2. Process Modeling and Simulation

2.1 SYSTEMATIC APPROACH TO MODEL BUILDING

THE PROCESS SYSTEM AND THE MODELLING GOAL

- *A* system is a part of the real world with well-defined physical boundaries.

- A system is influenced by its surroundings or environment via its *inputs and generates influences* on its surroundings by its *outputs which occur through its boundary. This is seen in* Fig. 2.1.

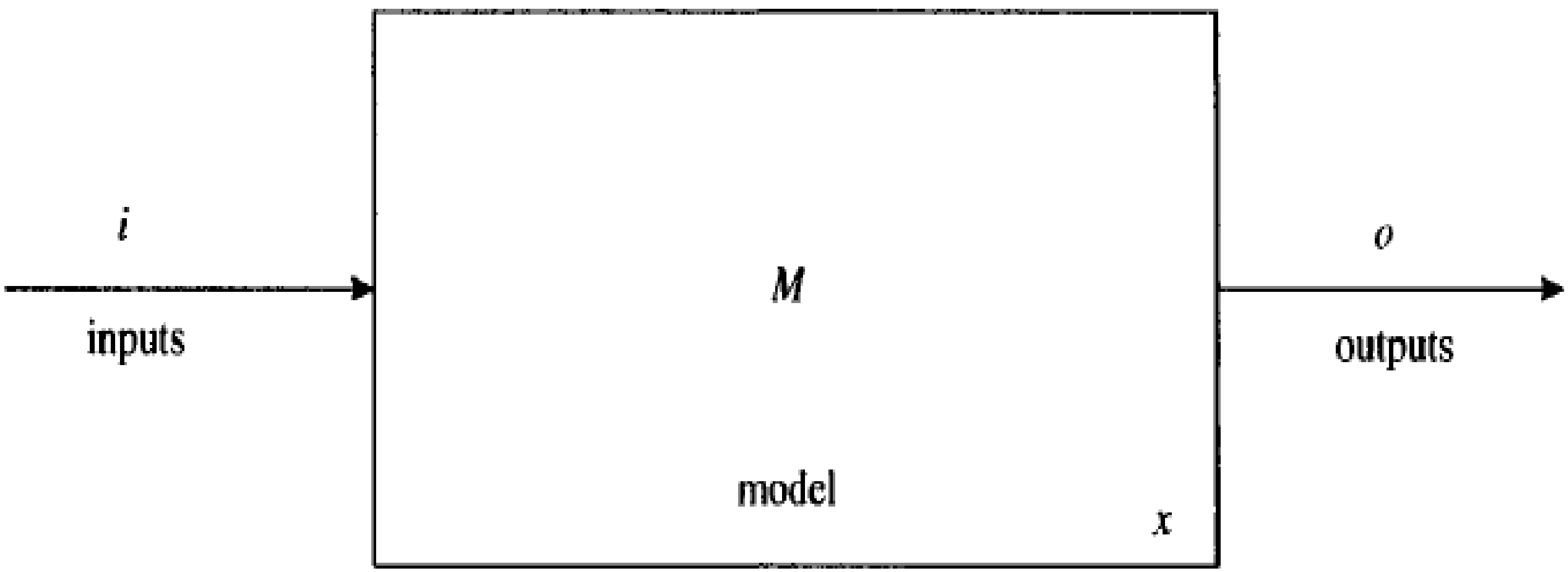


Fig. 2.1 General model schematic

- We are usually interested in the behavior of the system *in time* $t \in \mathcal{T}$

- *A system* is by nature a dynamic object.

- The system inputs *u and the system outputs y can be* single valued, giving a single input, single output (SISO) system.

- Alternately, the system can be a multiple input, multiple output (MIMO) system.

- Both inputs and outputs are assumed to be time dependent possibly vector-valued functions which we call ***signals***.

- *A system can be viewed as* ***an operator*** *in abstract mathematical sense* ***transforming*** **its inputs** ***u to its outputs y***.

