3. ADVANCED PROCESS MODELLING AND MODEL ANALYSIS

3.1. BASIC TOOLS FOR PROCESS MODEL ANALYSIS

- The analysis of process system models leads to **mathematical problems of various types**.

- It is convenient and useful to formulate these mathematical problems in a formal way **specifying the inputs to the problem, the desired output or question to be solved and indicate the procedure or method of solution**.

- Such a formal problem description can also be useful when we want to analyse **the computational needs of a mathematical problem** or one of its solution methods.

- Problem statements where a yes/no Question is to be answered are called **decision problems**, whilst problems with a Find/Compute section are termed **search problems**.

- In the Method or Procedure section the key steps in solving the problem are usually given in the form of a conceptual problem solution.

- The ingredients of a conceptual problem solution are as follows:

1. Solvability/feasibility analysis

- Here we answer the following key questions: Do we have a solution at all? If yes, is it unique?

2. Solution method (algorithm)

- Here we set out the way in which the output is computed or the approach for arriving at a decision.

3. Analysis of the problem and its solution method

- Here we provide an analysis of how many computational steps are needed for solution and how this number of steps depends on the problem size.

The Notion of a System, Linear and Time-Invariant Systems

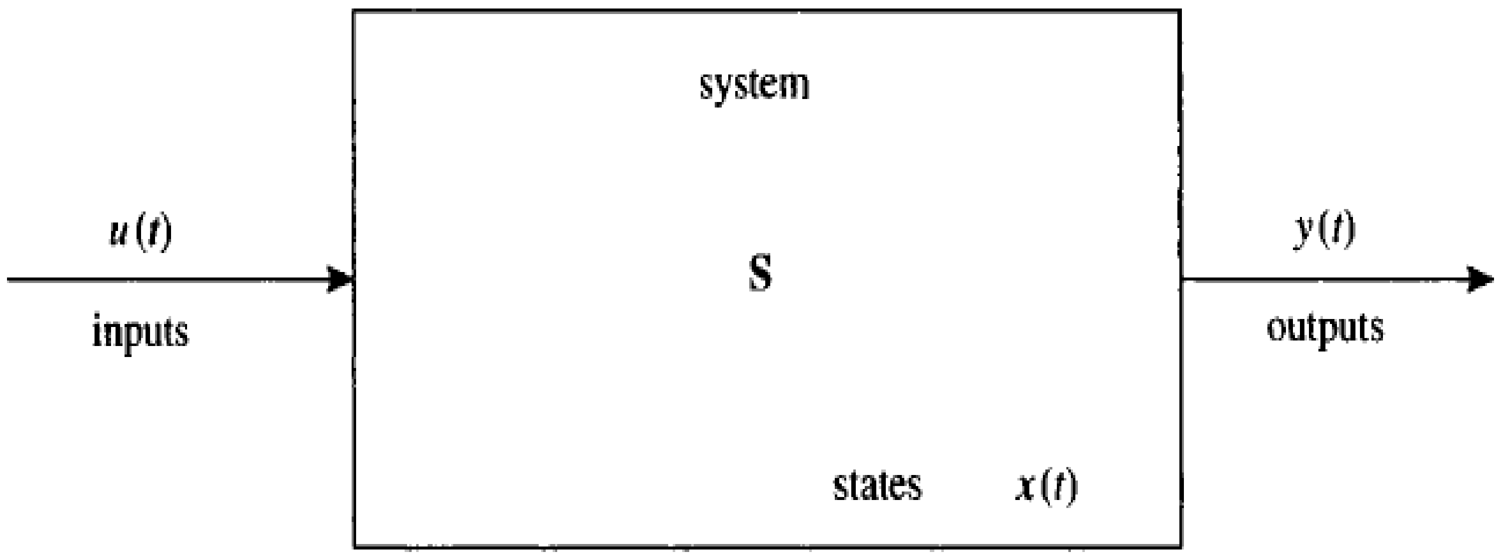
- We understand the system to be **part of the real world with a boundary between the system and its environment**.

- The system interacts with its environment only **through its boundary**.

- The effects of the environment on the system are described by time dependent ***input*** **functions** ***u(t)*** *from a given set of possible inputs* $u \in U$

- while the effect of the system on its environment is described by the ***output functions y(t)*** *taken from a set* of possible outputs $y \in y$.

-The schematic *signal flow diagram of a system S with its* input and output signals is shown in Fig. below



Signal flow diagram of a system

- The system can be described as an operator S which maps inputs u(t) into outputs y(t), expressed as:

$$\mathbf{S} : \mathcal{U} \rightarrow \mathcal{Y}, \quad y = \mathbf{S}[u].$$

- For process control applications, we often distinguish between manipulated input variables u(t) and disturbance variables d(t) within the set of input variables to the system.

- Both manipulated input and disturbance variables act upon the system to produce the system behavior.

