathrm{d}C_B}{\mathrm{d}t} = k_1 C_A - k_2 C_B$$

$$\frac{\mathrm{d}C_C}{\mathrm{d}t} = k_2 C_B$$

Solving using polymath

1. Click on dx on the tool bar (see Figure A.2).



POLYMATH 6.0 Educational Release - [Ordinary Differential Equations Solver]

RKF45 ☐ Table ☐ Graph ☑ Report

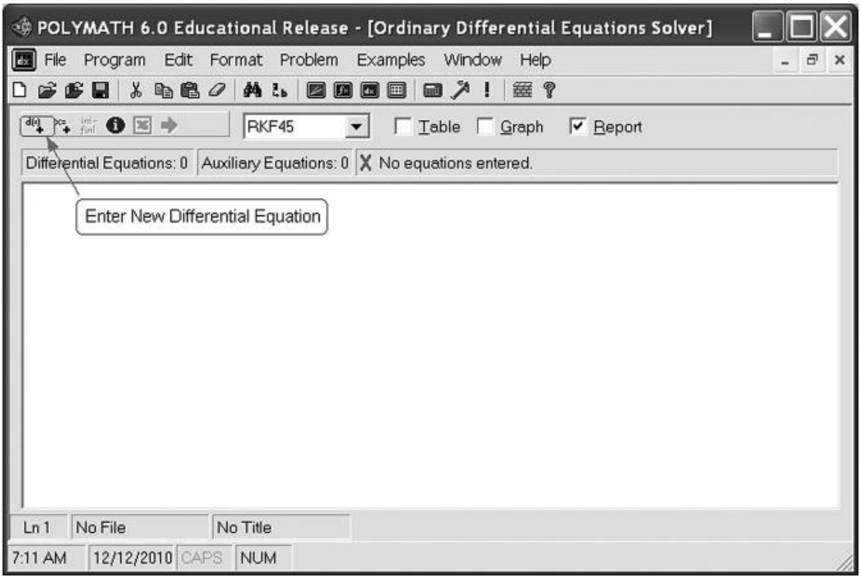
Differential Equations: 0 Auxiliary Equations: 0 No equations entered.

Solve system of Ordinary Differential Equations

Ln 1 No File No Title

7:18 AM 12/12/2010 CAPS NUM

FIGURE A.2
Solve systems of ordinary differential equations.



RKF45 ☐ Table ☐ Graph ☑ Report

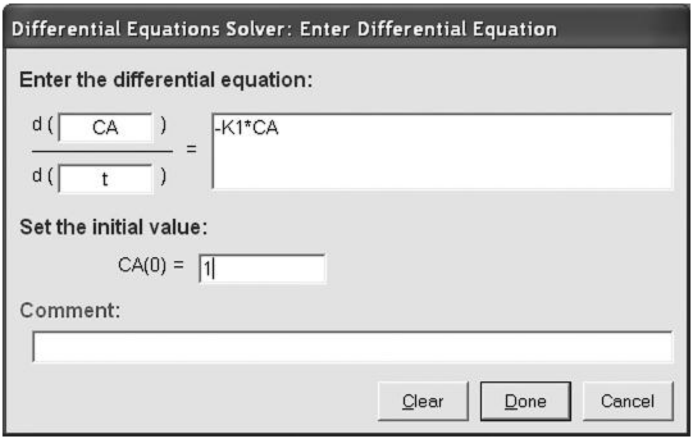
Differential Equations: 0 | Auxiliary Equations: 0 | X No equations entered.

Ln 1 | No File | No Title

7:11 AM | 12/12/2010 | CAPS | NUM

FIGURE A.3
Entering a new differential equation menu.

2. Click on d(*x*)+ on the left side [Ordinary differential Equations Solver] (see Figure A.3).
3. Fill in the first equation and click on *Done* (Figure A.4).



Enter the differential equation:

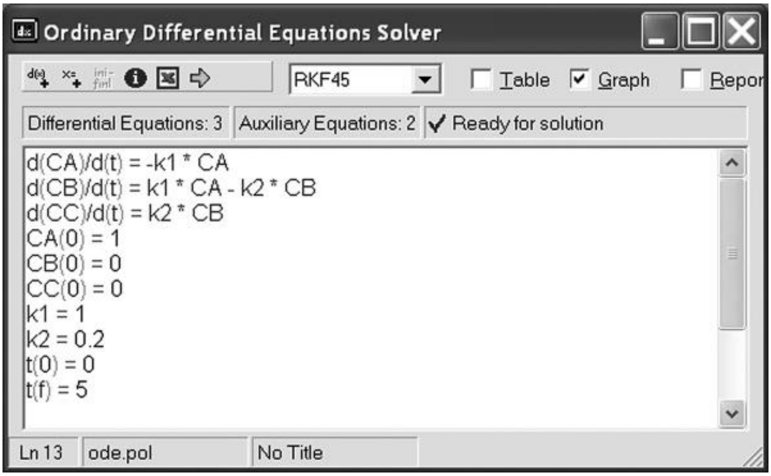
d(CA) / d(t) = -K1*CA

Set the initial value:

CA(0) = 1

Comment:

FIGURE A.4
Enter a differential equation window.



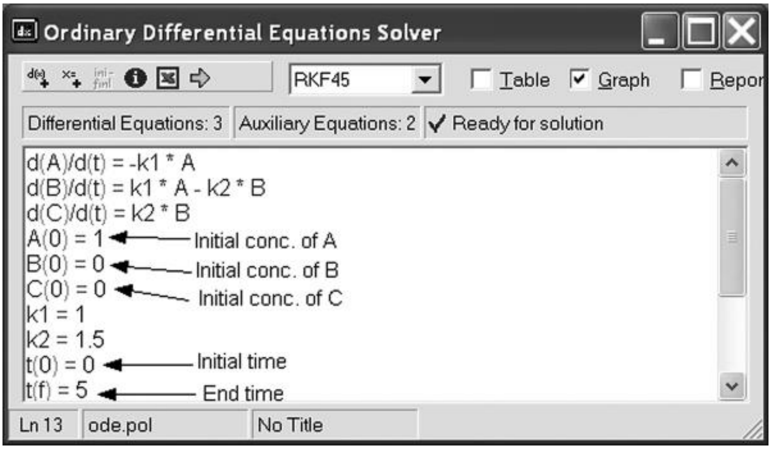
Differential Equations: 3 | Auxiliary Equations: 2 | ✓ Ready for solution

```
d(CA)/d(t) = -k1 * CA
d(CB)/d(t) = k1 * CA - k2 * CB
d(CC)/d(t) = k2 * CB
CA(0) = 1
CB(0) = 0
CC(0) = 0
k1 = 1
k2 = 0.2
t(0) = 0
t(f) = 5
```

Ln 13 | ode.pol | No Title

FIGURE A.5
Program code.

4. Repeat the same for the rest of the equations (Figure A.5).
5. Select Graph and note the Solve arrow appears which means "Ready for solution" (Figure A.6).



Differential Equations: 3 | Auxiliary Equations: 2 | ✓ Ready for solution

```
d(A)/d(t) = -k1 * A
d(B)/d(t) = k1 * A - k2 * B
d(C)/d(t) = k2 * B
A(0) = 1
B(0) = 0
C(0) = 0
k1 = 1
k2 = 1.5
t(0) = 0
t(f) = 5
```

Ln 13 | ode.pol | No Title

FIGURE A.6
Polymath codes with brief explanation.

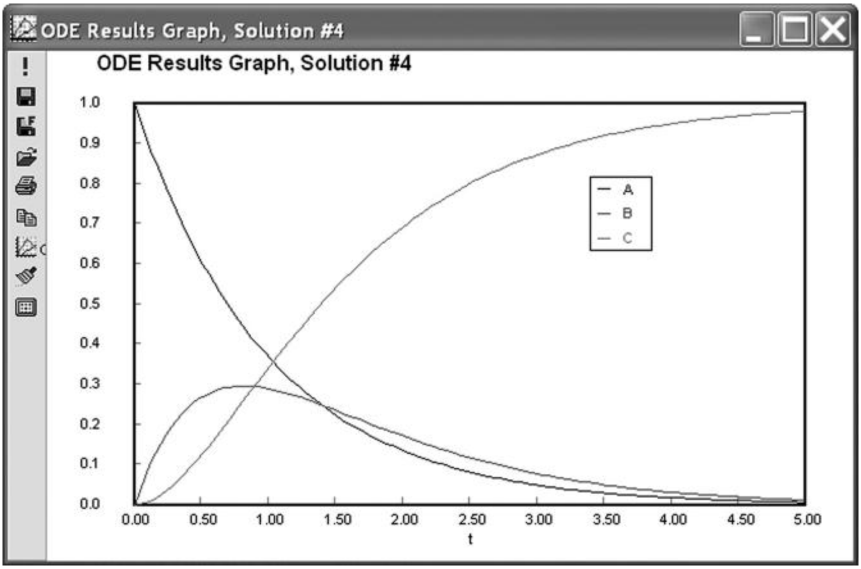
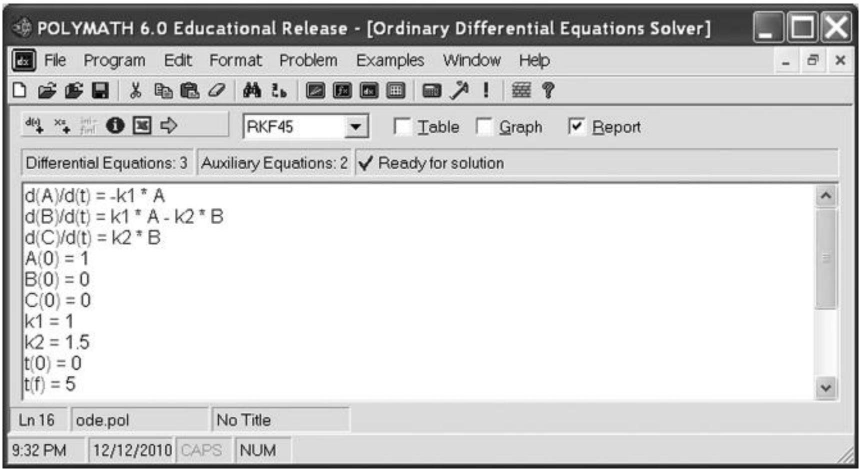


FIGURE A.7
Solution of a set of ODE, $k_2 = 1.5$.

6. Click on the Solve arrow (Figure A.7).
7. Repeat for $k_1 = 1$, $k_2 = 1.5$, and different entry of the equations (Figure A.8).



RKF45 ☐ Table ☐ Graph ☑ Report

Differential Equations: 3 Auxiliary Equations: 2 ✓ Ready for solution

```
d(A)/d(t) = -k1 * A
d(B)/d(t) = k1 * A - k2 * B
d(C)/d(t) = k2 * B
A(0) = 1
B(0) = 0
C(0) = 0
k1 = 1
k2 = 1.5
t(0) = 0
t(f) = 5
```

Ln 16 ode.pol No Title

9:32 PM 12/12/2010 CAPS NUM

FIGURE A.8
Polymath code for $k_1 = 1$ and $k_2 = 1.5$.

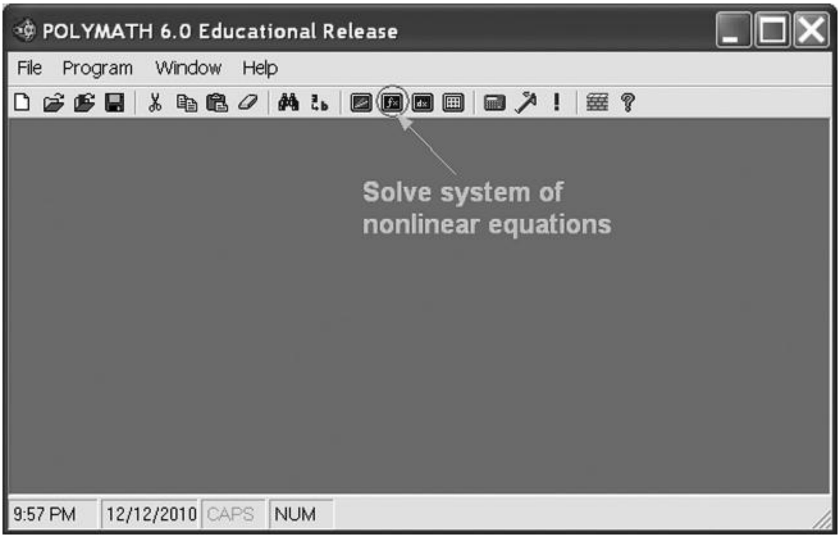


FIGURE A.9
Polymath windows for the solution of nonlinear equations.

Example A.2: Solving System of Linear Algebraic Equation

1. Open polymath and click on *fx* (Figure A.9).
2. To enter nonlinear equations *f*(*x*) (Figure A.10).

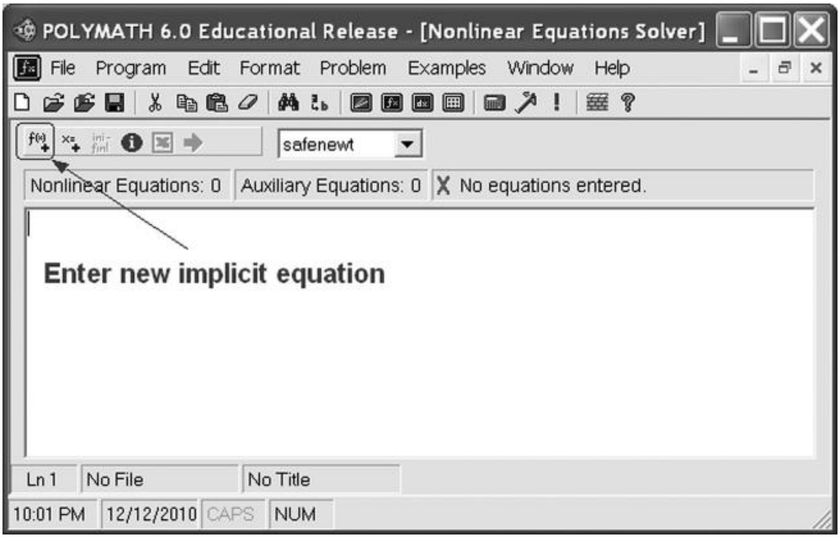


FIGURE A.10
Entering of a new implicit equation.

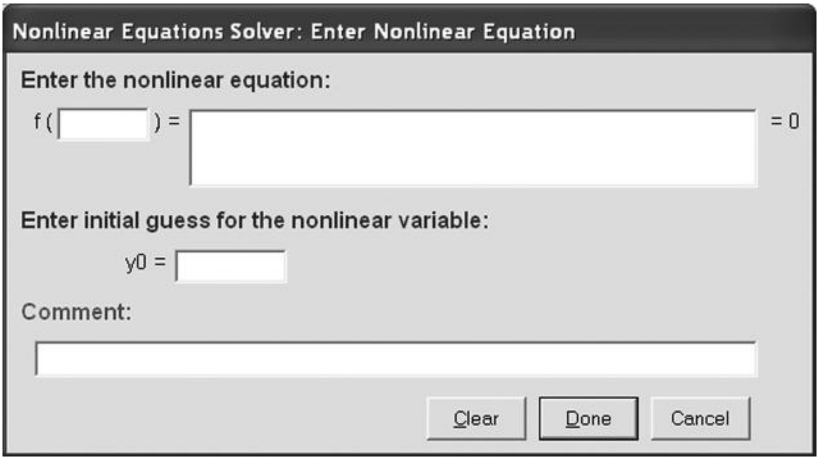


FIGURE A.11
Entering of a nonlinear equation.

3. For nonlinear equations click on *f*(*x*) (Figure A.11).
4. Click on "*x* = " (Figure A.12).

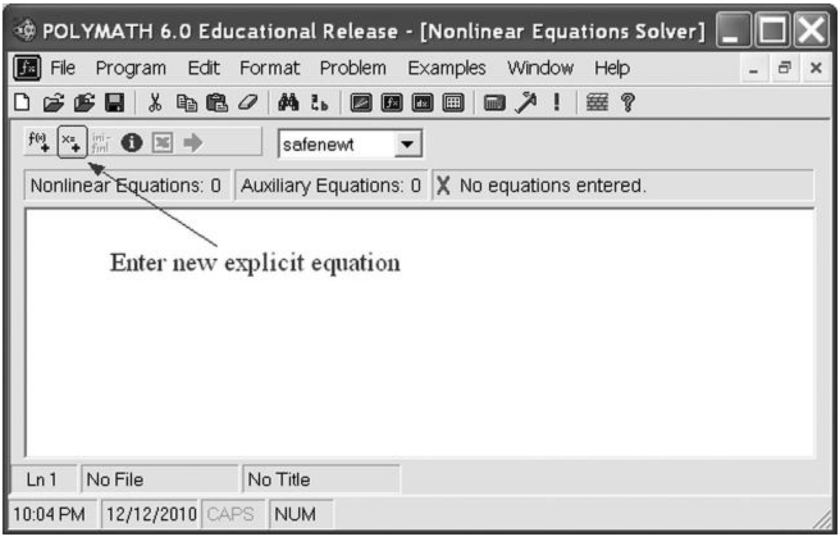


FIGURE A.12
Entering of a new explicit equation.