- *The states of the system are* ***represented by the vector X*** *and are usually associated with the mass, energy and momentum holdups in the* system.

- ***A process system*** *is then a system in which physical and chemical processes are* taking place, these being the main interest to the modeller.

- The system to be modelled could be seen as **the whole process plant, its environment**, **part of the plant**, **an operating unit** or an item of equipment.

- Hence, to define our system we need to *specify its* ***boundaries****, its* ***inputs*** *and* ***outputs*** *and* ***the physicochemical processes*** *taking place within the system*

- Process systems are conventionally specified in terms *of* ***a flowsheet which defines the boundaries together with inputs and*** **outputs**.

- Information is normally available about the internal structure of the system in terms of the **operating units** and **their connections**.

The Modeling Goal

- The *modeling goal specifies the* ***intended use of the model****.*

- *The modeling goal has a* major impact on the **level of detail and on the mathematical form of the model** which will be built.

- The use of the model can take various forms depending upon what is assumed to be known and what is to be computed.

- Amongst the most important and widely use modeling goals in process engineering are the following:

- ***Dynamic simulation***

  – With the process model developed to **represent changes in time**, it is possible to predict the outputs *o* ***given all inputs i, the model structure M and parameters p****.*

- ***Static or steady-state simulation***

  – Here, the process system is **assumed to be at steady state**, representing an operating point of the system. Again the simulation problem computes the output values *o given* specific inputs i, a model structure *M and its parameters p. This is sometimes known* as a "rating" problem.

- ***Design problem***

  – Here, we are interested in **calculating the values of certain parameters p’ from the set of parameters p**, given known inputs i and desired outputs *o and a fixed structure* M.

  – This type of problem is normally solved using an optimization technique which finds the parameter values which generates the desired outputs.

  – It is also called a **"specification" problem**.

- ***Process control***
  - The fundamental problems in process control are to consider a dynamic process model together with measured inputs i and/or outputs *o in order to:*
    - design an input for which the system responds in a prescribed way, which gives a '***regulation or state driving control problem***'.

- find the structure of the model *M with its parameters p using the input and* output data, thus giving a ***system identification problem****;*

- *find the internal states in M given a structure for the model, thus giving a* **state estimation problem** *which is typically solved using a form of least squares* solution;

- find faulty modes and/or system parameters which correspond to measured input and output data, leading *to* ***fault detection and diagnosis problems****.*

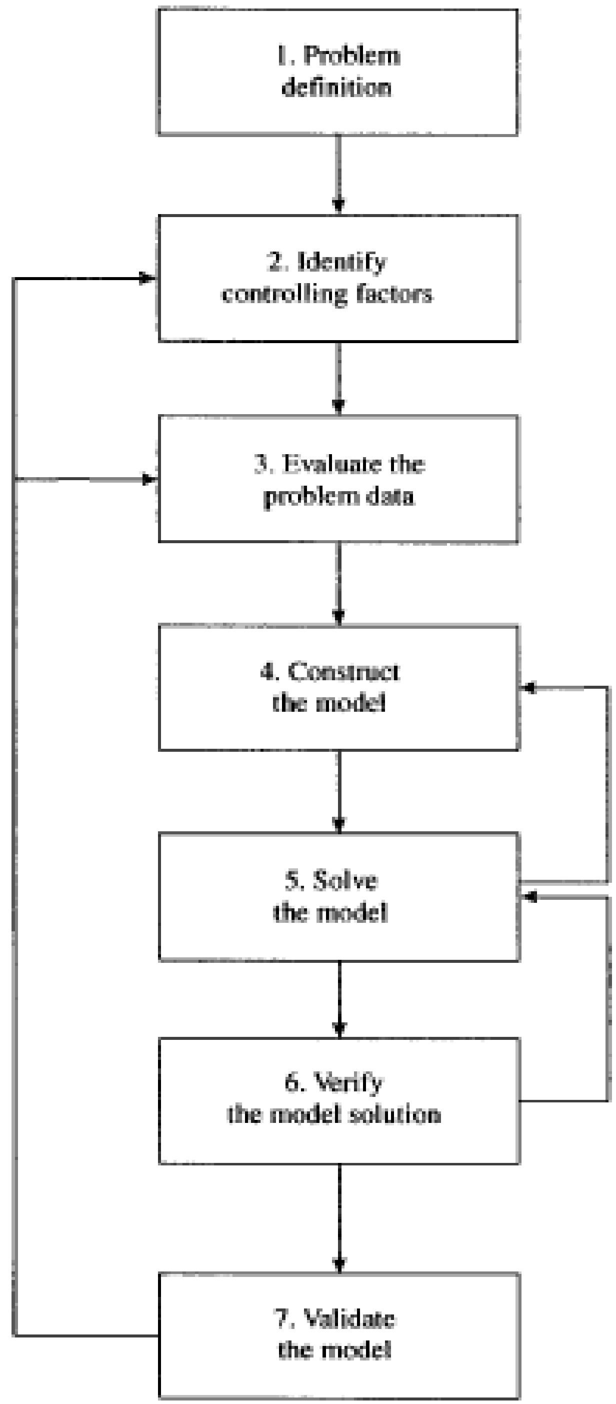
- It follows from the above *that a problem definition in process modeling should* contain at least two sections:
  - the **specification of the process system** to be modeled,
  - the **modeling goal**.