- There are systems with special properties which are especially interesting and easy to handle from the viewpoint of their analysis and control. Here we investigate a number of these systems.

Linear Systems

- The first property of special interest is linearity. A system S is called *linear if it* responds to a linear combination of its possible input functions with the same linear combination of the corresponding output functions.
- Thus, for the linear system we note that

$$\mathbf{S}[c_1 u_1 + c_2 u_2] = c_1 y_1 + c_2 y_2$$

with $c_1, c_2 \in \mathcal{R}$, $u_1, u_2 \in \mathcal{U}$, $y_1, y_2 \in \mathcal{Y}$ and $\mathbf{S}[u_1] = y_1$, $\mathbf{S}[u_2] = y_2$.

Time-Invariant Systems

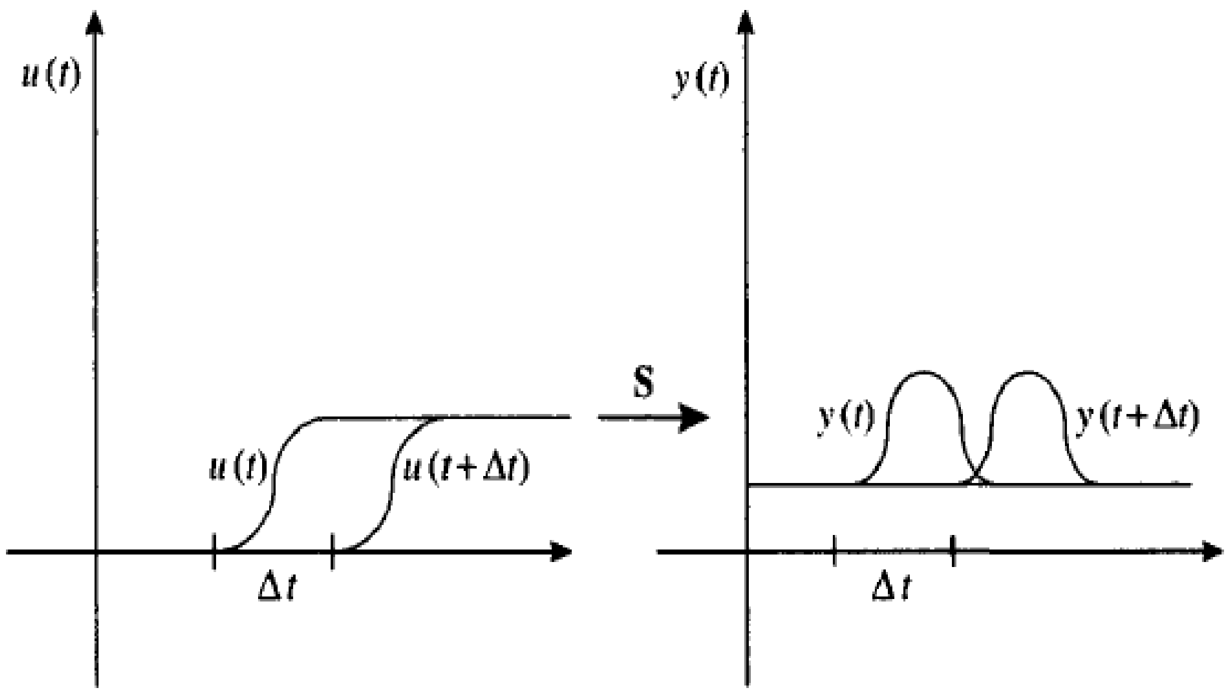
- The second interesting class of systems are time-invariant systems.

- A system S is time-invariant if its response to a given input is invariant under time shifting.

- Time-invariant systems do not change their system properties in time.

- If we were to repeat an experiment under the same circumstances at some later time, we get the same response as originally observed.

- The notion of time invariance is illustrated in Fig. below, where we see two identical inputs to the system separated by a time Δt and note that the time shifted outputs are also identical.



Notion of time invariance

- In many process system applications, this can be a reasonable assumption over a short time frame.

- In other cases, phenomena such as catalyst deactivation or heat transfer fouling lead to **non time-invariant systems**.

- An in-depth knowledge of the system mechanisms as well as the time frame of the intended analysis often resolves the validity of the time-invariant assumption.

- *Time-invariant systems have constant or time-independent parameters in their system models.*

- Linear and time-invariant systems are termed **LTI systems**

Different Descriptions of Linear Time-Invariant Systems

- The system S can be described in alternative ways :
  - in the time domain,
  - in the operator domain,
  - in the frequency domain.

- The operator and frequency domain description of systems is only used for linear systems, most frequently for LTI systems.

- These descriptions can be obtained by using Laplace transformation or Fourier transformation of the time domain description of systems to obtain the operator domain or frequency domain description respectively.

- Process models are naturally and conventionally set up in the time domain

- Continuous time LTI systems may be described in the time domain by
    - input-output models,
    - state space models.
- Input-output models are further subdivided into linear differential equation models and impulse response models.