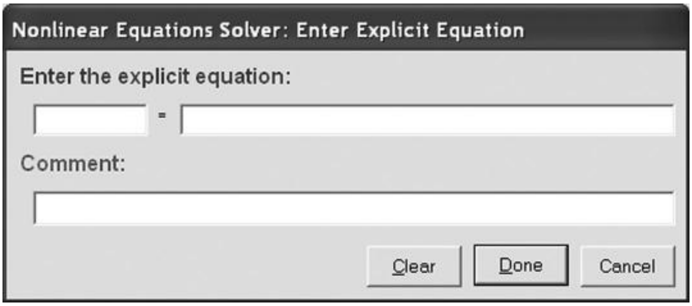


FIGURE A.13
Menu for entering of a new explicit equation.

5. Once you click on "$x =$" a window pops up as shown in Figure A.13.

Example A.3: Solving Linear Algebraic Equations

1. Click on the icon of linear equations solver as shown in Figure A.14.

Once you click on the linear equations icon, a window pops up as shown in Figure A.15.

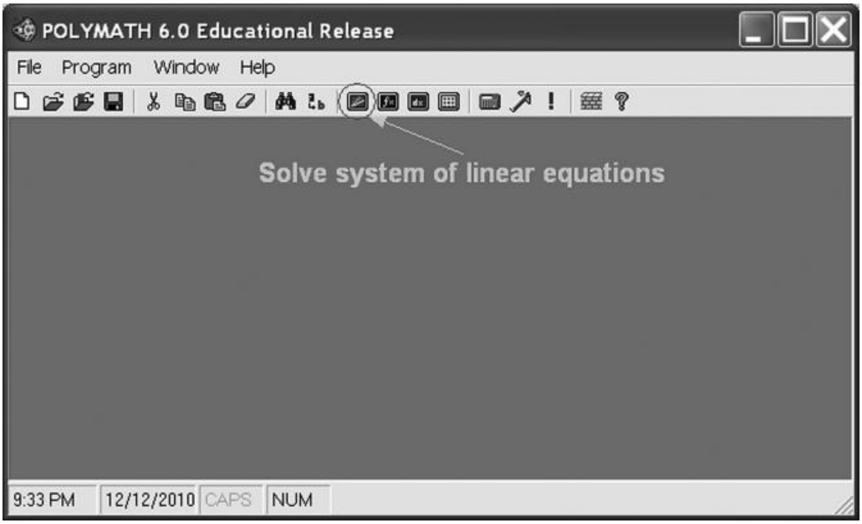
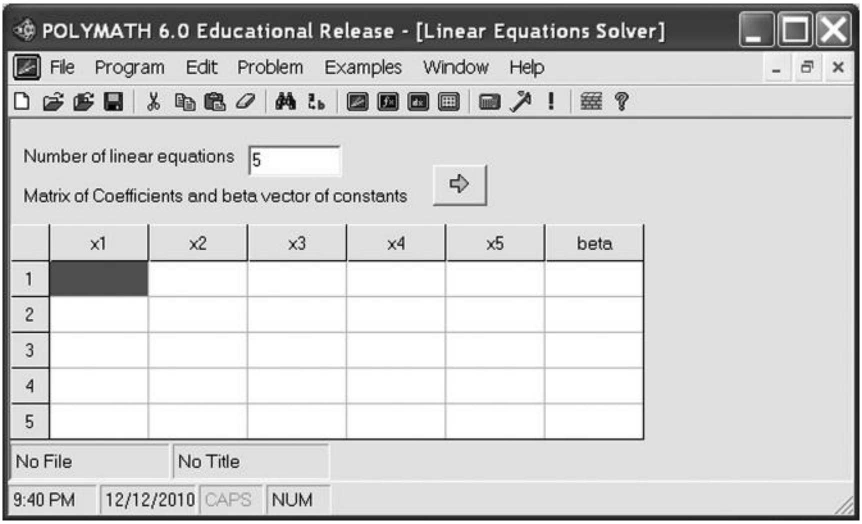


FIGURE A.14
Solving system of linear equations.



Number of linear equations 5

Matrix of Coefficients and beta vector of constants

	x1	x2	x3	x4	x5	beta
1						
2						
3						
4						
5						

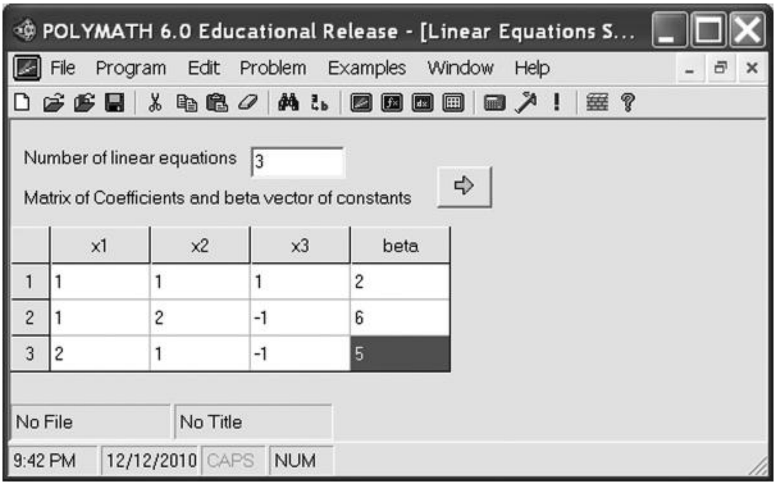
FIGURE A.15
Linear equation solver.

$$x + y + z = 2$$

$$x + 2y - z = 6$$

$$2x + y - z = 5$$

2. Fill in the coefficient of each equation as shown in Figure A.16.

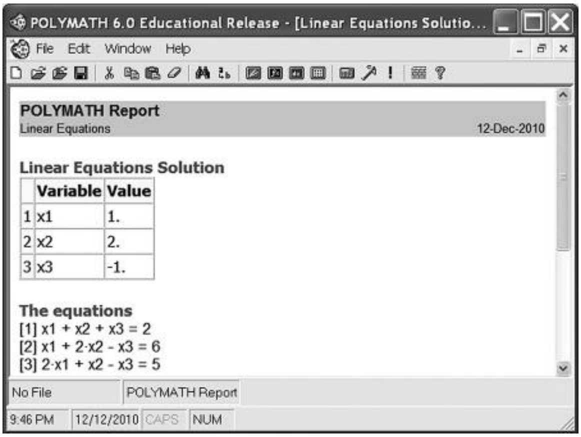


Number of linear equations 3

Matrix of Coefficients and beta vector of constants

	x1	x2	x3	beta
1	1	1	1	2
2	1	2	-1	6
3	2	1	-1	5

FIGURE A.16
Coefficients of the three linear equations.



POLYMATH Report
Linear Equations 12-Dec-2010

Linear Equations Solution

	Variable	Value
1	x1	1.
2	x2	2.
3	x3	-1.

The equations
[1] x1 + x2 + x3 = 2
[2] x1 + 2·x2 - x3 = 6
[3] 2·x1 + x2 - x3 = 5

FIGURE A.17
Results of three linear equations.

3. Click on the Solve arrow to solve the set of equations (Figure A.17).

Example A.4: System of Nonlinear Algebraic Equation

A pitot tube is inserted in a flow as shown in Figure A.18. The flowing fluid is air and the manometer liquid is mercury. Find the flow speed.

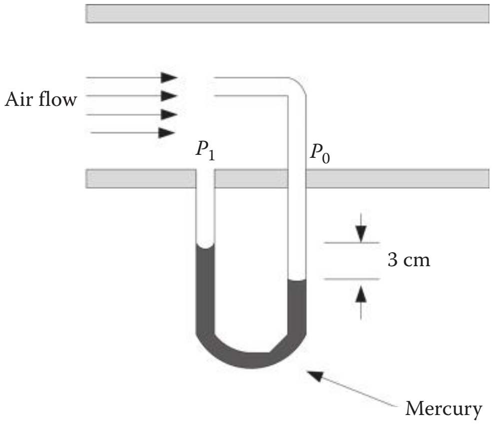


FIGURE A.18
Schematic of pitot tube.

Basic mechanical energy balance equations.

$$\frac{P}{\rho} + \frac{V^2}{2} + gz = \text{constant}$$

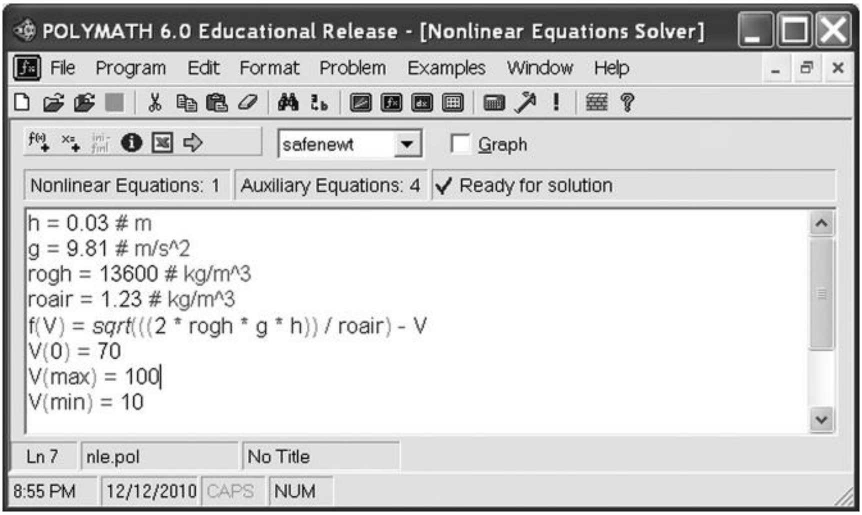
Writing Bernoulli's equation between 0 and 1 at the same level,

$$\frac{P_1}{\rho} + \frac{V^2}{2} = \frac{P_0}{\rho}$$

Rearranging the equation,

$$V = \sqrt{\frac{2(P_0 - P_1)}{\rho_{\text{air}}}} = \sqrt{\frac{2(\rho_{\text{Hg}} g h)}{\rho_{\text{air}}}}$$

Solve using polymath (Figure A.19).
Results: See Figure A.20.

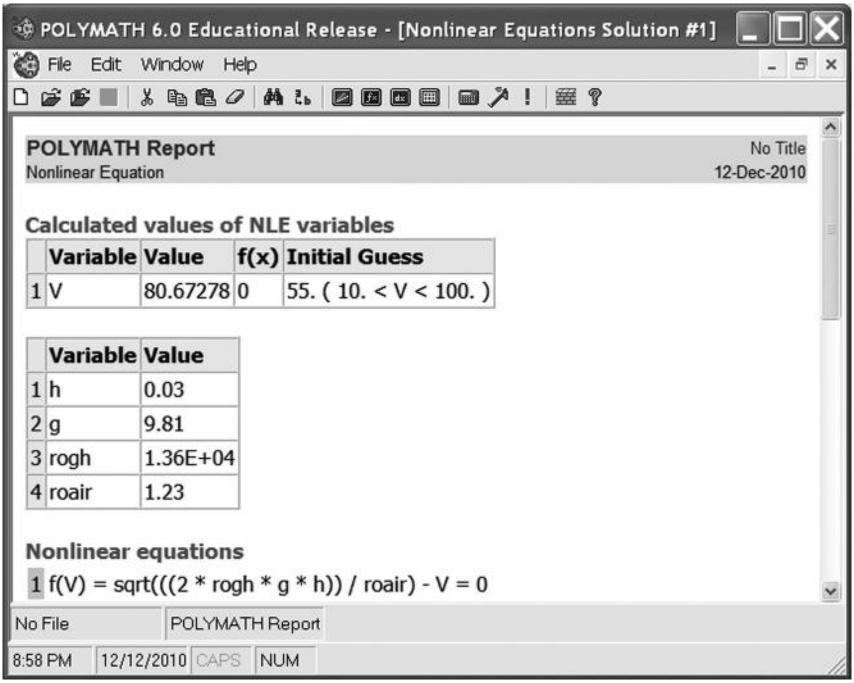


safenewt ☐ Graph

Nonlinear Equations: 1 Auxiliary Equations: 4 ✓ Ready for solution

```
h = 0.03 # m
g = 9.81 # m/s^2
rogh = 13600 # kg/m^3
roair = 1.23 # kg/m^3
f(V) = sqrt(((2 * rogh * g * h)) / roair) - V
V(0) = 70
V(max) = 100
V(min) = 10
```

FIGURE A.19
Polymath codes of nonlinear equations.



POLYMATH Report
Nonlinear Equation
No Title
12-Dec-2010

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	V	80.67278	0	55. (10. < V < 100.)

	Variable	Value
1	h	0.03
2	g	9.81
3	rogh	1.36E+04
4	roair	1.23

Nonlinear equations

1 f(V) = sqrt(((2 * rogh * g * h)) / roair) - V = 0

FIGURE A.20
Polymath results of nonlinear equations.

Example A.5: Use of Polymath for Data Regression

1. Enter the data after clicking on "Regression and analysis data" (Figure A.21).
2. A new data sheet is opened Figure A.22.
3. Fill in the data and label the column (Figure A.23).

FIGURE A.21
Regression and analysis data icon (surrounded by box).

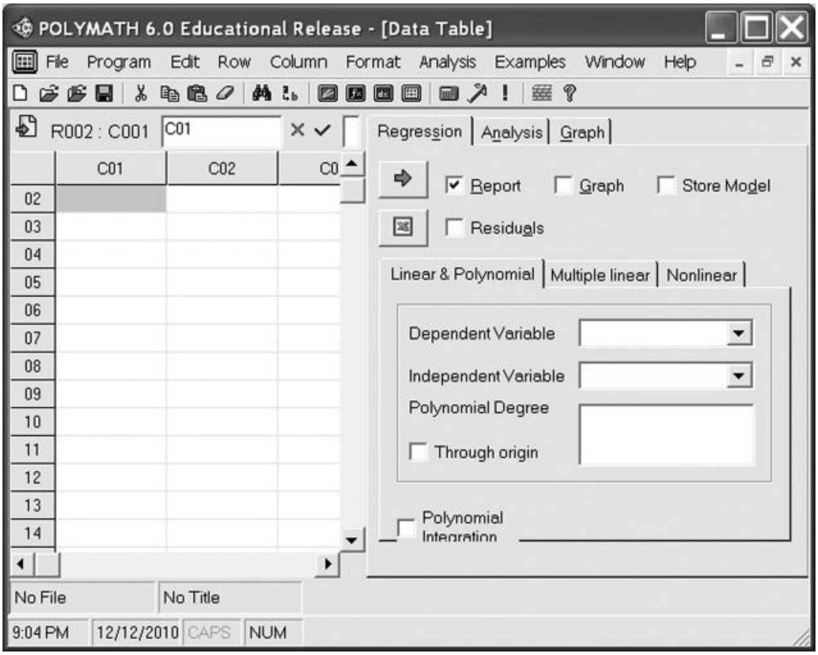
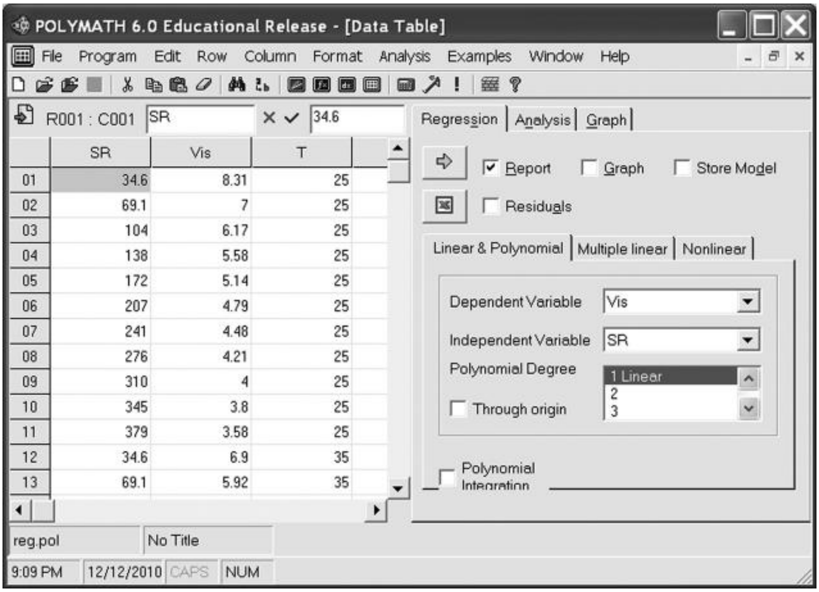
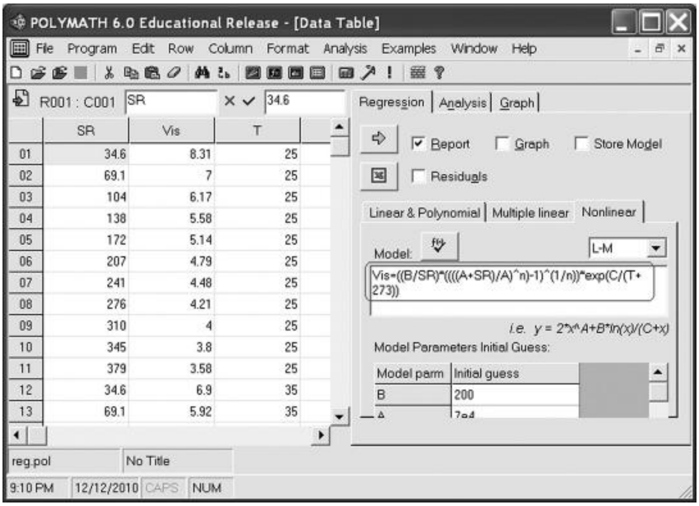


FIGURE A.22
Data table.