A SYSTEMATIC MODELLING PROCEDURE

- Like other engineering tasks, good practice requires models to be constructed following a well defined **sequence of steps**.

- These steps are arranged in a "Seven Step Modeling Procedure" which is introduced below and shown schematically in figure below.

- *Before starting to setup a process model the problem definition should be clearly stated. This defines the* ***process, the modeling goal and the validation criteria****.*


1. Problem definition
2. Identify controlling factors
3. Evaluate the problem data
4. Construct the model
5. Solve the model
6. Verify the model solution
7. Validate the model

1. Define the problem

- This step involves the description of the process system with the modeling goal. Moreover, it fixes the degree of detail relevant to the modeling goal and specifies:
  - inputs and outputs
  - hierarchy(ordered grouping) level relevant to the model or hierarchy levels of the model in the case of hierarchical models
  - the type of spatial distribution (distributed or lumped model)
  - the necessary range and accuracy of the model and
  - the time characteristics (static versus dynamic) of the process model.

2. *Identify the controlling factors or mechanisms*

- The next step is to investigate the physico-chemical processes and phenomena taking place in the system relevant to the modelling goal. These are termed *controlling factors or mechanisms. The most important and common controlling factors include:*

    - chemical reaction
    - diffusion of mass
    - conduction of heat
    - forced convection heat transfer
    - free convection heat transfer
    - radiation heat transfer
    - evaporation
    - turbulent mixing
    - heat or mass transfer through a boundary layer
    - fluid flow

3. *Evaluate the data for the problem*

- As it has been already noted, models of real process systems are of the grey-box type, therefore, we almost always need to use either measured process data directly or estimated parameter values in our models.

- *It is very important to consider both measured process data and parameter values together with their uncertainties or precision. Some default precision values* might be:
  - industrial measured data is ±10 to 30%,
  - estimated parameters from laboratory or pilot-plant data is ±5 to 20%,
  - reaction kinetic data is ±10 to 500%, if nothing else is specified.

- At this step, we may find out that there are neither suitable parameter values found in the literature nor measured data to estimate them.

- This situation may force us to reconsider our decisions in steps 1 and 2 and to return there to change them.

4. *Develop a set of model equations*

- The model equations in a process model are either differential (both partial and ordinary differential equations may appear) or algebraic equations.