Linear Differential Equations with Constant Coefficients

- If we consider the system input and output and their possibly higher order derivatives as

$$u(t), \frac{\mathrm{d}u}{\mathrm{d}t}, \frac{\mathrm{d}^2u}{\mathrm{d}t^2}, \ldots; \quad y(t), \frac{\mathrm{d}y}{\mathrm{d}t}, \frac{\mathrm{d}^2y}{\mathrm{d}t^2}, \ldots,$$

- the general form of the input-output model for an LTI SISO system is given by the following higher order linear differential equation with constant coefficients:

$$a_n \frac{d^n y}{dt^n} + a_{n-1} \frac{d^{n-1} y}{dt^{n-1}} + \cdots + a_1 \frac{dy}{dt} + a_0 y = b_0 u + b_1 \frac{du}{dt} + \cdots + b_r \frac{d^r u}{dt^r}.$$

State Space Representation

- Input-output representations describe the system with zero initial conditions.

- Given the assumption of zero initial condition, we needed the impulse response function h(t) or its Laplace transform, the transfer function H(s),
- state of the system at t_0 contains all past information on the system up to time t_0.

- To compute *y(t) for t* $\geq t_o$ *(all future values) we only need u(t), t* $> t_o$ *and* the state at t = t_0.

- The development of a state space model of a process system normally involves identifying a number of classes of variables in the system. These include:

- state variable vector $x \in \mathcal{R}^n$;
- (manipulable) input variable vector $u \in \mathcal{R}^l$ which is used to manipulate the states;
- disturbance variable vector $d \in \mathcal{R}^v$;
- output variable vector $y \in \mathcal{R}^m$ which is usually the measurements taken on the system. These can be directly related to the states.
- system parameter vector $p \in \mathcal{R}^w$.

- The general form of SSR or state space model of a MIMO LTI system without considering disturbances separately from manipulated inputs is in the following form:

$$\dot{x}(t) = \mathbf{A}x(t) + \mathbf{B}u(t), \quad \text{(state equation)},$$
$$y(t) = \mathbf{C}x(t) + \mathbf{D}u(t), \quad \text{(output equation)}$$

with given initial condition $x(t_0) = x(0)$ and

$$x(t) \in \mathcal{R}^n, \quad y(t) \in \mathcal{R}^m, \quad u(t) \in \mathcal{R}^r$$

being vectors of finite-dimensional spaces and

$$\mathbf{A} \in \mathcal{R}^{n \times n}, \quad \mathbf{B} \in \mathcal{R}^{n \times r}, \quad \mathbf{C} \in \mathcal{R}^{m \times n}, \quad \mathbf{D} \in \mathcal{R}^{m \times r}$$

- A is called a state matrix, B is the input matrix, C is the output matrix and D is the input-to-output coupling matrix.

- EXAMPLE (A simple stable SISO LTI system). Consider a simple LTI SISO system model in the form:

$$\frac{dx_1}{dt} = -4x_1 + 3x_2 + 7u_1,$$

$$\frac{dx_2}{dt} = 5x_1 - 6x_2 + 8u_1,$$

$$y = x_1.$$

1. Construct the state space model representation matrices.

- The standard matrix-vector form of the system model above is in the form of STATE SPACE Eq. with the following vectors and matrices

$$\dot{x}(t) = \mathbf{A}x(t) + \mathbf{B}u(t),$$
$$y(t) = \mathbf{C}x(t) + \mathbf{D}u(t),$$

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad u = [u_1], \quad y = [y],$$

$$\mathbf{A} = \begin{bmatrix} -4 & 3 \\ 5 & -6 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 7 \\ 8 \end{bmatrix}, \quad \mathbf{C} = [\ 1\ \ 0\ ], \quad \mathbf{D} = [0].$$

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LUMPED DYNAMIC MODELS AS DYNAMIC SYSTEM MODELS

- Lumped dynamic models are in the form of DAE systems where the

  - differential equations **originate from conservation balances of conserved extensive quantities** (mass, component masses, energy or momentum) for every balance volume;

  - algebraic equations are of mixed origin **derived from constitutive relations**. These are normally **nonlinear** algebraic equations. They are often of full structural rank indicating that the differential index of the DAE model is 1. Higher index models result when this system is rank deficient.

- Therefore, lumped dynamic models can be often transformed to set of explicit first-order NLDEs with given initial condition.

System Variables for Process Systems

- In order to develop a state space model of a process system, we need to identify the **system variables**.

- This includes the **state, input, disturbance and output variables** of the system. For process systems these choices are dictated by the development of the lumped parameter dynamic model of the process and by the setup of the measurements and any control system.

- More precisely, **state variables are fixed by the lumped parameter dynamic model** while input, disturbance and output variables are fixed **by the design, instrumentation and purpose of the model**. We now consider these variable categories.