	SR	Vis	T
01	34.6	8.31	25
02	69.1	7	25
03	104	6.17	25
04	138	5.58	25
05	172	5.14	25
06	207	4.79	25
07	241	4.48	25
08	276	4.21	25
09	310	4	25
10	345	3.8	25
11	379	3.58	25
12	34.6	6.9	35
13	69.1	5.92	35

FIGURE A.23
Viscosities versus shear rate at different temperatures.


POLYMATH 6.0 Educational Release - [Data Table]

R001 : C001 SR 34.6

	SR	Vis	T
01	34.6	8.31	25
02	69.1	7	25
03	104	6.17	25
04	138	5.58	25
05	172	5.14	25
06	207	4.79	25
07	241	4.48	25
08	276	4.21	25
09	310	4	25
10	345	3.8	25
11	379	3.58	25
12	34.6	6.9	35
13	69.1	5.92	35

☑ Report ☐ Graph ☐ Store Model

☐ Residuals

Model: L-M

Vis=((B/SR)*((((A+SR)/A)^n)-1)^(1/n))*exp(C/(T+273))

*i.e. y = 2*x^A+B*ln(x)/(C+x)*

Model Parameters Initial Guess:

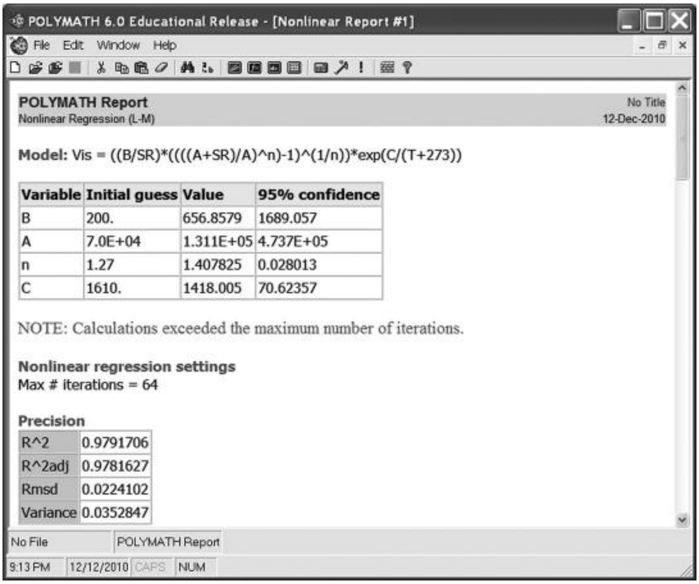
Model parm	Initial guess
B	200
A	7e4

reg.pol No Title

9:10 PM 12/12/2010 CAPS NUM

FIGURE A.24
Nonlinear regression and user-defined menu.

4. Select "Regression" and "Nonlinear" (Figure A.24).
5. Click on the Solve arrow (Figures A.25 through A.28).


POLYMATH 6.0 Educational Release - [Nonlinear Report #1]

POLYMATH Report No Title
Nonlinear Regression (L-M) 12-Dec-2010

Model: Vis = ((B/SR)*((((A+SR)/A)^n)-1)^(1/n))*exp(C/(T+273))

Variable	Initial guess	Value	95% confidence
B	200.	656.8579	1689.057
A	7.0E+04	1.311E+05	4.737E+05
n	1.27	1.407825	0.028013
C	1610.	1418.005	70.62357

NOTE: Calculations exceeded the maximum number of iterations.

Nonlinear regression settings
Max # iterations = 64

Precision

R^2	0.9791706
R^2adj	0.9781627
Rmsd	0.0224102
Variance	0.0352847

No File POLYMATH Report

9:13 PM 12/12/2010 CAPS NUM

FIGURE A.25
Results of nonlinear regression and parameters of empirical equations.

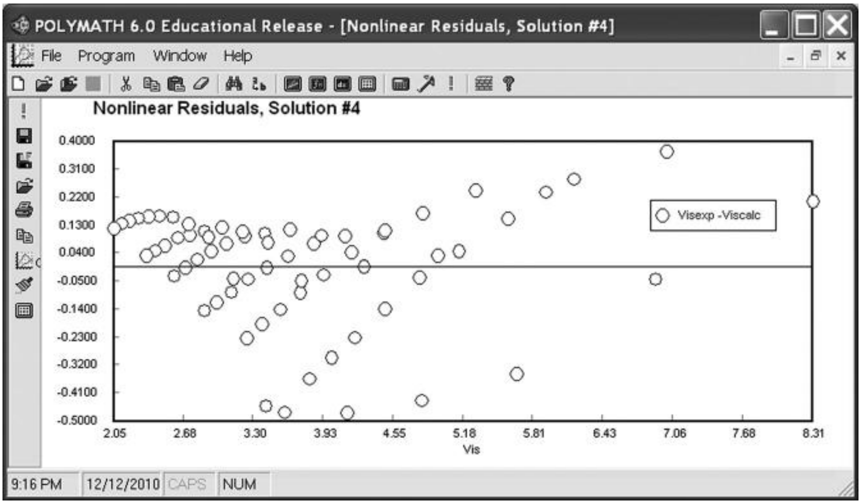


FIGURE A.26
Residual solutions.

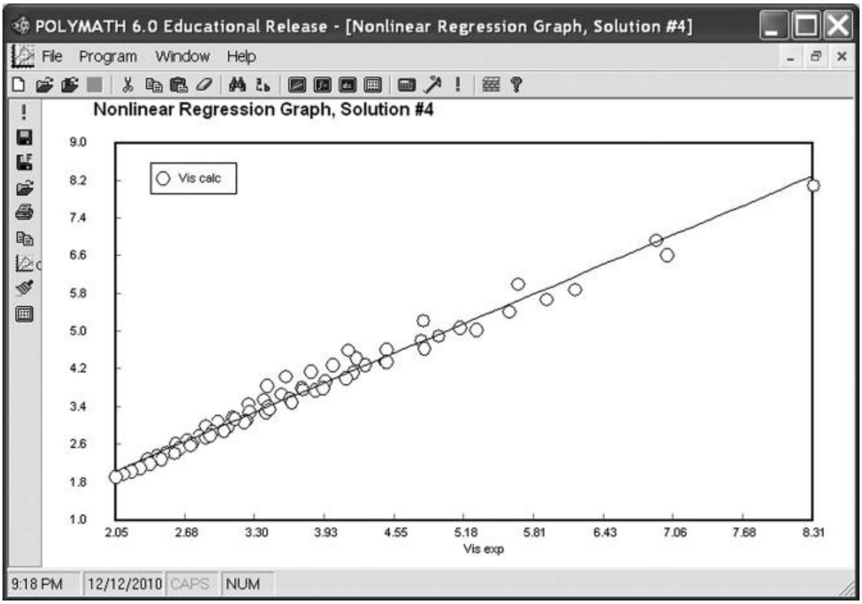
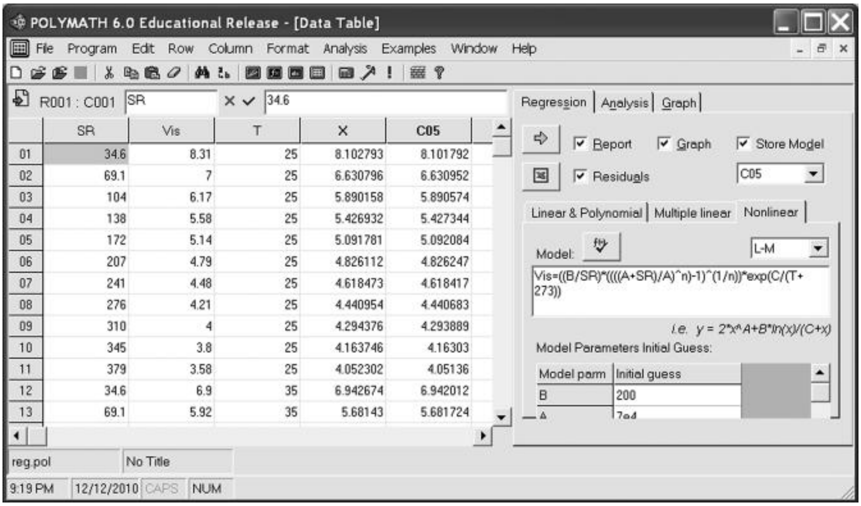


FIGURE A.27
Calculated versus experimental data.



R001 : C001 SR 34.6

	SR	Vis	T	X	C05
01	34.6	8.31	25	8.102793	8.101792
02	69.1	7	25	6.630796	6.630952
03	104	6.17	25	5.890158	5.890574
04	138	5.58	25	5.426932	5.427344
05	172	5.14	25	5.091781	5.092084
06	207	4.79	25	4.826112	4.826247
07	241	4.48	25	4.618473	4.618417
08	276	4.21	25	4.440954	4.440683
09	310	4	25	4.294376	4.293889
10	345	3.8	25	4.163746	4.16303
11	379	3.58	25	4.052302	4.05136
12	34.6	6.9	35	6.942674	6.942012
13	69.1	5.92	35	5.68143	5.681724

reg.pol No Title

9:19 PM 12/12/2010 CAPS NUM

☑ Report ☑ Graph ☑ Store Model

☑ Residuals C05

Model: L-M

```
Vis=((B/SR)*((((A+SR)/A)^n)-1)^(1/n))*exp(C/(T+273))
```

*i.e. y = 2*x^A+B*ln(x)/(C+x)*

Model Parameters Initial Guess:

Model parm	Initial guess
B	200
A	7e4

FIGURE A.28
Predicted results.

Appendix B: E-Z Solve Software

With E-Z Solve software (Figure B.1) you can solve systems consisting of the following forms:

1. Solve linear equations.
2. Solve nonlinear equations.
3. Solve differential equations.
4. Fit a set of experimental data using the regression option using REG option.
    a. Input of a set of data in a table.
    b. Use linear and polynomial regression for fitting data.
    c. Use multiple linear regressions.
    d. Use nonlinear regression.

Example B.1: Solving Set of ODEs

Consider the following reaction taking place in a batch reactor

$$A \xrightarrow{k_1} B$$

$$B \xrightarrow{k_2} C$$

FIGURE B.1
E-Z Solve software program.

Find the concentrations of A, B, and C as a function of time for 3 min, $k_1 = 0.1$, $k_2 = 0.2$. Initial concentration of A is 1 mol/L; B and C are zero.

SOLUTION

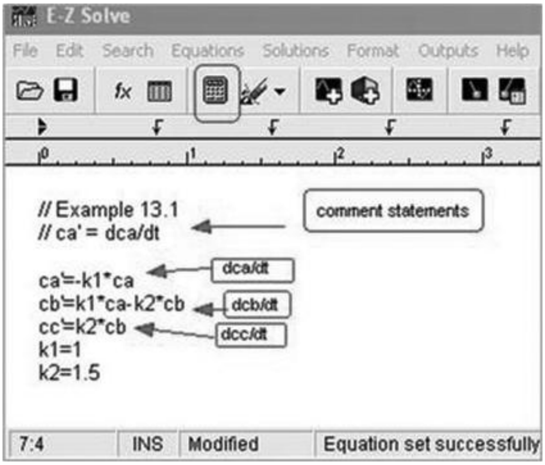
$$\frac{dC_A}{dt} = -k_1C_A$$

$$\frac{dC_B}{dt} = k_1C_A - k_2C_B$$

$$\frac{dC_C}{dt} = k_2C_B$$

1. Solving using "E-Z Solve," fill the above equations as shown in Figure B.2.
2. Click on the calculator above; to plot the result from "Add 2D plot" select new (see Figure B.3).
3. Click on "Add" button and select the variable you want to plot; to change the color of each line click on "Attribute" button (see Figures B.4 through B.6).

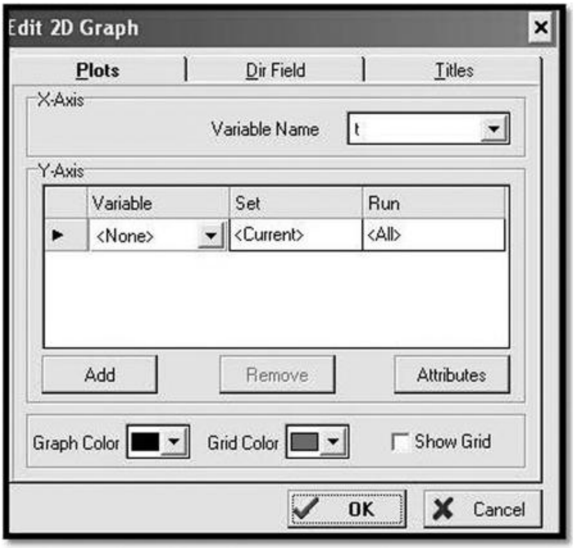
To change the plot click on "Edit" at the top right of the graph.



```
// Example 13.1
// ca' = dca/dt

ca'=-k1*ca
cb'=k1*ca-k2*cb
cc'=k2*cb
k1=1
k2=1.5
```

FIGURE B.2
Code of E-Z Solve for solving system of ODE.



Variable Name: t

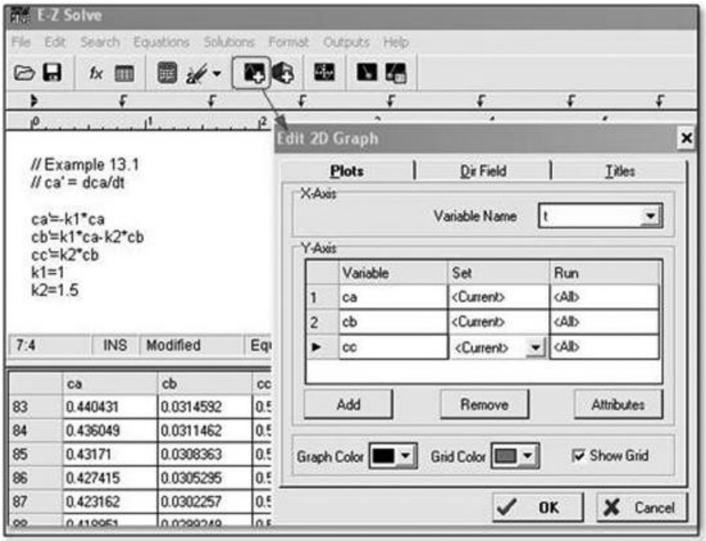
Variable	Set	Run
<None>	<Current>	<All>

Graph Color ■ Grid Color ■ ☐ Show Grid

FIGURE B.3
Plotting menu.

<None> every 1 pt(s)
Size 2
Style ——— Width 0
Color
☑ Show
☑ Include IC

FIGURE B.4
Selecting color of plotting curves.



```
// Example 13.1
// ca' = dca/dt

ca'=-k1*ca
cb'=k1*ca-k2*cb
cc'=k2*cb
k1=1
k2=1.5
```

7:4 INS Modified

	ca	cb
83	0.440431	0.0314592
84	0.436049	0.0311462
85	0.43171	0.0308363
86	0.427415	0.0305295
87	0.423162	0.0302257

X-Axis
Variable Name: t

Y-Axis

	Variable	Set	Run
1	ca	<Current>	<All>
2	cb	<Current>	<All>
►	cc	<Current>	<All>

Graph Color ■ Grid Color ■ ☑ Show Grid

FIGURE B.5
Two-dimensional plots.

Example B.2: Solution of Linear Algebraic Equation

$$x + y + z = 2$$

$$x + 2y - z = 6$$

$$2x + y - z = 5$$

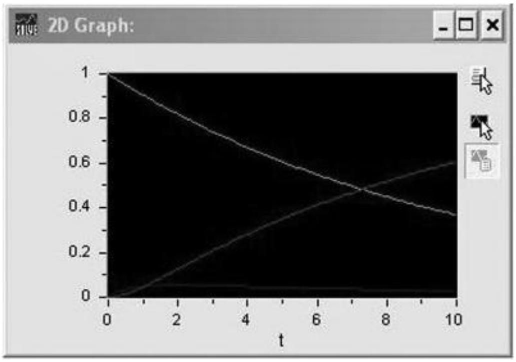
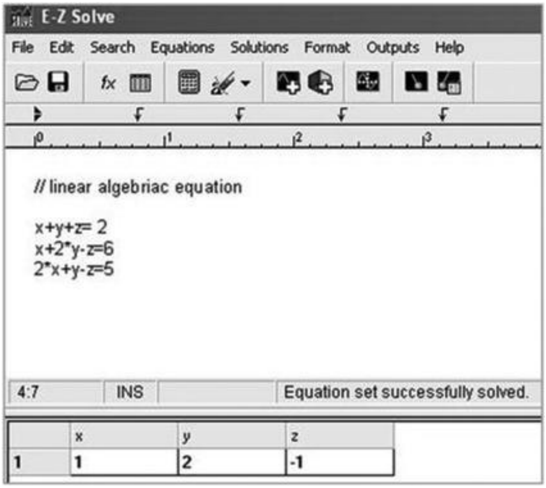


FIGURE B.6
Reactant and product concentrations versus time.



```
// linear algebriac equation

x+y+z= 2
x+2*y-z=6
2*x+y-z=5
```

4:7 INS Equation set successfully solved.

	x	y	z
1	1	2	-1

FIGURE B.7
Code of linear algebraic equations.

1. Fill in the equation as shown in Figure B.7 and click on the calculator icon to run.

Example B.3: Solving System of Nonlinear Algebraic Equation

A pitot tube is inserted in a flow as shown in Figure B.8. The flowing fluid is air and the manometer liquid is mercury. Find the flow speed.