- The *differential equations originate from conservation balances; therefore they can be termed **balance equations**.*

- *The algebraic equations are usually of mixed origin: they will be called **constitutive equations**.*

5. *Find and implement a solution procedure*

- Having set up a mathematical model, we must identify its mathematical form and find **or implement a solution procedure**.
- In all cases, we must ensure that the model is well posed such that the "excess" variables or **degrees of freedom are satisfied**.
- Lack of solution techniques may prevent a modeler using a particular type of process model and **can lead to additional simplifying assumptions to obtain a solvable model**.
- This can be the case with distributed parameter process models.

6. *Verify the model solution*

- Having a solution is just the start of the analysis. Verification is determining whether **the model is behaving correctly**.
- Is it coded correctly and giving you the answer you intended?
- This is not the same as model validation where we check the model against reality.
- You need to check carefully that the model is correctly implemented.

7. *Validate the model*

- Once a mathematical model has been set up, one should try to validate it. This checks the quality of the resultant model **against independent observations or assumption**s.

- Usually, **only partial validation** is carried out in practical cases depending on the modeling goal.

- There are various possibilities to validate a process model. The actual validation method strongly depends on the process system, on the modeling goal and on the possibilities of getting independent information for validation.

- The possibilities include but are not limited to:

  - verify experimentally the simplifying assumptions,
  - compare the model behavior with the process behavior,
  - develop analytical models for simplified cases and compare the behavior,
  - compare with other models using a common problem,
  - compare the model directly with process data.

- The tools to help carry out this task include the use of sensitivity studies to identify the key controlling inputs or system parameters as well as the use of statistical validation tests.

- These can involve hypothesis testing and the use of various measures such as averages, variances, maxima, minima and correlations. If the validation results show that **the developed model is not suitable for the modeling goal then one has to return to step 2 and perform the sequence again**.

- Usually, validation results indicate how to improve the model. We can often identify the **inadequate areas in our model development and, therefore, not all modeling efforts are lost**.

- Note that the final model is impossible to obtain in one pass through the modeling procedure. **Some iterations should be expected.**

- Step 4(***Develop a set of model equations)*** in the above SEVEN STEP MODELING PROCEDURE is a composite step in itself. It is broken down to sub-steps which are to be carried out sequentially but with inherent loops.

- The steps of this sub-procedure are as follows:

4.0 System and subsystem boundary and balance volume definitions

- The outcome of this step is the set of balance volumes for mass, energy and momentum leading to the conserved extensive quantities normally considered in process systems, such as total system mass, component masses or energy.

- In order to define the balance volumes we need to identify within our system the regions where mass, energy or momentum are likely to accumulate. These are termed the system "**holdups**".

- The accumulation of conserved quantities such as energy or mass are often dictated by the physical equipment or phase behavior within that equipment.

4.1. *Define the characterizing variables*

- Here, we need to define the **variables which will characterize the system being studied**.

- These variables are associated with the inputs, outputs and internal states of the system.

- The variable we use will be **strongly determined by our modelling goals.** For the inputs and outputs we can consider **component flows, total flow, mass or molar concentrations**.

- **Temperatures and pressures** may also be important, depending on whether energy is considered important.

- For the internal states of the system, the characterizing variables are related to the variables representing the main mass, energy and momentum holdups.

4.2. *Establish the balance equations*

- Here, we set up conservation balances for mass, energy and momentum for each balance volume.

4.3. *Transfer rate specifications*

- The rate expressions for **transfer of heat, mass and momentum between different balance volumes** in the conservation balances are specified here, usually as functions of intensive quantities, such as concentrations and temperature.

4.4. *Property relation specifications*

- These are mostly algebraic relationships expressing thermodynamic knowledge such as equations of state and the dependence of physico-chemical properties on thermodynamic state variables such as pressure, temperature and composition.

4.5. *Balance volume relation specifications*

- An equipment with a fixed physical volume is often divided into several balance volumes if multiple phases are present.
- A balance volume relation describes the relationship between balance volumes and physical volumes.

4.6. *Equipment and control constraint specifications*

- There is inevitably the need to define constraints on process systems.