State variables x(t)

- The differential equations in a lumped dynamic model **originate from conservation balances** for the conserved extensive quantities over each balance volume.

- As the state variables are the differential variables in these balance equations, the natural set of state variables of a process system **is the set of conserved extensive variables** or their intensive counterparts for each balance volume.

- This fact fixes the number of state variables. Hence, the dimension of the state space model is **equal to the number of conserved extensive quantities**.

- If there are c components in the system, then in general we can write c component mass balances for each species plus an energy balance.

- Thus, the total number of states n is obtained by multiplying (c + 1) by the number of balance volumes n_{Σ}: $n = (c+1)n_{\Sigma}$

- Moreover the physical meaning of the state variables is also fixed by this correspondence.

Manipulated input and disturbance variables u(t), d(t)

- In order to identify potential input variables and disturbances one should look carefully at the process to identify **all dynamic effects from the environment which act upon the system** to affect its behaviour.

- Those potential input variables which can be influenced by a device such as a control valve through an instrumentation system or changed manually **form the set of potential manipulated input variables.**

- The actual **purpose of the modelling decides which variables will be regarded as actual disturbances and manipulated input variables** from the overall set.

- Typically, the following type of signals are used as manipulated input variables in a process system:
  - flowrates,
  - split and recycle ratios,
  - utility flowrates and temperatures,
  - pressures,
  - current and voltage controlling heaters, shaft rotation, motors or valves.
  - switches.

Output variables, y(t)

- The set of potential output variables is fixed by the measurement devices and each measured variable can be regarded as an output of the system.

- The modelling goal is the one which finally **determines which variables are actually used for a given purpose from the possible set**.

- Typically, the following types of signals are used as output variables in a process system:
  - temperatures,
  - pressures,
  - concentration related physical quantities like mole or mass fraction,
  - level related physical quantities like weight, head or total mass,
  - flowrate related physical quantities.

EXAMPLE (Nonlinear state space model form of a CSTR model). Consider the nonlinear model describing the dynamics of a non-isothermal CSTR.

- The reaction is first order, A —> B and is exothermic.
- The reactor is cooled by coolant at temperature Tc.
- The feed is at temperature Ti. It is assumed that the physical properties remain constant and that inlet and outlet flows are equal.

- The mass and energy balances lead to the following equations:

$$V\frac{\mathrm{d}C_A}{\mathrm{d}t} = FC_{A_\mathrm{i}} - FC_A - kVC_A,$$

$$V\rho c_P\frac{\mathrm{d}T}{\mathrm{d}t} = F\rho c_P(T_\mathrm{i} - T) + kVC_A(-\Delta H_\mathrm{R}) - UA(T - T_\mathrm{C})$$

with the volume *V being constant.*

- These can be rearranged to give

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = \frac{F}{V}(C_{A_\mathrm{i}} - C_A) - kC_A,$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{F}{V}(T_\mathrm{i} - T) + \frac{kC_A}{\rho c_P}(-\Delta H_\mathrm{R}) - \frac{UA}{V\rho c_P}(T - T_\mathrm{C}).$$

- Now the *state variables of the nonlinear state space model of the CSTR are*

$$x = [C_A, T]^{\mathrm{T}}$$

- Let us select the flowrate and the coolant temperature as manipulated input variables, thus:

$$u = [F, T_{\mathrm{C}}]^{\mathrm{T}}$$

Constructing a Nonlinear State Space Model from Lumped Dynamic Model

- The construction is done in the following Steps:

1. **Transform the model equations**

   Take the lumped process model with its balance and constitutive equations. Making use of the equation structure of the constitutive algebraic part, we substitute the algebraic equations into the differential ones.

2. **State equations and state variables**

   The transformed differential balance equations will form the set of state equations with the differential variables being the state variables of the system.

3**. Potential input variables**

The potential input variables are the time-dependent variables on the right `hand side of the transformed model equations (state equations) which are *not* state variables and affect the variation of the state variables.