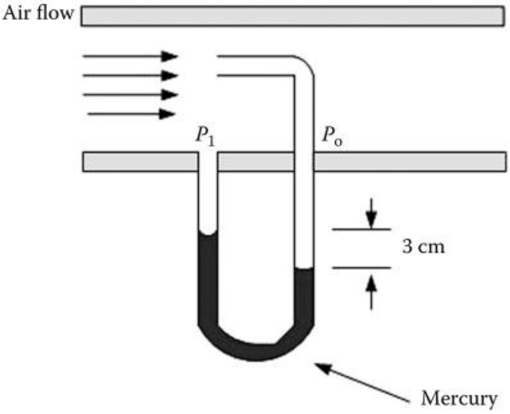


FIGURE B.8
Schematic diagram of pitot tube.

SOLUTION

Basic mechanical energy balance equations

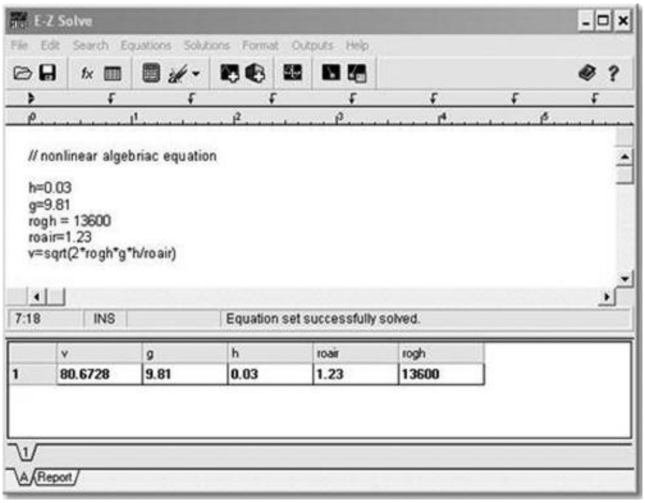
$$\frac{P}{\rho} + \frac{V^2}{2} + gz = \text{constant}$$

Writing Bernoulli's equation between 0 and 1 at the same level

$$\frac{P_1}{\rho} + \frac{V^2}{2} = \frac{P_o}{\rho}$$

$$V = \sqrt{\frac{2(P_o - P_1)}{\rho_{air}}} = \sqrt{\frac{2(\rho_{Hg} gh)}{\rho_{air}}}$$

Solve using polymath (Figure B.9).



```
// nonlinear algebriac equation

h=0.03
g=9.81
rogh = 13600
roair=1.23
v=sqrt(2*rogh*g*h/roair)
```

```
7:18    INS    Equation set successfully solved.
```

	v	g	h	roair	rogh
1	80.6728	9.81	0.03	1.23	13600

FIGURE B.9
E-Z Solve code of nonlinear algebraic equations.

Appendix C: MATLAB®/Simulink®

Introduction

Simulink is a software package for modeling, simulating, and analyzing dynamic systems. It supports linear and nonlinear systems, modeled in continuous time, sampled time, or a hybrid of the two. Simulink is also practical. With thousands of engineers around the world using it to model and solve real problems, knowledge of this tool will serve you well throughout your professional career.

Commonly used blocks (Figure C.1).

Plotting blocks (Figure C.2).

Example C.1: Solving Sets of ODE

Solve the following two ordinary differential equations using MATLAB/ SIMULINK (Figure C.3).

$$dCA_1/dt = (CA_0 - CA_1)$$

$$dCA_2/dt = (CA_1 - CA_2)$$

Example C.2: System of ODE

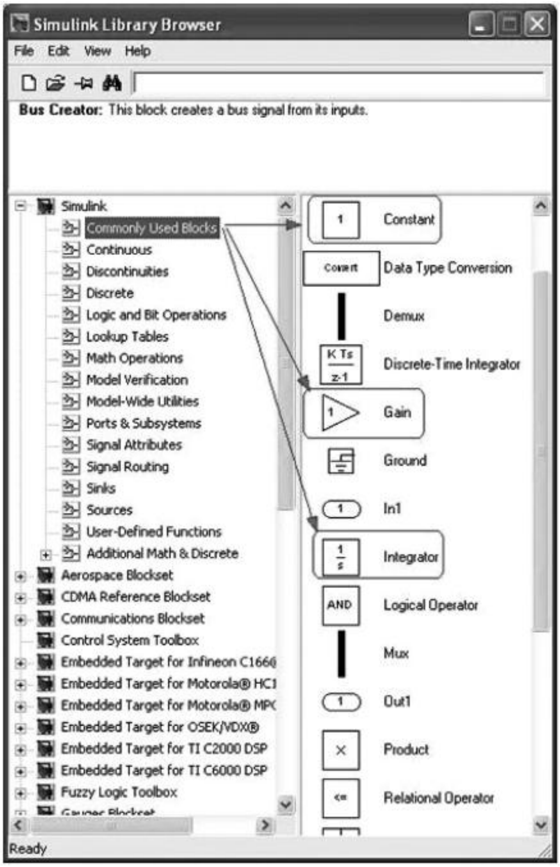
Solve the following set of ordinary differential equation with initial concentration of A (1 mol/L) and zero concentration of B.

$$dC_A/dt = -2C_A + C_B$$

$$dC_B/dt = 3(C_A - C_B)$$

$$C_A(0) = 1; \quad C_B(0) = 0$$

1. Double click on the first integral sign and enter initial concentration of A (i.e., $C_A(0) = 1$) (Figure C.4).
2. Double click on the second integral and enter initial concentration of B (i.e., $C_B(0) = 0$) (Figure C.5).



Bus Creator: This block creates a bus signal from its inputs.

FIGURE C.1
SIMULINK library browsers.

Example C.3: Multiple Reactions in Batch Reactors

Solving a set of three ordinary differential equations

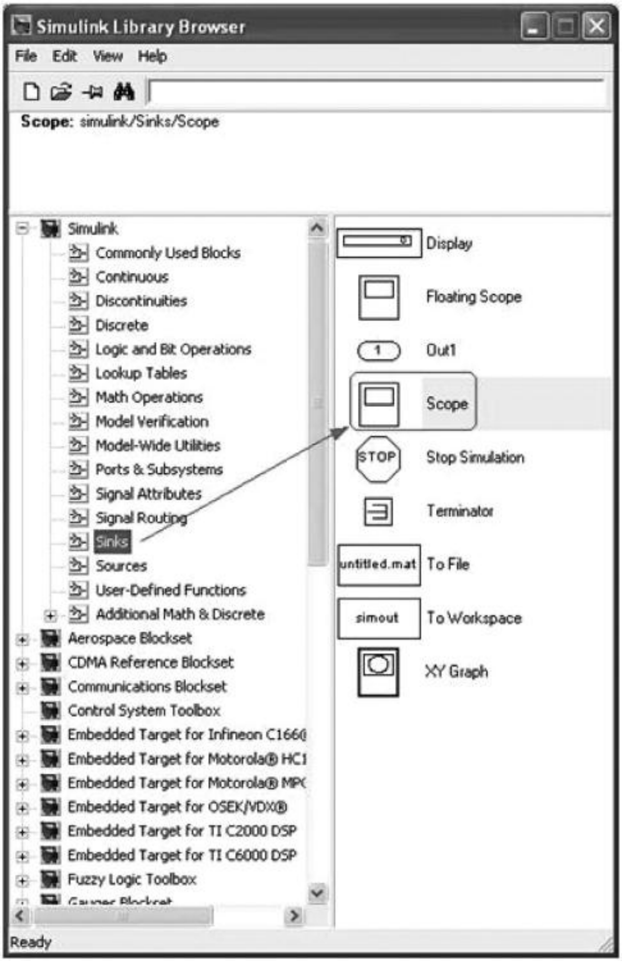
Consider the following reactions in series:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$\frac{dC_A}{dt} = -k_1 * C_A$$

$$\frac{dC_B}{dt} = k_1 * C_A - k_2 * C_B$$

$$\frac{dC_C}{dt} = k_2 * C_B$$



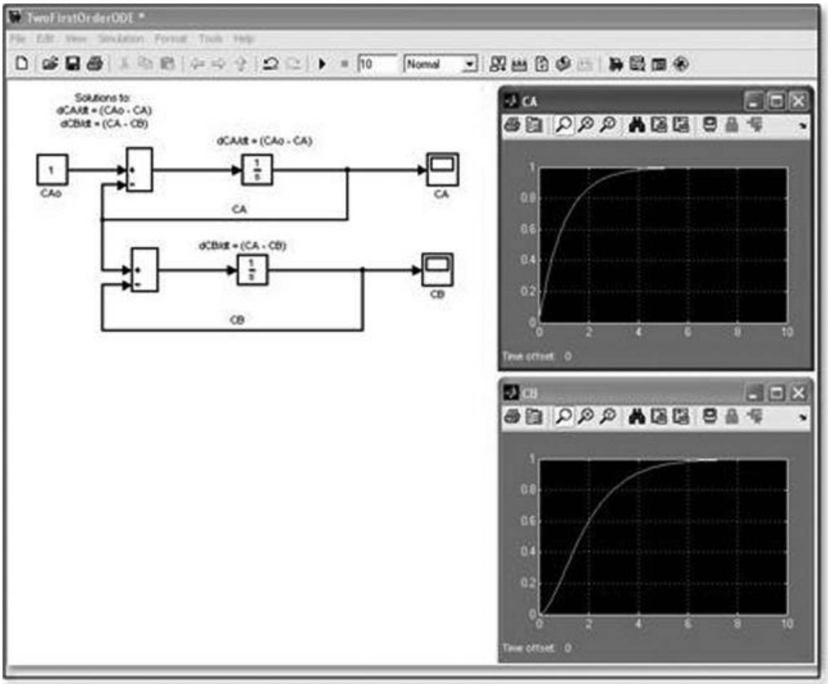
Scope: simulink/Sinks/Scope

FIGURE C.2
Sinks objects.

Example C.4: Solution of Second-Order Differential Equations

Solve the following equation using SIMULINK (Figure C.6):

$$\frac{d^2x}{dt^2} + 2\frac{dx}{dt} + 3x = 1$$

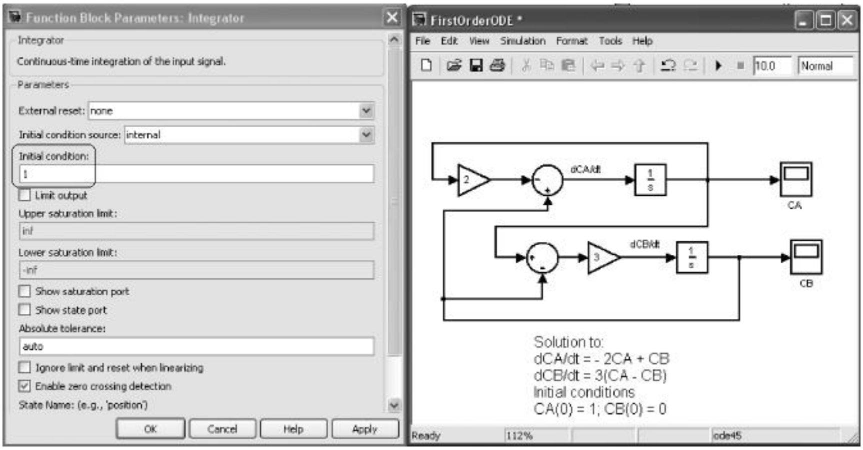


Solutions to:
dCA/dt = (CAo - CA)
dCB/dt = (CA - CB)

dCA/dt = (CAo - CA)

dCB/dt = (CA - CB)

FIGURE C.3
Solution of two ordinary differential equations.



Integrator

Continuous-time integration of the input signal.

Parameters

External reset: none

Initial condition source: internal

Initial condition: 1

☐ Limit output

Upper saturation limit: inf

Lower saturation limit: -inf

☐ Show saturation port

☐ Show state port

Absolute tolerance: auto

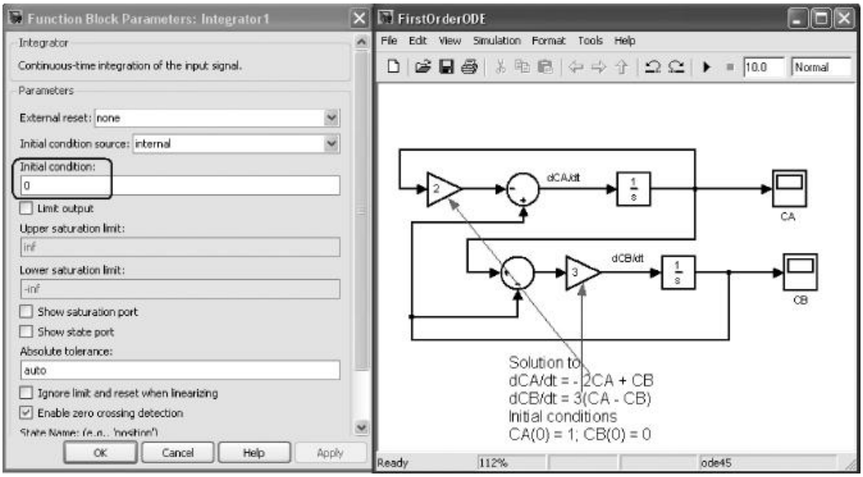
☐ Ignore limit and reset when linearizing

☑ Enable zero crossing detection

State Name: (e.g., 'position')

Solution to:
dCA/dt = - 2CA + CB
dCB/dt = 3(CA - CB)
Initial conditions
CA(0) = 1; CB(0) = 0

FIGURE C.4
Initial conditions of A.



Function Block Parameters: Integrator1

Integrator

Continuous-time integration of the input signal.

Parameters

External reset: none

Initial condition source: internal

Initial condition: 0

☐ Limit output

Upper saturation limit: inf

Lower saturation limit: -inf

☐ Show saturation port

☐ Show state port

Absolute tolerance: auto

☐ Ignore limit and reset when linearizing

☑ Enable zero crossing detection

State Name: (e.g., 'position')

Solution to
dCA/dt = -2CA + CB
dCB/dt = 3(CA - CB)
Initial conditions
CA(0) = 1; CB(0) = 0

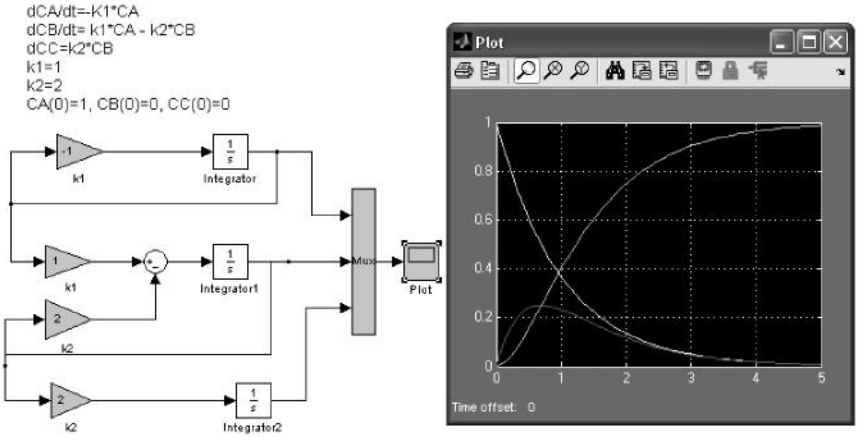
FIGURE C.5
Initial conditions of B.

Example C.5: Nonlinear Algebraic Equations

Find the value of Ca in the following nonlinear algebraic equations:
Nonlinear algebraic equation (Figure C.7):

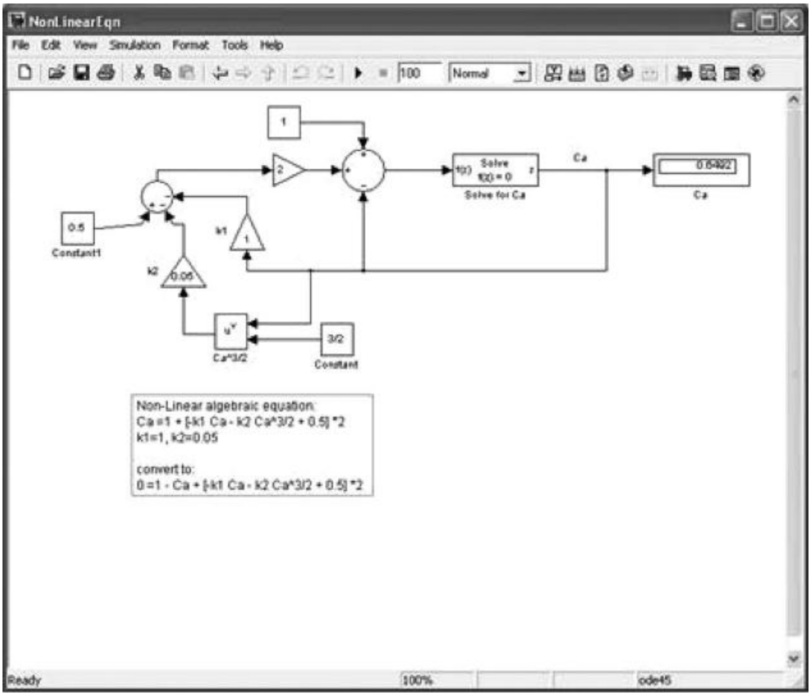
$$\mathrm{Ca} = 1 - 2[0.5 - k_1\mathrm{Ca} - k_2\mathrm{Ca}^{3/2}]$$

$$k_1 = 1, \quad k_2 = 0.05$$



dCA/dt=-K1*CA
dCB/dt= k1*CA - k2*CB
dCC=k2*CB
k1=1
k2=2
CA(0)=1, CB(0)=0, CC(0)=0

FIGURE C.6
Solution of second-order ODE.