- These are typically in the form of equipment operating constraints (for the pressures, temperatures etc.) and in terms of control constraints, which define relations between manipulated and controlled variables in the system.

4.7. *Modeling assumptions*

- When developing a particular model we apply modeling assumptions to get our model equations. These assumptions form an integral part of the resultant model.

- Therefore, they are regarded as *ingredients of a process model together with the* model equations, their initial and boundary conditions.

INGREDIENTS OF PROCESS MODELS

- The SEVEN STEP MODELLING PROCEDURE described above shows that a process model resulting from this procedure is not simply a set of equations.

- It incorporates a lot more information. In order to encourage the clarity of presentation and the consistency of the process model, a *structural presentation incorporating all key ingredients is very important*.

1. *Assumptions—which include but are not limited to*

- time characteristics
- spatial characteristics
- flow conditions
- controlling mechanisms or factors
- neglected dependencies, such as
  - temperature dependence of physico-chemical properties
  - concentration dependence of physico-chemical properties
- required range of states and associated accuracy

2. *Model equations and characterizing variables*

- Here, we have differential (balance) equations for
  - overall mass, component masses for all components for all phases in all equipment at all hierarchical levels (where applicable).
  - energy (or enthalpy),
  - momentum;
- constitutive equations for
  - *transfer rates: mass transfer, heat/energy transfer, and reaction rates,*
- *property relations: thermodynamical constraints and relations, such as the* dependence of thermodynamical properties on the thermodynamical state variables (temperature, pressure and compositions), equilibrium relations and state equations,

- *balance volume relations: relationships between the defined mass and energy* balance regions,
- equipment and control constraints; and the variables which characterize the system:
  - flows, temperatures, pressures, concentrations, enthalpies,
  - mass, energy and momentum holdups.

3. *Initial conditions (where applicable)*

- Initial conditions are needed for the differential (balance) equations in dynamic process models. Initial conditions for all algebraic variables are also important since most solutions are numerical.

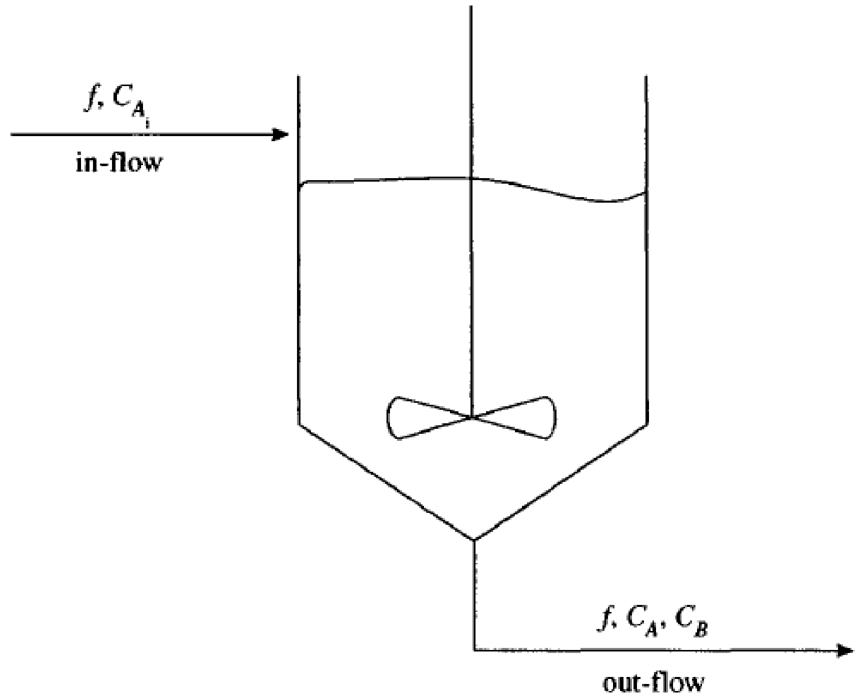
4. *Boundary conditions (where applicable)*

- Boundary conditions must be specified for the differential (balance) equations in spatially distributed process models.