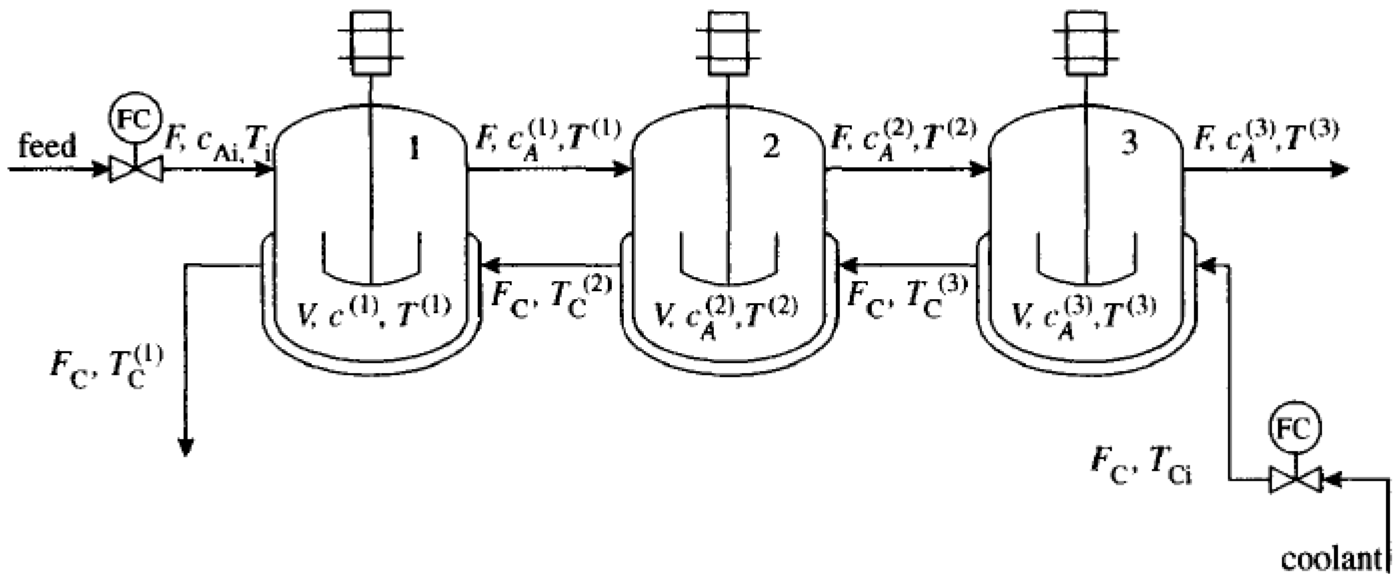
4. **Manipulable input variables and disturbances**

- From the set of input variables, we can select those which can be directly manipulable based on the instrumentation diagram of the flowsheet and based on the modelling goal. The rest are regarded as disturbance variables.

5. **Output variables and output equations**

- Using the instrumentation diagram, we can find out the quantities we measure for the system and their relationship to the state variables. These will be the output variables. Their relationships to state (and sometimes to input) variables form the output equations.

- EXAMPLE (State space model of three jacketted CSTRs in series). Consider a process system consisting of three jacketted CSTRs in series with cooling provided in a countercurrent direction. The cascade is shown in Fig. below.



- Develop the nonlinear state space model of the system from its lumped dynamic system model.

- Assumptions

A 1 . Perfect mixing in each of the tanks and in their jackets.

A2. There is a single first-order A -> B exothermic reaction with the reaction rate

$$r_A = kC_A \quad \left[\frac{\text{kmol}}{\text{s m}^3}\right]$$

A3. The reaction rate coefficient k obeys Arrhenius law, i.e.

$$k = k_0 \, \mathrm{e}^{-E/(RT)}$$

- A4. The volume of the mixture in the reactors and that in the cooling jackets is constant.
- A5 . The corresponding volumes and heat transfer area in the three CSTRs are the same.
- A6. Countercurrent flow of the reaction mixture and the cooling water.
- A7. The heat capacity of the wall is negligible.
- A8. The physico-chemical properties are constant.

- **Model equations**

The dynamic model of the ith CSTR consists of the following balances:

- *Component mass balance for component A in the reactor*

$$V\frac{dC_A^{(i)}}{dt} = FC_A^{(i-1)} - FC_A^{(i)} - VC_A^{(i)}k_0e^{-E/RT}.$$

- *Energy balance of the reaction mixture*

$$c_P\rho V\frac{dT^{(i)}}{dt} = c_P\rho FT^{(i-1)} - c_P\rho FT^{(i)} - \Delta HVC_A^{(i)}k_0\,e^{-E/RT} + K_TA(T_C^{(i)} - T^{(i)})$$

- Energy balance for the water in the jacket

$$c_{PC}\rho_C V_C \frac{dT_C^{(i)}}{dt} = c_{PC}\rho_C F_C T_C^{(i+1)} - c_{PC}\rho_C F_c T_C^{(i)} + K_T A(T^{(i)} - T_C^{(i)})$$

- The following "boundary conditions" specify the inlet and the outlet conditions for the reaction mixture and the cooling water respectively:

$$C_A^{(0)} = C_{A_i}, \quad T^{(0)} = T_i, \quad T_C^{(4)} = T_{C_i}$$

- Moreover, we need proper initial conditions for every differential variable at time t = 0

$$C_A^{(i)}(0), \quad T^{(i)}(0), \quad T_C^{(i)}(0), \quad i = 1, 2, 3.$$

- *State variables and state equations*

  The state variables of the system consisting of the three jacketted CSTRs are dictated by the balance equations to be

$$x = \left[C_A^{(i)}, T^{(i)}, T_C^{(i)} \mid i = 1, 2, 3 \right]^T$$

- *Input and output variables*

  The potential input variables are the non-differential variables on the right-hand side of the balance equations which affect its solution, can vary in time and possibly can be manipulated:

$$C_A^{(0)} = C_{A_i}, \quad T^{(0)} = T_i, \quad T_C^{(4)} = T_{Ci}, \quad F, \quad F_C.$$