Non-Linear algebraic equation:
Ca =1 + [-k1 Ca - k2 Ca^3/2 + 0.5] *2
k1=1, k2=0.05

convert to:
0 =1 - Ca + [-k1 Ca - k2 Ca^3/2 + 0.5] *2

FIGURE C.7
Solution of nonlinear algebraic equations.

convert to

$$1 - \mathrm{Ca} + 2[0.5 - k_1\,\mathrm{Ca} - k_2\,\mathrm{Ca}^{3/2}] = 0.$$

Example C.6: Algebraic Equation

Given the temperature in degrees Celsius, convert to degrees Fahrenheit (Figure C.8).

Example C.7: Liquid Level in a Cylindrical Tank (Figures 7.9 and 7.10)

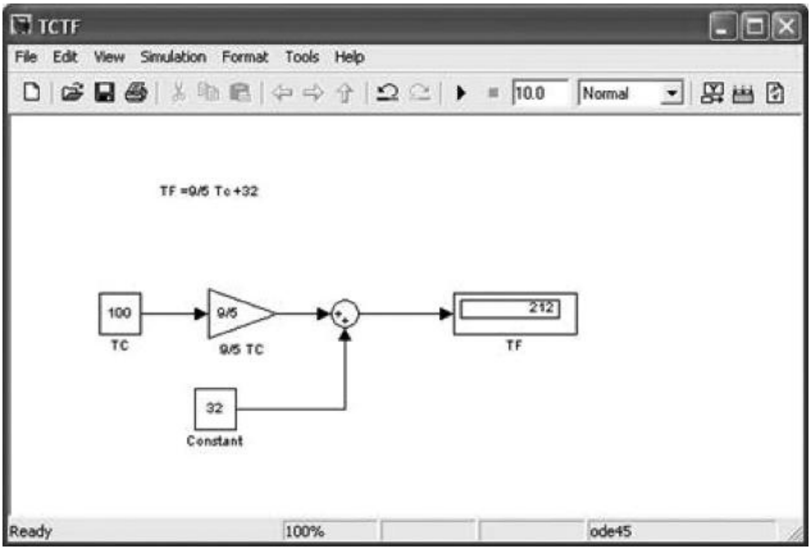


FIGURE C.8
Convert temperatures from degrees Celsius to degrees Fahrenheit.

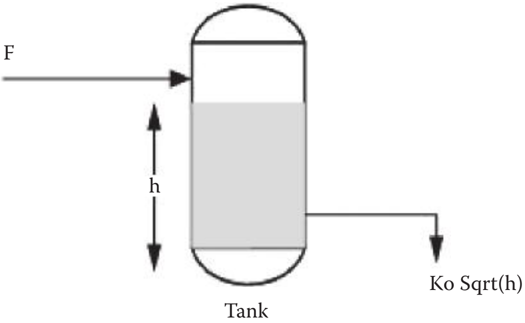


FIGURE C.9
Water in a cylindrical tank.

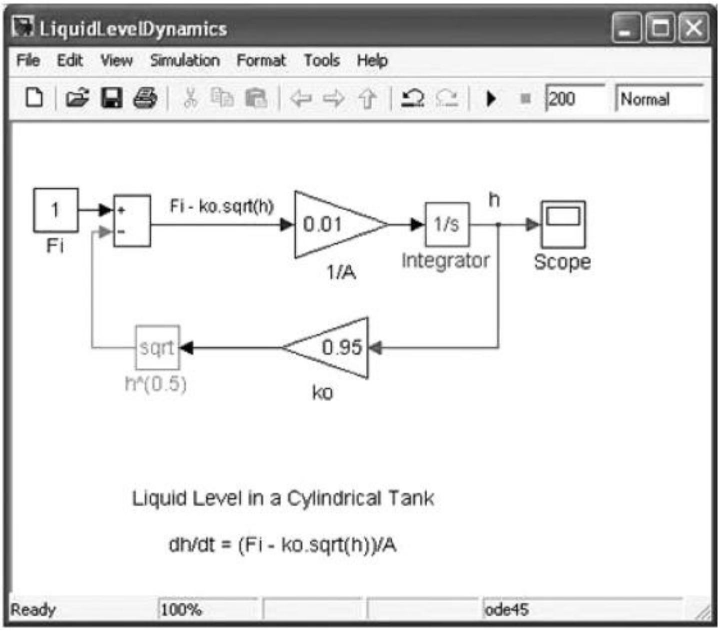


FIGURE C.10
Simulation of liquid level in a cylindrical tank.

Appendix D: Nonlinear Regression of Experimental Data

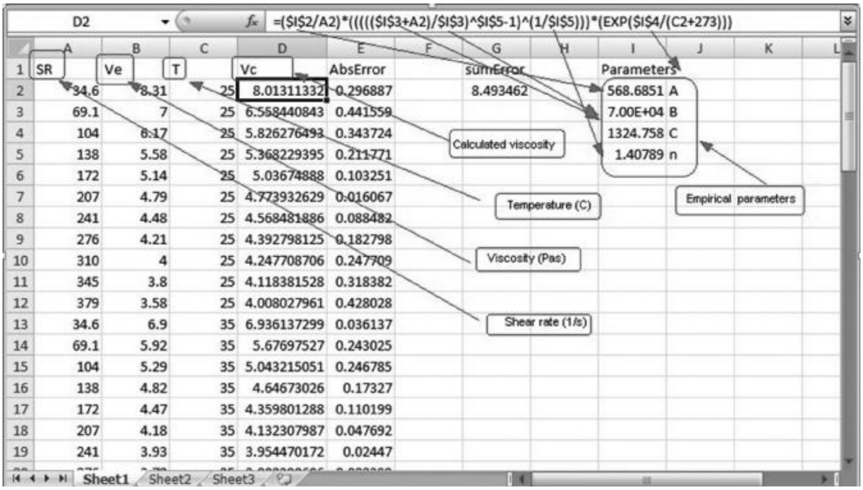
D.1 Nonlinear Regression Using Excel

In the present example, it is required to derive empirical equations to predict the experimental shear rate, viscosity, and temperature data. The proposed equation is as follows:

$$\eta = \frac{A}{\dot{\gamma}}\left[\left(\frac{B+\dot{\gamma}}{\dot{\gamma}}\right)^{m} - 1\right]^{1/m} e^{C/(T+273)}$$

where SR is the shear rate (1/s), Ve is the experimental viscosity in Pa.s, and *T* is the temperature in degrees Celsius (Figures D.1 through D.3).

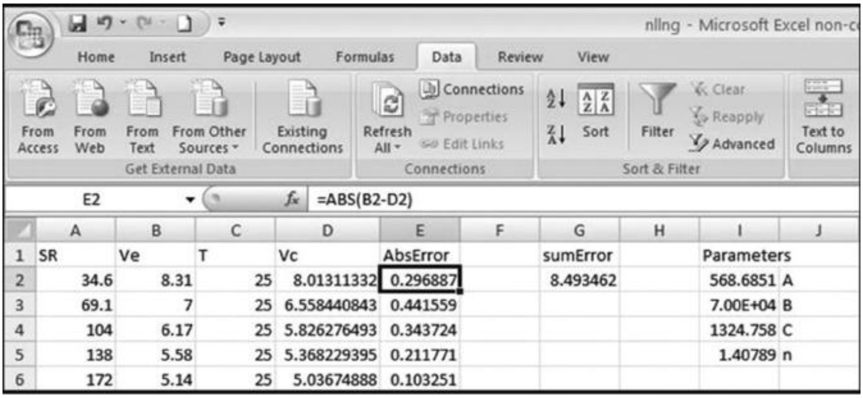
Click on Data from the Excel tool bar (Figure D.4).



D2 =($I$2/A2)*(((((($I$3+A2)/$I$3)^$I$5-1)^(1/$I$5)))*(EXP($I$4/(C2+273)))

	A	B	C	D	E	F	G	H	I	J
1	SR	Ve	T	Vc	AbsError		sumError		Parameters	
2	34.6	8.31	25	8.01311332	0.296887		8.493462		568.6851	A
3	69.1	7	25	6.558440843	0.441559				7.00E+04	B
4	104	6.17	25	5.826276493	0.343724				1324.758	C
5	138	5.58	25	5.368229395	0.211771				1.40789	n
6	172	5.14	25	5.03674888	0.103251					
7	207	4.79	25	4.773932629	0.016067					
8	241	4.48	25	4.568481886	0.088482					
9	276	4.21	25	4.392798125	0.182798					
10	310	4	25	4.247708706	0.247709					
11	345	3.8	25	4.118381528	0.318382					
12	379	3.58	25	4.008027961	0.428028					
13	34.6	6.9	35	6.936137299	0.036137					
14	69.1	5.92	35	5.67697527	0.243025					
15	104	5.29	35	5.043215051	0.246785					
16	138	4.82	35	4.64673026	0.17327					
17	172	4.47	35	4.359801288	0.110199					
18	207	4.18	35	4.132307987	0.047692					
19	241	3.93	35	3.954470172	0.02447					

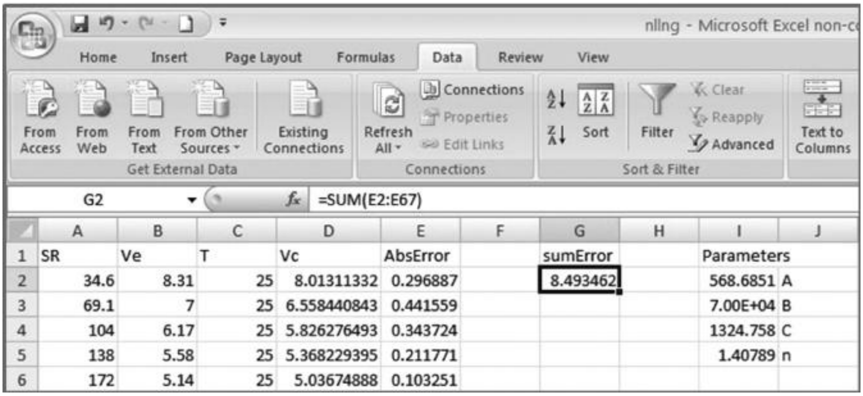
FIGURE D.1
Generating empirical correlation using Excel.



E2 =ABS(B2-D2)

	A	B	C	D	E	F	G	H	I	J
1	SR	Ve	T	Vc	AbsError		sumError		Parameters	
2	34.6	8.31	25	8.01311332	0.296887		8.493462		568.6851	A
3	69.1	7	25	6.558440843	0.441559				7.00E+04	B
4	104	6.17	25	5.826276493	0.343724				1324.758	C
5	138	5.58	25	5.368229395	0.211771				1.40789	n
6	172	5.14	25	5.03674888	0.103251					

FIGURE D.2
Calculation of absolute error.



G2 =SUM(E2:E67)

	A	B	C	D	E	F	G	H	I	J
1	SR	Ve	T	Vc	AbsError		sumError		Parameters	
2	34.6	8.31	25	8.01311332	0.296887		8.493462		568.6851	A
3	69.1	7	25	6.558440843	0.441559				7.00E+04	B
4	104	6.17	25	5.826276493	0.343724				1324.758	C
5	138	5.58	25	5.368229395	0.211771				1.40789	n
6	172	5.14	25	5.03674888	0.103251					

FIGURE D.3
Calculation of the sum of absolute errors.

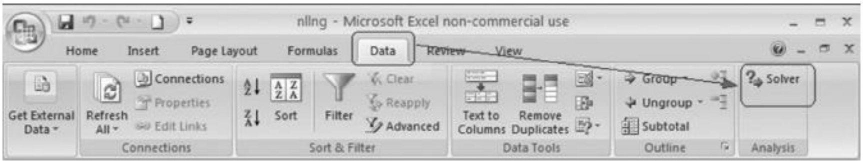
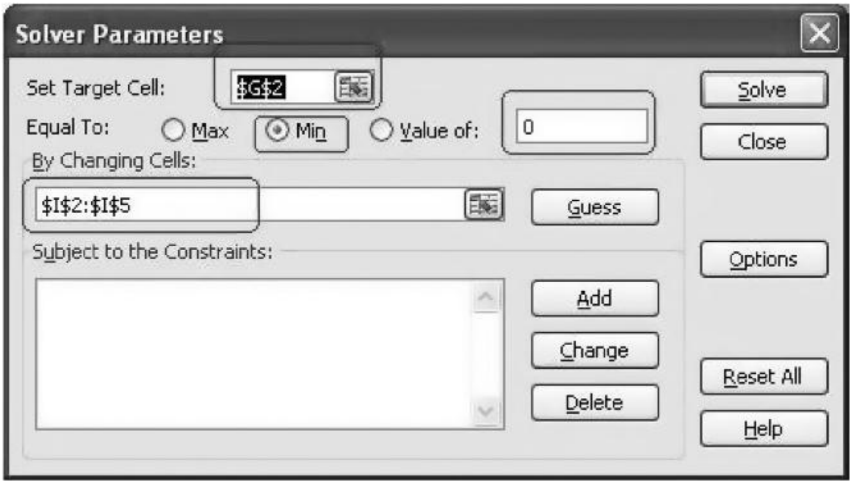


FIGURE D.4
Using Solver to generate parameters.



Set Target Cell: $G$2

Equal To: ○ Max ● Min ○ Value of: 0

By Changing Cells: $I$2:$I$5

Subject to the Constraints:

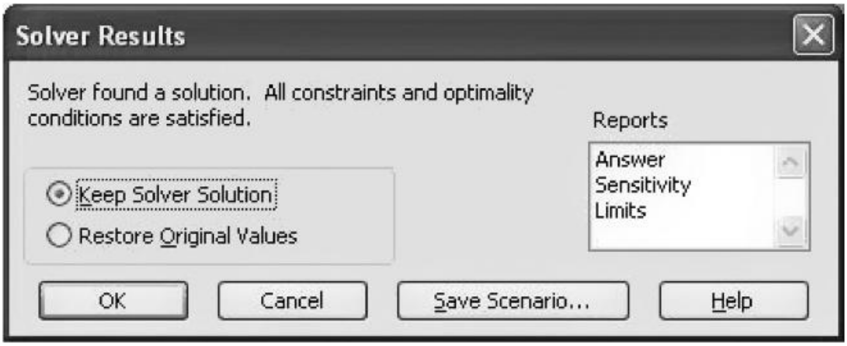
FIGURE D.5
Solver parameters.

Click on the Solver button; a window pops up as shown in Figures D.5 and D.6.

D.2 Nonlinear Regression Using SigmaPlot

In this example, we will create a nonlinear regression equation from scratch (Figure D.7).

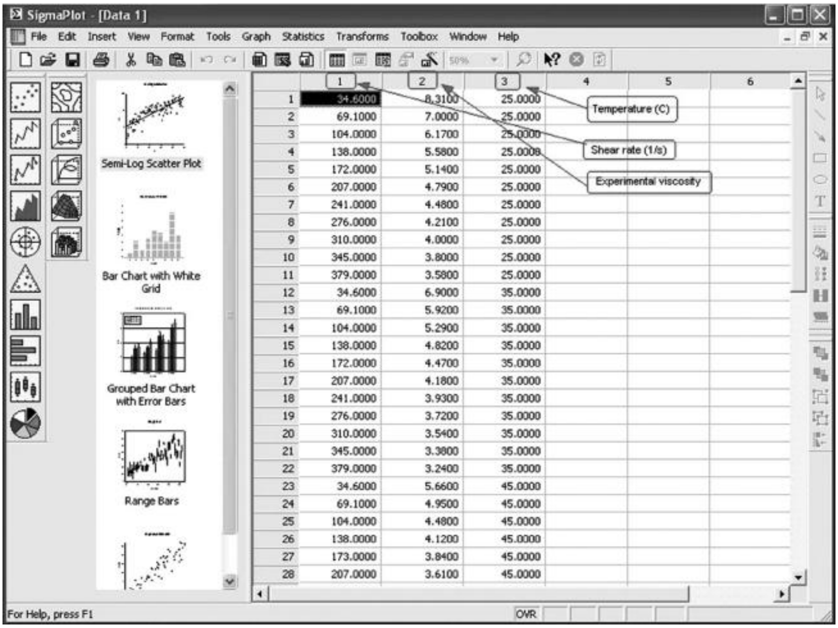
First, on the Statistics menu, click Regression Wizard (Figures D.8 and D.9).



Solver found a solution. All constraints and optimality conditions are satisfied.

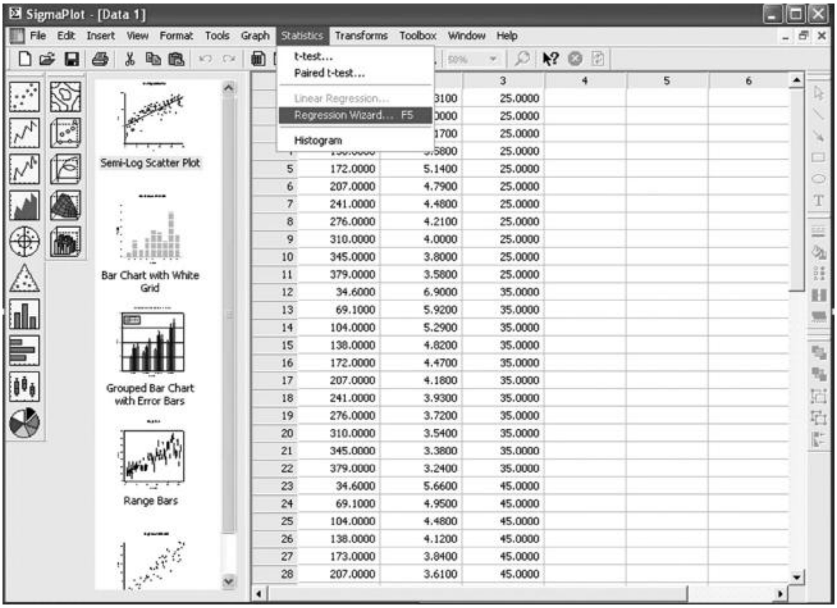
● Keep Solver Solution
○ Restore Original Values

FIGURE D.6
Solver results.