5. *Parameters*

- As a result of step 3 in the SEVEN STEP MODELLING PROCEDURE the value and/or source of the model parameters are specified here with their units and precision. This also applies to all variables in the model.

- **EXAMPLE 2.1. (Modelling example: CSTR).**
  Develop a process model of the continuously stirred tank and with a single first-order chemical reaction taking place:



Flow sheet of CSTR

- The feed contains the reactant in an inert fluid.
- Let us assume that the tank is adiabatic, such that its wall is perfectly insulated from the surroundings.
- Let us model for dynamic prediction and control purposes following the SEVEN STEP MODELLING PROCEDURE with all of its ingredients

1. Problem definition

- The process system to be modeled is a continuously stirred tank with continuous fluid flow in and out and with a single first order chemical reaction A→ B taking place in an inert solvent.

- The tank is adiabatic with its wall perfectly insulated from the environment.

- The modeling goal is **to predict the behavior of the principal mass and energy states of the tank contents if the inlet concentration is changed over a stated range**.

- The accuracy of the predictions should be ±10% of the real process.

2. *Controlling factors or mechanisms*

- chemical reaction
- perfect mixing

3. *Data for the problem*

- No measured data is specified; therefore, we use the following parameter type data:
  - Reaction kinetic data, heat of reaction
  - physico-chemical properties
  - equipment parameters from the literature or given by the process documentation.

4. *Process model*

- *Assumptions:*
  - *perfect mixing,*
  - *constant physico-chemical properties*
  - equal inflow and outflow (implying constant liquid volume with V = *constant),*
  - *single first-order reaction, A →P,*
  - adiabatic operation.

Model equations and characterizing variables:

- *Differential (balance) equations in molar units*

$$\frac{dm_A}{dt} = f_{A_i} - f_A - rV,$$

$$V\rho c_p \frac{dT}{dt} = f c_{p_i} \rho_i (T_i - T) + rV(-\Delta H_R).$$

- *Constitutive equations*

$$r = k_0 \, e^{-E/(RT)} C_A,$$

$$m_A = C_A V,$$

$$f_{A_i} = f C_{A_i},$$

$$f_A = f C_A.$$

Variables

t	time [s]
C_A	concentration in the tank [mol/m^3]
V	liquid volume [m^3]
f	volumetric flowrate [m^3/s]
C_{A_i}	inlet concentration [mol/m^3]
r	reaction rate [mol/(s·m^3)]
c_p	specific heat of mixture [J/(mol K)]
c_{p_i}	specific heat of feed i [J/(mol K)]
T	temperature in the tank [K]
T_i	inlet temperature [K]
ΔH_R	heat of reaction [J/mol]
E	activation energy [J/mol]
k_0	pre-exponential factor [s^{-1}]
R	universal gas constant, 8.314 [J/(mol K)]
ρ	density of mixture [mol/m^3]

ρ_i	density of feed i [mol/m^3]
m_A	moles of A [mol]
f_{A_i}	inlet flowrate of species A [mol/s]

- **Initial conditions**

$$C_A(0) = C_{A_i}, \quad T(0) = T_i$$

- **Boundary conditions**
  - None
- **Parameters**
  - Values for the following parameters with 10% precision:

$$V,\ f,\ C_{A_i},\ T_i,\ c_p,\ c_{p_i},\ \rho,\ \rho_i$$

  - and for the reaction parameters with 30% precision:

$$k_0,\ E,\ \Delta H_R$$

5. *Solution procedure*

Solve using an ODE or differential-algebraic equation solver.

6. *Model verification*

Implement model equations using structured programming principles. Check code for correct execution. Check output trends against expected trends for reactor given step changes in feed variables. Also, check predicted steady-state values after a feed disturbance.

7. *Model validation*

Provide measured data from pilot plant or real process. Analyze plant data quality. Carry out validation of predicted outputs from step test of system using least squares estimation of error.