- Let us assume that the flowrates are kept constant, therefore, the vector of potential input variables is

$$u^* = [C_{Ai},\ T_i,\ T_{C_i}]^T$$

- The set of possible output variables is the same as the vector of state variables if we assume that the concentration of component A can be directly measured, i.e.

$$y^* = x.$$

STATE SPACE MODELS AND MODEL LINEARIZATION

- Almost without exception, process models are nonlinear in their form. Nonlinear models **are difficult to analyse directly**, since **there is little nonlinear analysis theory** which is easy to apply.

- Also many models are used at, or nearby to a particular operating point and as such **a linear form of the model may be adequate for analysis purposes**, providing we do not use it far from the intended point of operation.

- There is also the fact that **many powerful and extensive linear analysis tools are available** to the process engineer. These include tools for assessing performance and designing control systems based on linear systems theory. In the area of control design, the use of linear models dominates the available techniques.

- Hence, **it can be beneficial and even vital to develop linear approximations to the original nonlinear model**.

Linearization of Single Variable Differential Equations

- Most of the models which we develop are nonlinear, since terms in the equations are raised to a power or multiplied together.

- We usually refer to the model as being "nonlinear in certain variables". Some variables may occur in a linear form such as cx where c is a constant or in nonlinear form such as cX^2, or cX_1X_2.

- Example

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{1}{A}\left\{C_{v_1}(P_1 - P_0 - \rho g h)^{1/2} - C_{v_2}(P_0 + \rho g h - P_3)^{1/2}\right\}$$

- *Is Non-linear with h.*

$$\frac{\mathrm{d}T_s}{\mathrm{d}t} = \frac{1}{\tau}(T - T_s)$$ *is linear with respect to Ts.*

- Linearization is based on the application of Taylor's expansion about a particular operating point. For the general dynamic model in one variable, *x we can write:*

$$\frac{dx}{dt} = f(x, t)$$

- and the expansion of the nonlinear function f(x,t) gives

$$f(x, t) = f(x_0, t) + \left.\frac{df}{dx}\right|_{x_0} (x - x_0) + \left.\frac{d^2 f}{dx^2}\right|_{x_0} \frac{(x - x_0)^2}{2!} + \cdots ,$$

where x_0 is the operating point and $d^i f/dx^i$ is the ith derivative of f with respect to x evaluated at x_0.

- If we truncate after the first derivative, we obtain the linear approximation

$$f(x,t) \simeq f(x_0,t) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} (x - x_0)$$

- and so the original equation can be written as

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x_0,t) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} (x - x_0),$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\hat{x} + x_0) = f(x_0,t) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} (x - x_0),$$

since

$$\frac{\mathrm{d}x_0}{\mathrm{d}t} = f(x_0,t) \quad \text{and} \quad \hat{x} = x - x_0,$$

we can subtract this to get

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} (\hat{x}); \quad \hat{x}(0) = 0,$$

- Which is our final linearized state space equation in the deviation variable x’.

- Often we drop the terminology x’ and simply write x, noting that this is a deviation variable.

Multi-variable Linearization

- We can extend the single variable linearization to the case where we have many variables in our model. Hence, consider the set of ODEs given by

$$\frac{dx}{dt} = f(x)$$

$$\begin{aligned}
\frac{dx_1}{dt} &= f_1(x_1, x_2, x_3, \ldots, x_n), \\
\frac{dx_2}{dt} &= f_2(x_1, x_2, x_3, \ldots, x_n), \\
&\vdots \\
\frac{dx_n}{dt} &= f_3(x_1, x_2, x_3, \ldots, x_n).
\end{aligned}$$

- Linearization means expanding the right-hand sides as a multi-variable Taylor series.

- which can be expanded about the point

$(x_{1_0}, x_{2_0}, \ldots, x_{n_0})$ to give:

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} \cong f_1(x_0) + \left.\frac{\partial f_1}{\partial x_1}\right|_{x_{1_0}} (x_1 - x_{1_0}) + \cdots + \left.\frac{\partial f_1}{\partial x_n}\right|_{x_{n_0}} (x_n - x_{n_0})$$

$$= f_1(x_0) + \sum_{j=1}^{n} \left.\frac{\partial f_1}{\partial x_j}\right|_{x_{j_0}} (x_j - x_{j_0}).$$

If we do this for all equations (1 , . . . , n) we obtain

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = f_i(x_0) + \sum_{j=1}^{n} \left.\frac{\partial f_i}{\partial x_j}\right|_{x_{j_0}} (x_j - x_{j_0}), \quad i = 1, \ldots, n.$$

- Finally, writing the linearized equations in deviation variable form we get

$$\frac{\mathrm{d}\hat{x}_i}{\mathrm{d}t} = \sum_{j=1}^{n} \frac{\partial f_i}{\partial x_j}\bigg|_{x_{j0}} (\hat{x}_i), \quad i = 1, \ldots, n.$$

- If we collect all *n equations together in matrix-vector form we obtain*

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{x} = \mathbf{J}\hat{x},$$

- where J is the system Jacobian (matrix of partial derivatives) evaluated at the steady state point Xjo.

$$\mathbf{J} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

Linearized State Space Equation Forms

- When we develop models of process systems we usually end up with a nonlinear set of differential equations accompanied by a set of algebraic equations.