	1	2	3	4	5	6
1	34.6000	8.3100	25.0000			
2	69.1000	7.0000	25.0000			
3	104.0000	6.1700	25.0000			
4	138.0000	5.5800	25.0000			
5	172.0000	5.1400	25.0000			
6	207.0000	4.7900	25.0000			
7	241.0000	4.4800	25.0000			
8	276.0000	4.2100	25.0000			
9	310.0000	4.0000	25.0000			
10	345.0000	3.8000	25.0000			
11	379.0000	3.5800	25.0000			
12	34.6000	6.9000	35.0000			
13	69.1000	5.9200	35.0000			
14	104.0000	5.2900	35.0000			
15	138.0000	4.8200	35.0000			
16	172.0000	4.4700	35.0000			
17	207.0000	4.1800	35.0000			
18	241.0000	3.9300	35.0000			
19	276.0000	3.7200	35.0000			
20	310.0000	3.5400	35.0000			
21	345.0000	3.3800	35.0000			
22	379.0000	3.2400	35.0000			
23	34.6000	5.6600	45.0000			
24	69.1000	4.9500	45.0000			
25	104.0000	4.4800	45.0000			
26	138.0000	4.1200	45.0000			
27	173.0000	3.8400	45.0000			
28	207.0000	3.6100	45.0000			

FIGURE D.7
Sigma plot data window.



	1	2	3	4	5	6
		3100	25.0000			
		0000	25.0000			
		1700	25.0000			
		5800	25.0000			
5	172.0000	5.1400	25.0000			
6	207.0000	4.7900	25.0000			
7	241.0000	4.4800	25.0000			
8	276.0000	4.2100	25.0000			
9	310.0000	4.0000	25.0000			
10	345.0000	3.8000	25.0000			
11	379.0000	3.5800	25.0000			
12	34.6000	6.9000	35.0000			
13	69.1000	5.9200	35.0000			
14	104.0000	5.2900	35.0000			
15	138.0000	4.8200	35.0000			
16	172.0000	4.4700	35.0000			
17	207.0000	4.1800	35.0000			
18	241.0000	3.9300	35.0000			
19	276.0000	3.7200	35.0000			
20	310.0000	3.5400	35.0000			
21	345.0000	3.3800	35.0000			
22	379.0000	3.2400	35.0000			
23	34.6000	5.6600	45.0000			
24	69.1000	4.9500	45.0000			
25	104.0000	4.4800	45.0000			
26	138.0000	4.1200	45.0000			
27	173.0000	3.8400	45.0000			
28	207.0000	3.6100	45.0000			

FIGURE D.8
Selection of regression wizard.

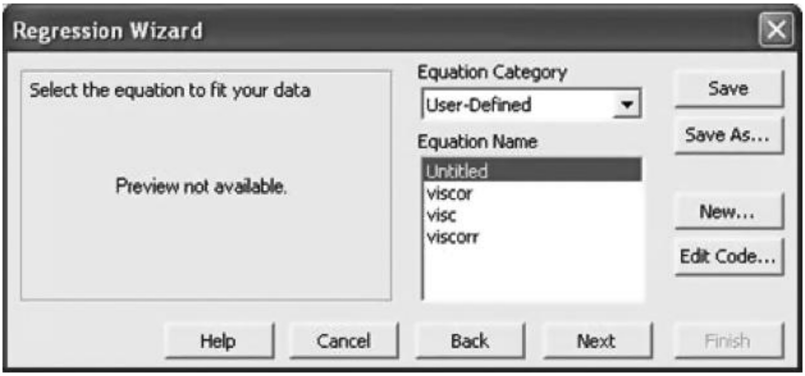
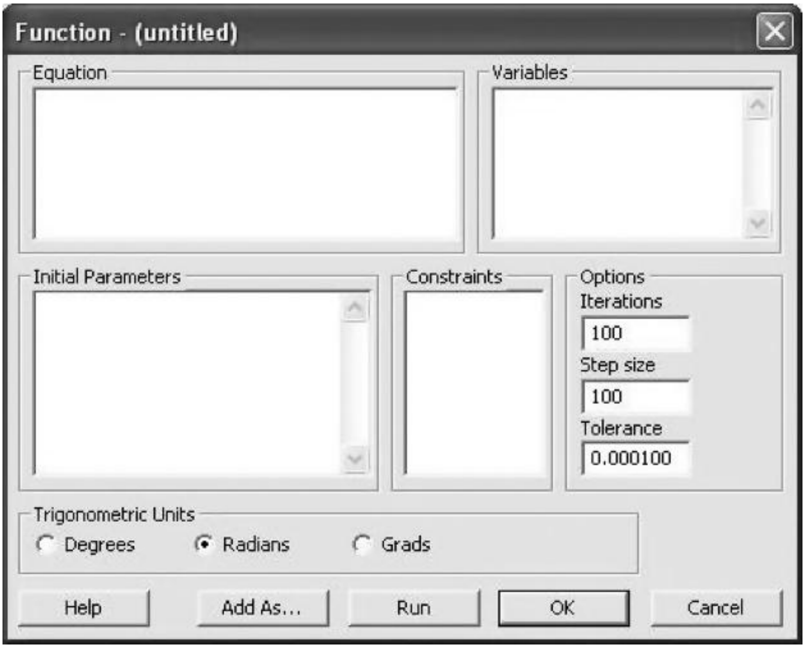


FIGURE D.9
Regression wizard.

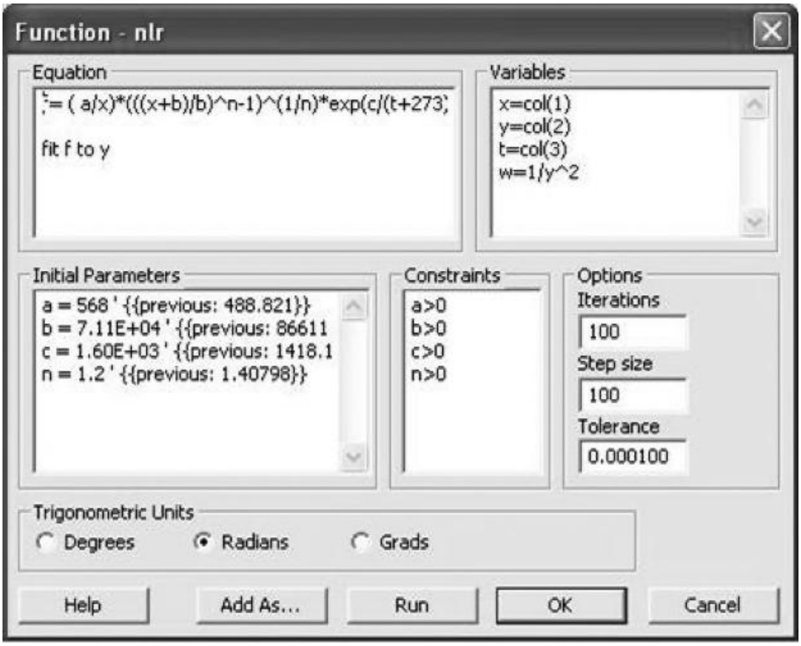
Click New in the Regression Wizard to open the Function dialog box (Figures D.10 and D.11).

Enter the following equations, variables, initial parameters, and constraints into the appropriate windows.



Iterations: 100
Step size: 100
Tolerance: 0.000100
Trigonometric Units: ○ Degrees ● Radians ○ Grads

FIGURE D.10
Editing of function window.



Function - nlr

Equation

```
= ( a/x)*(((x+b)/b)^n-1)^(1/n)*exp(c/(t+273)

fit f to y
```

Variables

```
x=col(1)
y=col(2)
t=col(3)
w=1/y^2
```

Initial Parameters

```
a = 568 ' {{previous: 488.821}}
b = 7.11E+04 ' {{previous: 86611
c = 1.60E+03 ' {{previous: 1418.1
n = 1.2 ' {{previous: 1.40798}}
```

Constraints

```
a>0
b>0
c>0
n>0
```

Options

Iterations: 100

Step size: 100

Tolerance: 0.000100

Trigonometric Units

○ Degrees ● Radians ○ Grads

FIGURE D.11
Nonlinear function, variables, and constraints.

For the equation, enter:

```
f = (a/x)*(((x + b)/b)^n – 1)^(1/n)*exp(c/(t + 273))
fit f to y
```

For the variables, enter:

```
x = col(1)
y = col(2)
t = col(3)
w = 1/y^2
```

For the initial parameters, enter as initial guess:

```
a = 568
b = 7.11E + 04
c = 1.60E + 03
n = 1.2
```

nlr

FIGURE D.12
Equation name window.

For the constraints, enter:

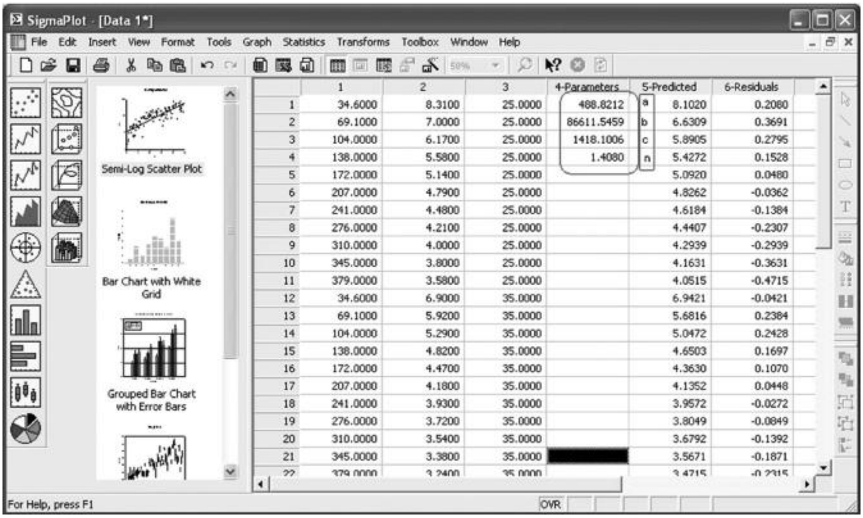
a > 0, b > 0, c > 0, n > 0

Click OK. "The Add As" dialog box appears.

Type equation name; in this example "nlr" and then click OK (Figure D.12). Click on "Run" button to complete the curve fit (Figure D.13).

D.3 Nonlinear Regression Using SYSTAT

Click on systat start-up file (Figure D.14).



	1	2	3	4-Parameters	5-Predicted	6-Residuals
1	34.6000	8.3100	25.0000	488.8212 a	8.1020	0.2080
2	69.1000	7.0000	25.0000	86611.5459 b	6.6309	0.3691
3	104.0000	6.1700	25.0000	1418.1006 c	5.8905	0.2795
4	138.0000	5.5800	25.0000	1.4080 n	5.4272	0.1528
5	172.0000	5.1400	25.0000		5.0920	0.0480
6	207.0000	4.7900	25.0000		4.8262	-0.0362
7	241.0000	4.4800	25.0000		4.6184	-0.1384
8	276.0000	4.2100	25.0000		4.4407	-0.2307
9	310.0000	4.0000	25.0000		4.2939	-0.2939
10	345.0000	3.8000	25.0000		4.1631	-0.3631
11	379.0000	3.5800	25.0000		4.0515	-0.4715
12	34.6000	6.9000	35.0000		6.9421	-0.0421
13	69.1000	5.9200	35.0000		5.6816	0.2384
14	104.0000	5.2900	35.0000		5.0472	0.2428
15	138.0000	4.8200	35.0000		4.6503	0.1697
16	172.0000	4.4700	35.0000		4.3630	0.1070
17	207.0000	4.1800	35.0000		4.1352	0.0448
18	241.0000	3.9300	35.0000		3.9572	-0.0272
19	276.0000	3.7200	35.0000		3.8049	-0.0849
20	310.0000	3.5400	35.0000		3.6792	-0.1392
21	345.0000	3.3800	35.0000		3.5671	-0.1871
22	379.0000	3.2400	35.0000		3.4715	-0.2315

FIGURE D.13
Sigma plot calculated results and residues.

Recent Data Files
D:\C&EData\viscosity.syz
D:\Documents and Settings\nayef.ACADEMICS\Desktop\viscosity.syz
D:\Documents and Settings\nayef.ACADEMICS\Desktop\vis-mod.syz
Recent Command Files
Recent Output Files

Themes: [Current Theme: Classic]
Classic
Default
Introductory_Statistics
Market_Research

Manuals
Data.pdf
GettingStarted.pdf
Graphics.pdf

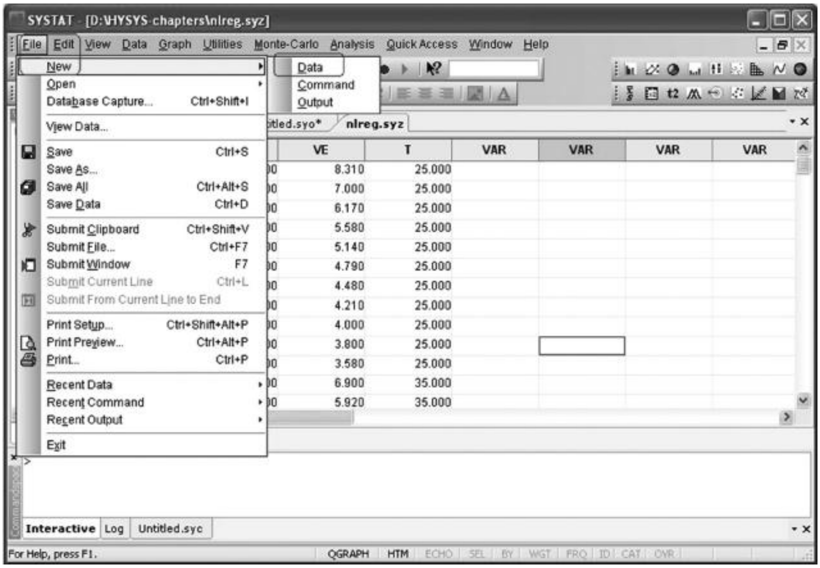
☑ Show at startup

Did you know...
You can directly submit a set of commands through Utilities -> User Menu -> Menu list.
[Next Tip]

Scratchpad

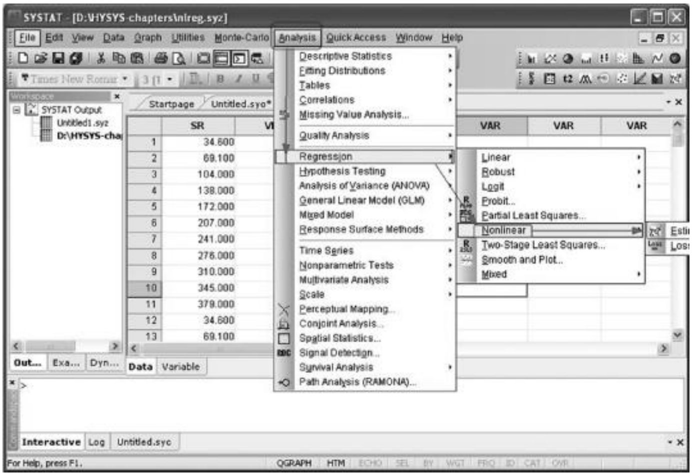
FIGURE D.14
Systat version 12 main menu.

From File, New, Data fill the data that will be used in fitting procedure (Figure D.15).



VE	T	VAR	VAR	VAR	VAR
8.310	25.000				
7.000	25.000				
6.170	25.000				
5.580	25.000				
5.140	25.000				
4.790	25.000				
4.480	25.000				
4.210	25.000				
4.000	25.000				
3.800	25.000				
3.580	25.000				
6.900	35.000				
5.920	35.000				

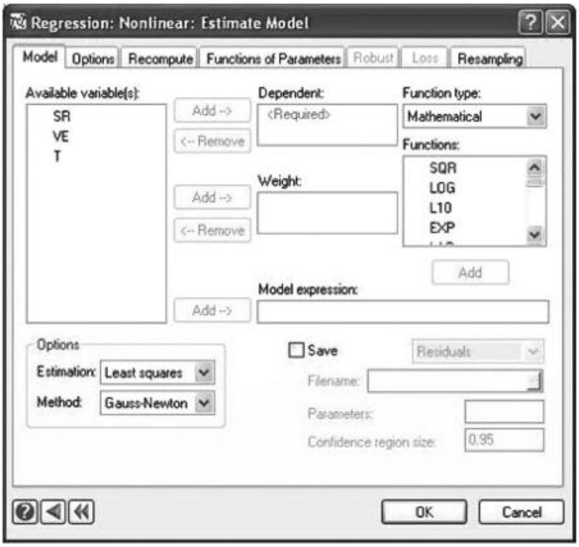
FIGURE D.15
Systat data window.



	SR
1	34.600
2	69.100
3	104.000
4	138.000
5	172.000
6	207.000
7	241.000
8	276.000
9	310.000
10	345.000
11	379.000
12	34.600
13	69.100

FIGURE D.16
Selection of nonlinear regression.

Analysis
Regression
Nonlinear
Estimate model
Insert the model in the Model expression (Figure D.16).
A window pops up as shown in Figure D.17.