- If we consider the state space model LTI system written in deviation variable form, then the state space matrices are **the partial derivatives of the state and output equations with respect to the state and the input variables** as follows:

$$\mathbf{A} = \left.\frac{\partial f}{\partial x}\right|_{x_0, u_0} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix},$$

$$\mathbf{B} = \left.\frac{\partial f}{\partial u}\right|_{x_0, u_0} = \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \cdots & \frac{\partial f_1}{\partial u_r} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \cdots & \frac{\partial f_2}{\partial u_r} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial f_n}{\partial u_1} & \frac{\partial f_n}{\partial u_2} & \cdots & \frac{\partial f_n}{\partial u_r} \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1r} \\ b_{21} & b_{22} & \dots & b_{2r} \\ \vdots & \vdots & \dots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nr} \end{pmatrix},$$

$$\mathbf{C} = \frac{\partial h}{\partial x}\bigg|_{x_0, u_0} = \begin{pmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & \cdots & \frac{\partial h_1}{\partial x_n} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & \cdots & \frac{\partial h_2}{\partial x_n} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial h_m}{\partial x_1} & \frac{\partial h_m}{\partial x_2} & \cdots & \frac{\partial h_m}{\partial x_m} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{pmatrix},$$

$$\mathbf{D} = \frac{\partial h}{\partial u}\bigg|_{x_0, u_0} = \begin{pmatrix} \frac{\partial h_1}{\partial u_1} & \frac{\partial h_1}{\partial u_2} & \cdots & \frac{\partial h_1}{\partial u_r} \\ \frac{\partial h_2}{\partial u_1} & \frac{\partial h_2}{\partial u_2} & \cdots & \frac{\partial h_2}{\partial u_r} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial h_m}{\partial u_1} & \frac{\partial h_m}{\partial u_2} & \cdots & \frac{\partial h_m}{\partial u_r} \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & \cdots & d_{1r} \\ d_{21} & d_{22} & \cdots & d_{2r} \\ \vdots & \vdots & \cdots & \vdots \\ d_{m1} & d_{m2} & \cdots & d_{mr} \end{pmatrix}$$

- EXAMPLE (Linearization of a CSTR model). Consider the nonlinear model describing the dynamics of a non-isothermal CSTR. The reaction is first order, *A —> B and is exothermic.* The reactor is cooled by coolant at temperature *TQ, It is assumed that the physical* properties remain constant and that inlet and outlet flows are equal.
- The mass and energy balances lead to the following equations:

$$V\frac{dC_A}{dt} = FC_{A_i} - FC_A - kVC_A,$$

$$V\rho c_P\frac{dT}{dt} = F\rho c_P(T_i - T) + kVC_A(-\Delta H_R) - UA(T - T_C).$$

- These can be rearranged to give

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A_i} - C_A) - kC_A,$$

$$\frac{dT}{dt} = \frac{F}{V}(T_i - T) + \frac{kC_A}{\rho c_P}(-\Delta H_R) - \frac{UA}{V\rho c_P}(T - T_C).$$

- Now we linearize the equations above in the following steps:
  - *First, we can classify the variables within the nonlinear state space formulation* as

$$x = [C_A, T]^{\mathrm{T}}, \quad y = [C_A, T]^{\mathrm{T}}, \quad u = [F, T_{\mathrm{C}}]^{\mathrm{T}}$$

other choices for *u are possible.*

  - *Second, convert the original nonlinear ODEs into linear state space form.*

The partial derivatives with respect to the states *x are given by*

$$\frac{\partial f_1}{\partial x_1} = \frac{\partial}{\partial C_A}\left(\frac{F}{V}(C_{A_i} - C_A)\right) - \frac{\partial}{\partial C_A}(kC_A)$$

$$= -\frac{F}{V} - k_0\,\mathrm{e}^{-E/(RT_0)},$$

$$\frac{\partial f_1}{\partial x_2} = \frac{\partial}{\partial T}\left(\frac{F}{V}(C_{A_i} - C_A)\right) - \frac{\partial}{\partial T}(kC_A)$$

$$= -k_0\left(\frac{E}{RT_0^2}\right)\mathrm{e}^{-E/(RT_0)}C_{A_0}.$$

$$
\begin{aligned}
\frac{\partial f_2}{\partial x_1} &= \frac{\partial}{\partial C_A}\left(\frac{F}{V}(T_{\mathrm{i}} - T)\right) + \frac{\partial}{\partial C_A}\left(\frac{kC_A}{\rho c_P}(-\Delta H_{\mathrm{R}})\right) \\
&\quad - \frac{\partial}{\partial C_A}\left(\frac{UA}{V\rho c_P}(T - T_{\mathrm{C}})\right) \\
&= \frac{k}{\rho c_P}(-\Delta H_{\mathrm{R}}) \\
&= \frac{k_0\,\mathrm{e}^{-E/(RT_0)}}{\rho c_P}(-\Delta H_{\mathrm{R}}),
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial f_2}{\partial x_2} &= \frac{\partial}{\partial T}\left(\frac{F}{V}(T_{\mathrm{i}} - T)\right) + \frac{\partial}{\partial T}\left(\frac{kC_A}{\rho c_P}(-\Delta H_{\mathrm{R}})\right) \\
&\quad - \frac{\partial}{\partial T}\left(\frac{UA}{V\rho c_P}(T - T_{\mathrm{C}})\right) \\
&= -\frac{F}{V} + k_0\left(\frac{E}{RT_0^2}\right)\mathrm{e}^{-E/(RT_0)} C_{A_0}\frac{(-\Delta H_{\mathrm{R}})}{\rho c_P} - \frac{UA}{V\rho c_P}.
\end{aligned}
$$

- The partial derivatives with respect to the inputs *u are*

$$\frac{\partial f_1}{\partial u_1} = \frac{\partial}{\partial F}\left(\frac{F}{V}(C_{A_i} - C_A)\right) - \frac{\partial}{\partial F}(kC_A)$$

$$= \frac{(C_{A_i} - C_{A_0})}{V},$$

$$\frac{\partial f_1}{\partial u_2} = \frac{\partial}{\partial T_C}\left(\frac{F}{V}(C_{A_i} - C_A)\right) - \frac{\partial}{\partial T_C}(kC_A)$$

$$= 0,$$

$$\frac{\partial f_2}{\partial u_1} = \frac{\partial}{\partial F}\left(\frac{F}{V}(T_i - T)\right) + \frac{\partial}{\partial F}\left(\frac{kC_A}{\rho c_P}(-\Delta H_R)\right)$$

$$- \frac{\partial}{\partial F}\left(\frac{UA}{V\rho c_P}(T - T_C)\right)$$

$$= \frac{(T_i - T)}{V},$$

$$\frac{\partial f_1}{\partial u_2} = \frac{\partial}{\partial T_C}\left(\frac{F}{V}(C_{A_i} - C_A)\right) - \frac{\partial}{\partial T_C}(kC_A)$$

$$= 0,$$

$$\frac{\partial f_2}{\partial u_1} = \frac{\partial}{\partial F}\left(\frac{F}{V}(T_i - T)\right) + \frac{\partial}{\partial F}\left(\frac{kC_A}{\rho c_P}(-\Delta H_R)\right)$$

$$- \frac{\partial}{\partial F}\left(\frac{UA}{V\rho c_P}(T - T_C)\right)$$

$$= \frac{(T_i - T)}{V},$$

$$\frac{\partial f_2}{\partial u_2} = \frac{\partial}{\partial T_C}\left(\frac{F}{V}(T_i - T)\right) + \frac{\partial}{\partial T_C}\left(\frac{kC_A}{\rho c_P}(-\Delta H_R)\right)$$

$$- \frac{\partial}{\partial T_C}\left(\frac{UA}{V\rho c_P}(T - T_C)\right)$$

$$= \frac{UA}{V\rho c_P.}$$

- *Finally, write the state space equations in deviation variable form as*

$$\begin{bmatrix} \frac{d\hat{C}_A}{dt} \\ \frac{d\hat{T}}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{F}{V} - k_0 e^{-E/(RT_0)} & -k_0 \left(\frac{E}{RT_0^2}\right) e^{-E/(RT_0)} C_{A_0} \\ +\frac{k_0 e^{-E/(RT_0)}(-\Delta H_R)}{\rho c_P} & -\frac{F}{V} + k_0 \left(\frac{E}{RT_0^2}\right) e^{-E/(RT_0)} C_{A_0} \frac{(-\Delta H_R)}{\rho c_P} - \frac{UA}{V \rho c_P} \end{bmatrix} \begin{bmatrix} \hat{C}_A \\ \hat{T} \end{bmatrix}$$

$$+ \begin{bmatrix} \frac{(C_{A_i} - C_{A_0})}{V} & 0 \\ \frac{(T_i - T_0)}{V} & \frac{UA}{V \rho c_P} \end{bmatrix} \begin{bmatrix} \hat{F} \\ \hat{T}_C \end{bmatrix}.$$