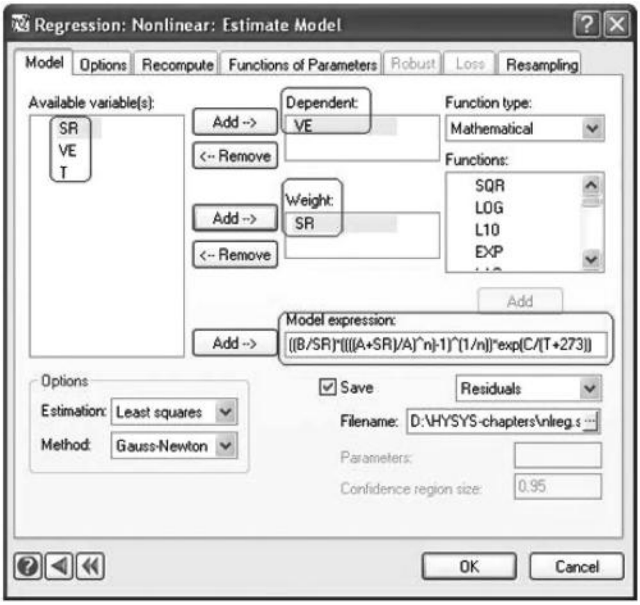


Function type: Mathematical

Options
Estimation: Least squares
Method: Gauss-Newton

Confidence region size: 0.95

FIGURE D.17
Windows of nonlinear regressions.



Dependent: VE

Weight: SR

Function type: Mathematical

Model expression: ((B/SR)*((((A+SR)/A)^n)-1)^(1/n))*exp(C/(T+273))

Estimation: Least squares

Method: Gauss-Newton

☑ Save Residuals

Filename: D:\HYSYS-chapters\nlreg.s

Confidence region size: 0.95

FIGURE D.18
Nonlinear regression available variables.

Fill in the dependent variable, experimental viscosity VE, the weight as shear rate SR, and the model expression (Figure D.18).

```
(a/SR)*(((SR+b)/b)^n-1)^(1/n)*exp(c/(T+273))
```

Click on the "Options" buttons and fill in the initial guess of the parameters (Figure D.19).

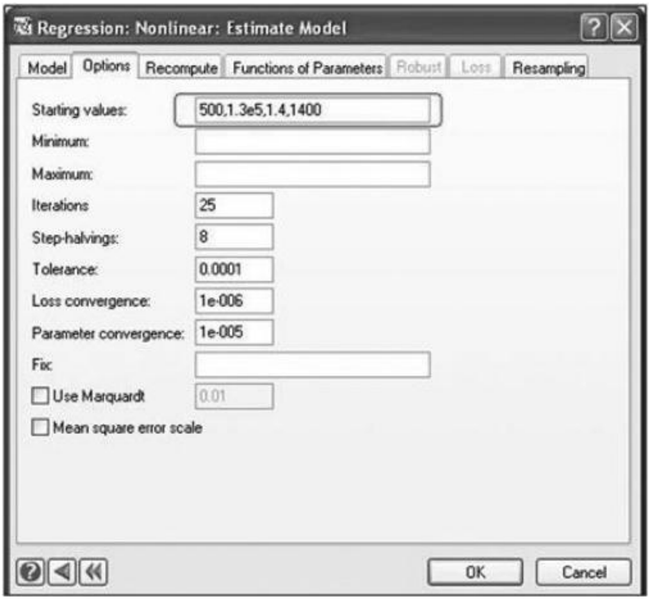
A, B, n, C

To display the estimated values on the same data (Figure D.20).

The output parameters results (Figure D.21).
The parameters values are:

$B = 837.57$
$A = 131{,}616.71$
$n = 1.46$
$C = 1281.65$

Comparison between experimental and estimated values is shown in Figure A.22.



Starting values: 500,1.3e5,1.4,1400

Minimum:

Maximum:

Iterations: 25

Step-halvings: 8

Tolerance: 0.0001

Loss convergence: 1e-006

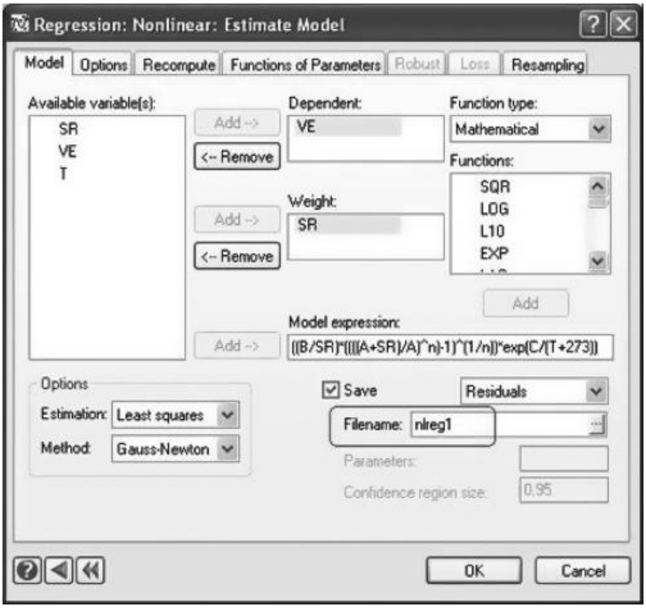
Parameter convergence: 1e-005

Fix:

☐ Use Marquardt 0.01

☐ Mean square error scale

FIGURE D.19
Nonlinear regression starting values.



Available variable(s): SR, VE, T

Dependent: VE

Weight: SR

Function type: Mathematical

Model expression: ((B/SR)*((((A+SR)/A)^n)-1)^(1/n))*exp(C/(T+273))

Options

Estimation: Least squares

Method: Gauss-Newton

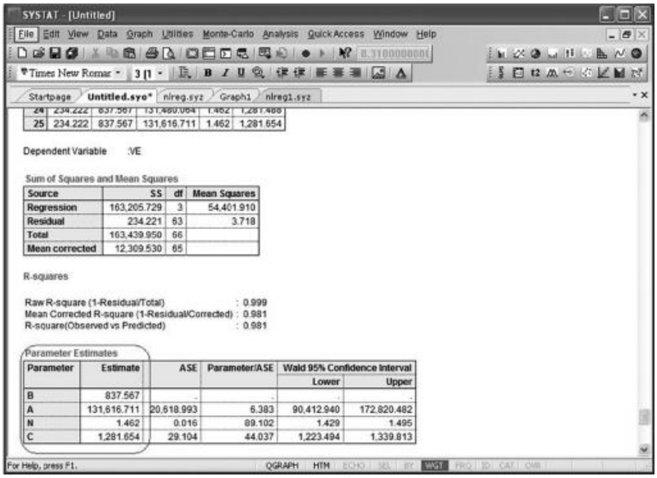
☑ Save Residuals

Filename: nlreg1

Parameters:

Confidence region size: 0.95

FIGURE D.20
Model regression windows.



25	234.222	837.567	131,616.711	1.462	1,281.654

Dependent Variable :VE

Sum of Squares and Mean Squares

Source	SS	df	Mean Squares
Regression	163,205.729	3	54,401.910
Residual	234.221	63	3.718
Total	163,439.950	66	
Mean corrected	12,309.530	65	

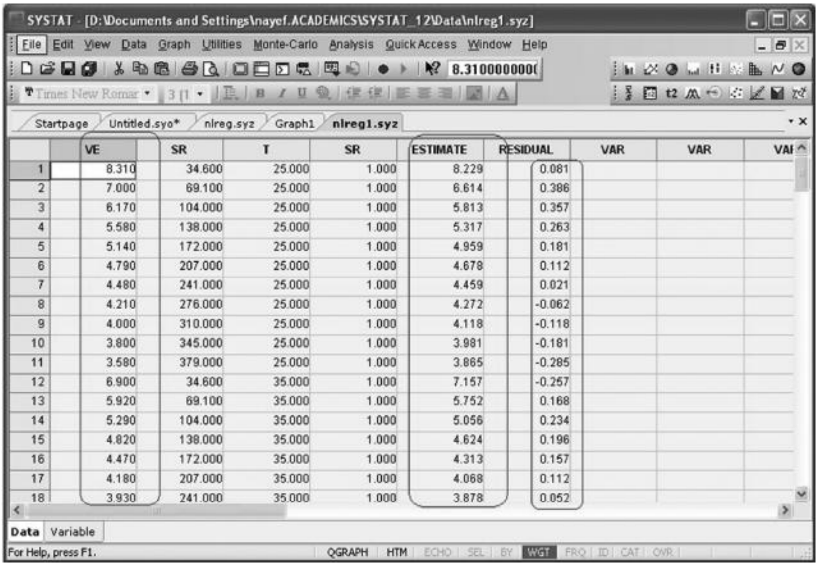
R-squares

Raw R-square (1-Residual/Total) : 0.999
Mean Corrected R-square (1-Residual/Corrected) : 0.981
R-square(Observed vs Predicted) : 0.981

Parameter Estimates

Parameter	Estimate	ASE	Parameter/ASE	Wald 95% Confidence Interval	
				Lower	Upper
B	837.567	.	.	.	.
A	131,616.711	20,618.993	6.383	90,412.940	172,820.482
N	1.462	0.016	89.102	1.429	1.495
C	1,281.654	29.104	44.037	1,223.494	1,339.813

FIGURE D.21
Results of nonlinear regression.



	VE	SR	T	SR	ESTIMATE	RESIDUAL	VAR	VAR	VAI
1	8.310	34.600	25.000	1.000	8.229	0.081			
2	7.000	69.100	25.000	1.000	6.614	0.386			
3	6.170	104.000	25.000	1.000	5.813	0.357			
4	5.580	138.000	25.000	1.000	5.317	0.263			
5	5.140	172.000	25.000	1.000	4.959	0.181			
6	4.790	207.000	25.000	1.000	4.678	0.112			
7	4.480	241.000	25.000	1.000	4.459	0.021			
8	4.210	276.000	25.000	1.000	4.272	-0.062			
9	4.000	310.000	25.000	1.000	4.118	-0.118			
10	3.800	345.000	25.000	1.000	3.981	-0.181			
11	3.580	379.000	25.000	1.000	3.865	-0.285			
12	6.900	34.600	35.000	1.000	7.157	-0.257			
13	5.920	69.100	35.000	1.000	5.752	0.168			
14	5.290	104.000	35.000	1.000	5.056	0.234			
15	4.820	138.000	35.000	1.000	4.624	0.196			
16	4.470	172.000	35.000	1.000	4.313	0.157			
17	4.180	207.000	35.000	1.000	4.068	0.112			
18	3.930	241.000	35.000	1.000	3.878	0.052			

FIGURE D.22
Estimated and residuals value.

Appendix E: Microsoft Visio

A Gantt chart helps you schedule your project tasks and then helps you track your progress.

1. Open Microsoft Visio; from the *File* menu, point to *New*, point to *Schedule*, and then click *Gantt chart* (Figure E.1).
2. On the *Date* tab, type the number of tasks you want to start with, the time units you want displayed, and the date range for the project (Figure E.2).

Choose the number of tasks, dates, and units you want to use on the Gantt chart timescale.

Number of Tasks

Enter the number of tasks you want to start within your Gantt chart. It is also possible to add more tasks in later stages.

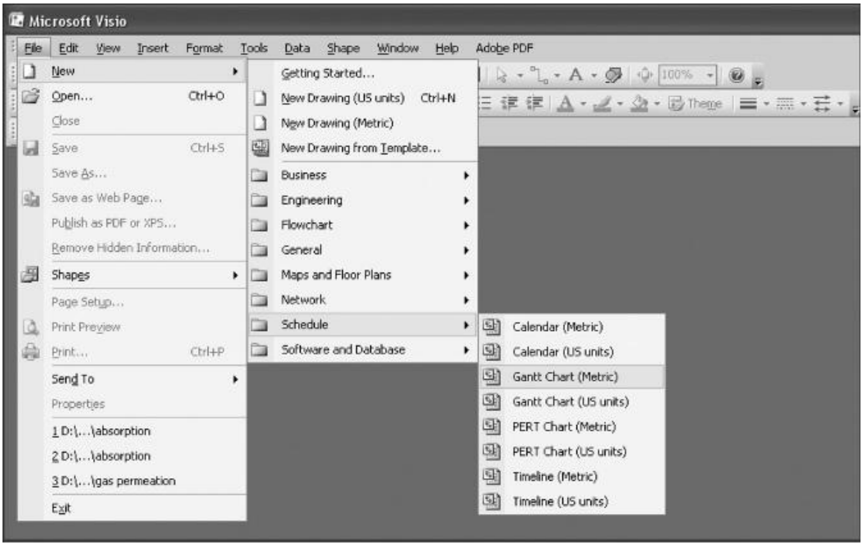
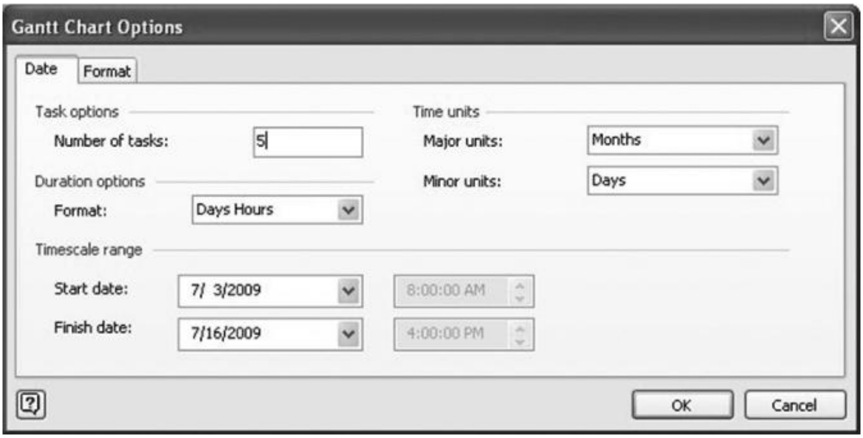


FIGURE E.1
Microsoft Visio.



Number of tasks: 5

Format: Days Hours

Start date: 7/ 3/2009 8:00:00 AM

Finish date: 7/16/2009 4:00:00 PM

Major units: Months

Minor units: Days

FIGURE E.2
Gantt chart options.

Major Units

Select the largest unit, such as years or months that you want to use in your timescale. Major units appear above the minor units on the Gantt chart timescale. The major and minor units largely determine the width of your Gantt chart. As a guideline, choose the major unit that best expresses the total length of your project, and choose a minor unit, one smaller than the major unit. For example, for a 2-year project, choose years for the major unit and months for the minor unit.

Minor Units

Select the smallest unit, such as days or hours, which you want to use in your timescale. Minor units appear below the major units on the Gantt chart timescale. The major and minor units largely determine the width of your Gantt chart.

Format

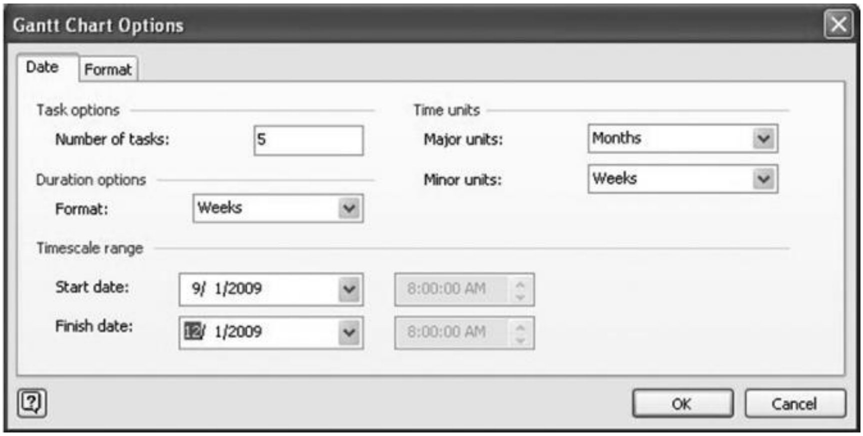
Select the time units you want to display in the *Duration* column in your Gantt chart.

Start Date

Enter the date and time when your project begins. The date you specify will be the date your Gantt chart timescale begins. You can select a start or finish time only when *Hours* is specified for *Minor units*.

Finish Date

Type the last date and time you want on the Gantt chart timescale. You can select a start or finish time only when *Hours* is specified for *Minor* (Figure E.3).



Number of tasks: 5

Format: Weeks

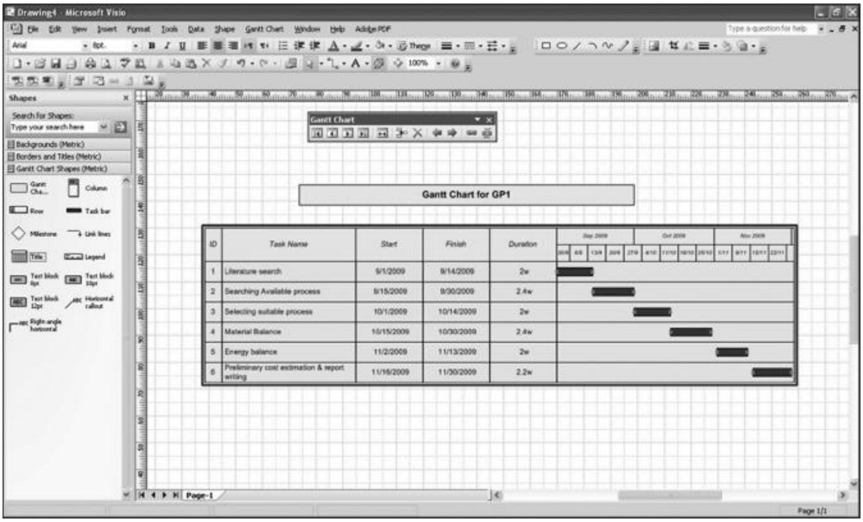
Start date: 9/ 1/2009 8:00:00 AM

Finish date: 12/ 1/2009 8:00:00 AM

Major units: Months

Minor units: Weeks

FIGURE E.3
Gantt chart tasks.

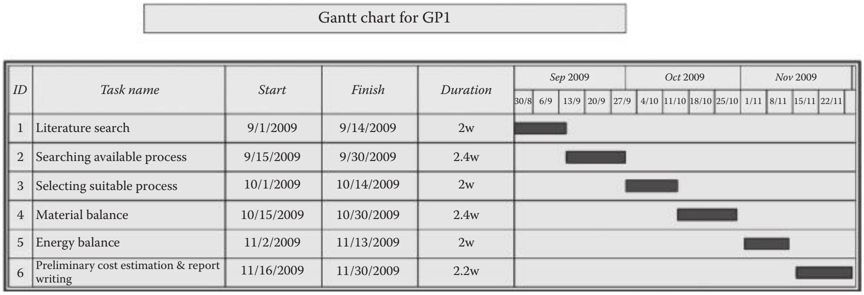


Gantt Chart for GP1

ID	Task Name	Start	Finish	Duration
1	Literature search	9/1/2009	9/14/2009	2w
2	Searching Available process	9/15/2009	9/30/2009	2.4w
3	Selecting suitable process	10/1/2009	10/14/2009	2w
4	Material Balance	10/15/2009	10/30/2009	2.4w
5	Energy balance	11/2/2009	11/13/2009	2w
6	Preliminary cost estimation & report writing	11/16/2009	11/30/2009	2.2w

FIGURE E.4
Completed Gantt chart.

Event number of tasks was 5; new task has been added (Figure E.4).
To copy the chart: while in Visio
Edit > copy drawing
Go to MS Office and paste (Figure E.5).



Gantt chart for GP1

ID	*Task name*	*Start*	*Finish*	*Duration*
1	Literature search	9/1/2009	9/14/2009	2w
2	Searching available process	9/15/2009	9/30/2009	2.4w
3	Selecting suitable process	10/1/2009	10/14/2009	2w
4	Material balance	10/15/2009	10/30/2009	2.4w
5	Energy balance	11/2/2009	11/13/2009	2w
6	Preliminary cost estimation & report writing	11/16/2009	11/30/2009	2.2w

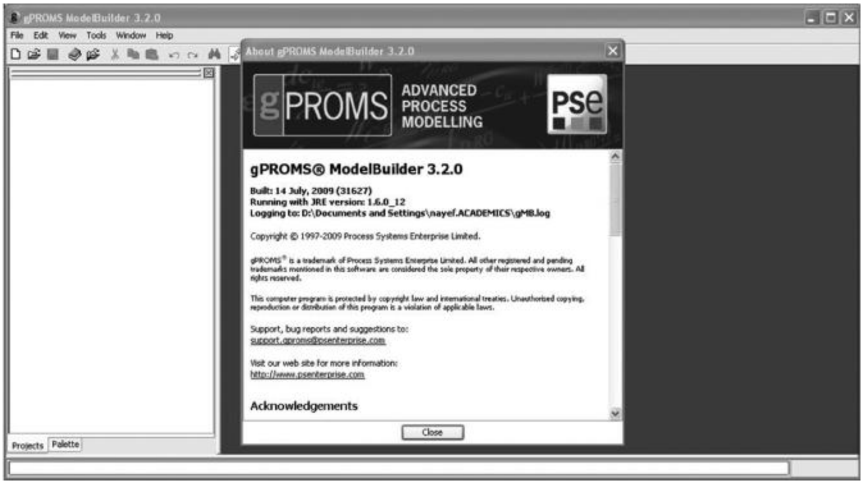
FIGURE E.5
Gantt chart pasted in MS Word.

Appendix F: General Process Modeling and Simulation (gPROMs)

In this appendix the set of ODEs and PDEs and integral equations generated to simulate the absorption of carbon dioxide using a mine flowing counter currently in a hollow fiber membrane contactor is solved using gPROMs software package (Figure F.1).

To create a new gPROMs project, select New from the Project menu. This will bring up a tree in the left-hand pane containing a number of folders:

- Variable Types
- Stream Types
- Connection Types
- Models
- Tasks
- Processes



gPROMS® ModelBuilder 3.2.0

Built: 14 July, 2009 (31627)
Running with JRE version: 1.6.0_12
Logging to: D:\Documents and Settings\nayef.ACADEMICS\gMB.log

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Support, bug reports and suggestions to:
support.gproms@psenterprise.com

Visit our web site for more information:
http://www.psenterprise.com

Acknowledgements

FIGURE F.1
gPROMs software.

Example F.1

Consider the single hollow fiber membrane as shown in Figure F.2.
The model equations are:
Dimensionless constants

$$\xi = \frac{r}{ri}, \quad \zeta = \frac{z}{l}, \quad \phi_{AI} = \frac{[CO_2]}{[CO_2]^{int}} = \frac{[CO_2]_l}{m[CO_2]_g}, \quad \phi_{BI} = \frac{[R_1R_2NH]}{C_T} \tag{F.1}$$

Dimensionless concentration of carbon dioxide

$$\frac{\partial \phi_{AI}}{\partial \zeta} = \left(\frac{1}{1-\xi^2}\right)\left\{\frac{2}{Gr_A}\left[\frac{\partial^2 \phi_{AI}}{\partial \xi^2} + \frac{1}{\xi}\frac{\partial \phi_{AI}}{\partial \xi}\right] - \frac{1}{2}\left(\frac{\beta_1 \phi_{BI}}{\beta_3 + \phi_{BI}}\right)\left[\phi_{AI}\phi_{BI} - \frac{(1-\phi_{BI})^2}{\beta_4 \phi_{BI}}\right]\right\} \tag{F.2}$$

Dimensionless concentrations of amine

$$\frac{\partial \phi_{BI}}{\partial \zeta} = \left(\frac{1}{1-\xi^2}\right)\left\{\frac{2}{Gr_B}\left[\frac{\partial^2 \phi_{BI}}{\partial \xi^2} + \frac{1}{\xi}\frac{\partial \phi_{BI}}{\partial \xi}\right] - \left(\frac{\beta_2 \phi_{BI}}{\beta_3 + \phi_{BI}}\right)\left[\phi_{AI}\phi_{BI} - \frac{(1-\phi_{BI})^2}{\beta_4 \phi_{BI}}\right]\right\} \tag{F.3}$$

Boundary conditions (Figure F.3)

$$\begin{gathered} \text{at } \zeta = 0, \quad \phi_{AI} = 0 \\ \phi_{BI} = 1 \quad \text{for any } 1 \geq \xi \geq 0 \\ \text{at } \zeta = 0, \quad \left|\frac{\partial \phi_{AI}}{\partial \xi}\right|_{\xi=0} = 0 \end{gathered} \tag{F.4}$$

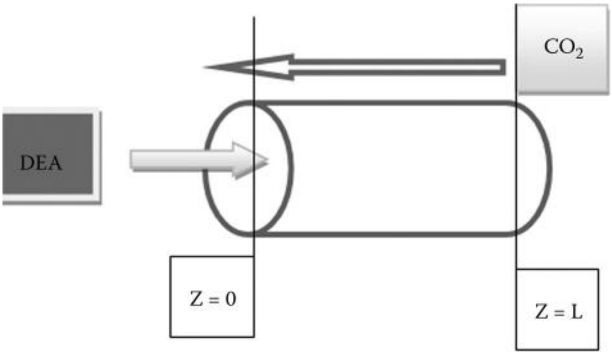


FIGURE F.2
Single hollow fiber module.

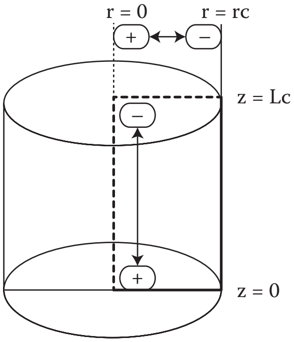


FIGURE F.3
Vertical hollow fiber modules.

$$\left|\frac{\partial \phi_{BI}}{\partial \xi}\right|_{\xi=0} = 0 \quad \text{for any } 1 \geq \xi \geq 0 \tag{F.5}$$

$$\text{at } \xi = 1, \quad \frac{\partial \phi_{AI}}{\partial \xi}\Big|_{\xi=1} = \frac{Sh_{\text{ext}}}{2}\Big[\Big|1 - \phi_{AI}\Big|_{\xi=} \tag{F.6}$$

$$\left|\frac{\partial \phi_{BI}}{\partial \xi}\right|_{\xi=0} = 0 \quad \text{for any } 1 \geq \zeta \geq 0 \tag{F.7}$$

$$Gr_A = \frac{v_z d_i^2}{l D_{CO_2}}, \quad Gr_B = \frac{v_z d_i^2}{l D_{R_1 R_2} NH} \tag{F.8}$$

Dimensionless parameters

$$\beta_1 = \frac{l K_Z C_t}{v_z} \beta_2 = \frac{l K_Z m [CO_2]_g}{v_z} \beta_2 = \frac{k - z}{k_{Bi} C_T} \beta_4 = 4 k_{eq} m [CO_2]_g \tag{F.9}$$

Cups rule for carbon dioxide exit concentrations

$$\phi_{AIo} = 4 \int_0^1 \xi (1 - \xi^2) \phi_{AI} \, d\xi \tag{F.10}$$

Cups rule for amine exit dimensionless concentrations

$$\phi_{Blo} = 4\int_0^2 \xi(1-\xi^2)\phi_{Bl}\, d\xi \tag{F.11}$$

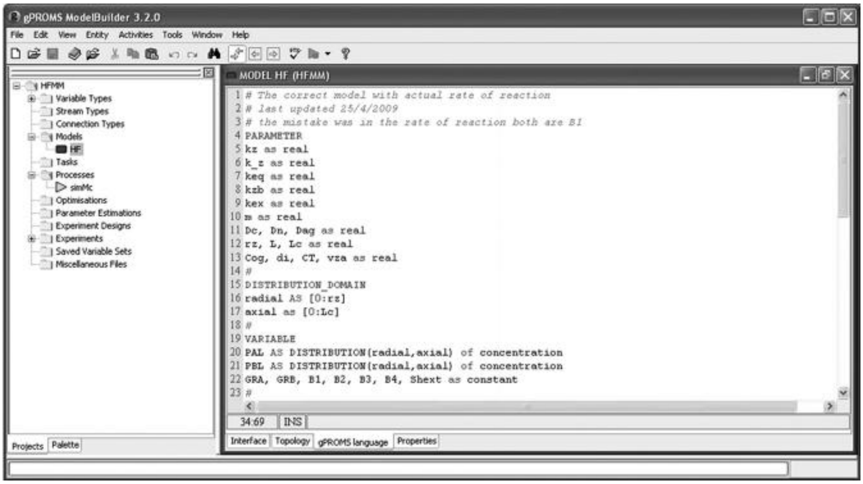
$$\eta_{CO_2} = \frac{[CO_2]_{li} - [CO_2]_{lo}}{[CO_2]_{li}} = 1 - \phi_{Alo} \tag{F.12}$$

Use the following data:

Kz = 3.17 m^2/s
k_z = 3.71E-6 m^2/s
keq = 1.43 m^2/s
kex = 10
kzb = 4580
m = 0.76 m
Dc = 1.92E-9 m
Dn = 3.83E-10 m
Dag = 1.56E-6
Cog = 41.60 mol/m^3
CT = 1000 $mole/m^3$
L = 0.2 m
Lc = 1.0
Vza = 0.01 m/s
di = 0.33 10^{-3}

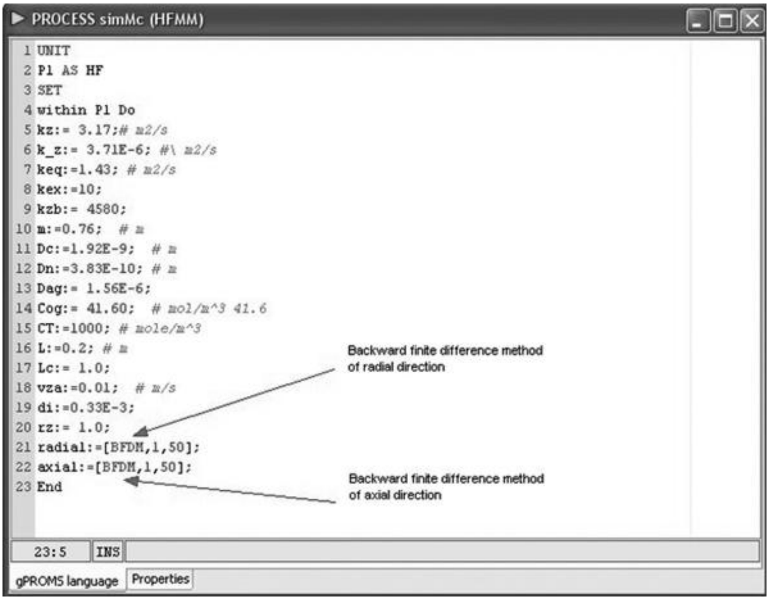
Solving the set of PDEs

The model code is demonstrated in Figure F.4.
The gPROMs process simulation file is shown in Figure F.5.
The set of the partial differential equations is written as shown in Figure F.6.



```
# The correct model with actual rate of reaction
# last updated 25/4/2009
# the mistake was in the rate of reaction both are B1
PARAMETER
kz as real
k_z as real
keq as real
kzb as real
kex as real
m as real
Dc, Dn, Dag as real
rz, L, Lc as real
Cog, di, CT, vza as real
#
DISTRIBUTION_DOMAIN
radial AS [0:rz]
axial as [0:Lc]
#
VARIABLE
PAL AS DISTRIBUTION(radial,axial) of concentration
PBL AS DISTRIBUTION(radial,axial) of concentration
GRA, GRB, B1, B2, B3, B4, Shext as constant
#
```

FIGURE F.4
gPROMs model for the hollow fiber module.



```
UNIT
P1 AS HF
SET
within P1 Do
kz:= 3.17;# m2/s
k_z:= 3.71E-6; #\ m2/s
keq:=1.43; # m2/s
kex:=10;
kzb:= 4580;
m:=0.76;  # m
Dc:=1.92E-9;  # m
Dn:=3.83E-10; # m
Dag:= 1.56E-6;
Cog:= 41.60;  # mol/m^3 41.6
CT:=1000; # mole/m^3
L:=0.2; # m
Lc:= 1.0;
vza:=0.01;  # m/s
di:=0.33E-3;
rz:= 1.0;
radial:=[BFDM,1,50];
axial:=[BFDM,1,50];
End
```

FIGURE F.5
gPROMs Process simulation file.

```
PARAMETER
kz as real
k_z as real
keq as real
kzb as real
kex as real
m as real
Dc, Dn, Dag as real
rz, L, Lc as real
Cog, di, CT, vza as real
#
DISTRIBUTION_DOMAIN
radial AS [0:rz]
axial as [0:Lc]
#
VARIABLE
PAL AS DISTRIBUTION(radial,axial) of concentration
PBL AS DISTRIBUTION(radial,axial) of concentration
GRA, GRB, B1, B2, B3, B4, Shext as constant
#
BOUNDARY
#
# tube side'
PAL(0|+:rz|-,0)=0;  #  at z=0; CO2 inlet concentration
PBL(0|+:rz|-,0)= 1; # at z=0;  amine inlet concentration
Partial(PAL(0|+:rz|-,Lc),axial)= 4*INTEGRAL(r:=0:1;r*(1-r^2)*PAL(0|+:rz|-,Lc)); #  at z=1
Partial(PBL(0|+:rz|-,Lc),axial)= 4*INTEGRAL(r:=0:1;r*(1-r^2)*PBL(0|+:rz|-,Lc)); # at z=1
#
PARTIAL(PAL(0,0:Lc),radial)=0; # at r=0  co2
PARTIAL(PBL(0,0:Lc),radial)=0; # at r=0  amine
PARTIAL(PAL(rz,0:Lc),radial)=Shext*(1-PAL(rz,0:Lc))/2; # at r=1  co2
PARTIAL(PBL(rz,0:Lc),radial)=0; # at r=1  amine

EQUATION
#tube side
  GRA = vza*di^2/(L*Dc);
  GRB = vza*di^2/(L*Dn);
  B1= L*kz*CT/vza;
  B2 = L*kz*m*Cog/vza;
  B3 = kzb/CT;  # kzb=k_z/KBi
  B4 = 4*keq*m*Cog;
  Shext = kex*di/Dag;
For r:= 0|+ TO rz|- DO
  For z:=0|+ TO Lc|- DO
    PARTIAL(PAL(r,z),axial)= (1/(1-r^2))*((2/GRA)*(PARTIAL(PAL(r,z),radial,radial)
        +(1/r)*PARTIAL(PAL(r,z),radial))-(1/2)*(B1/(B3+PBL(r,z)))*
        ((PAL(r,z)*(PBL(r,z)^2))-(1-PBL(r,z))^2/B4));
#
    PARTIAL(PBL(r,z),axial)= (1/(1-r^2))*((2/GRB)*(PARTIAL(PBL(r,z),radial,radial)
         +(1/r)*PARTIAL(PBL(r,z),radial))-(B2/(B3+PBL(r,z)))*
         ((PAL(r,z)*(PBL(r,z)^2))-(1-PBL(r,z))^2/B4));
  END
END
```

FIGURE F.6
gPROMs model.

CHEMICAL ENGINEERING

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