

2.2. DYNAMIC MODELS—LUMPED PARAMETER SYSTEMS

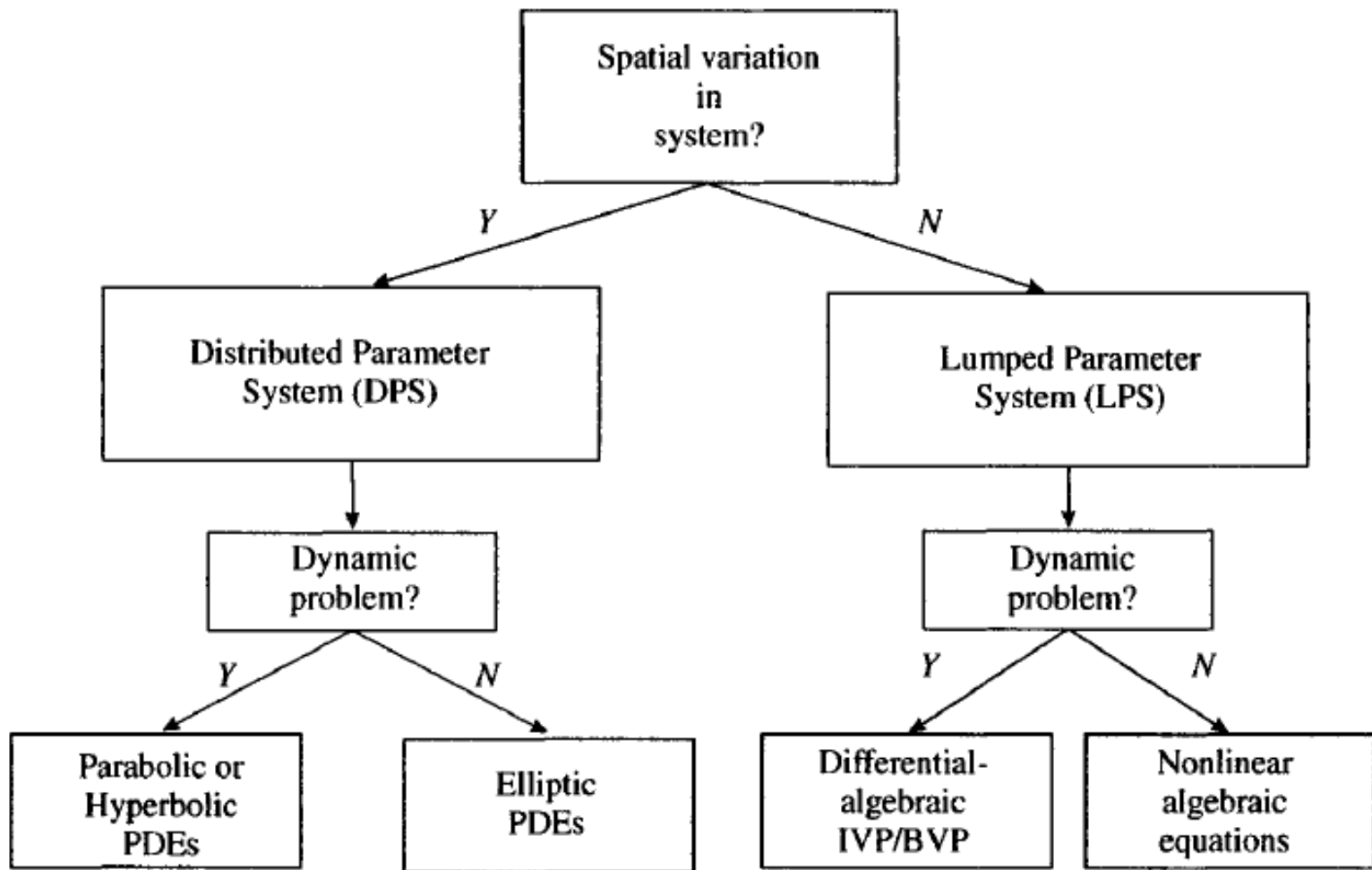
- This section focused on the underlying modelling principles for **lumped parameter systems (LPSs)** and the subsequent analysis of those models.
- Here, we are concerned about the **time varying behaviour of systems which are considered to have states which are homogeneous within the balance volume V**. Hence, the concept of "lumping" the scalar field into a representative single state value.
- Sometimes the term "**well mixed**" is applied to such systems where the **spatial variation** in the scalar field, which describes the state of interest, **is uniform**.
- In some cases, we may also consider the stationary behaviour of such systems which leads to **steady state model** descriptions.

- Lumped parameter dynamic models, or compartmental models are widely used **for control and diagnostic purposes**.
- They are frequently used as the basis for **engineering design**, startup and shutdown studies as well as **assessing safe operating procedures**.

Dynamic Models

- In terms of dynamic models we have two clearly identifiable classes:
 - distributed parameter dynamic models,
 - lumped parameter dynamic models.
- In the above classes, we identify the distributed parameter dynamic models with various forms of PDEs, principally **parabolic partial differential equations (PPDEs)**.

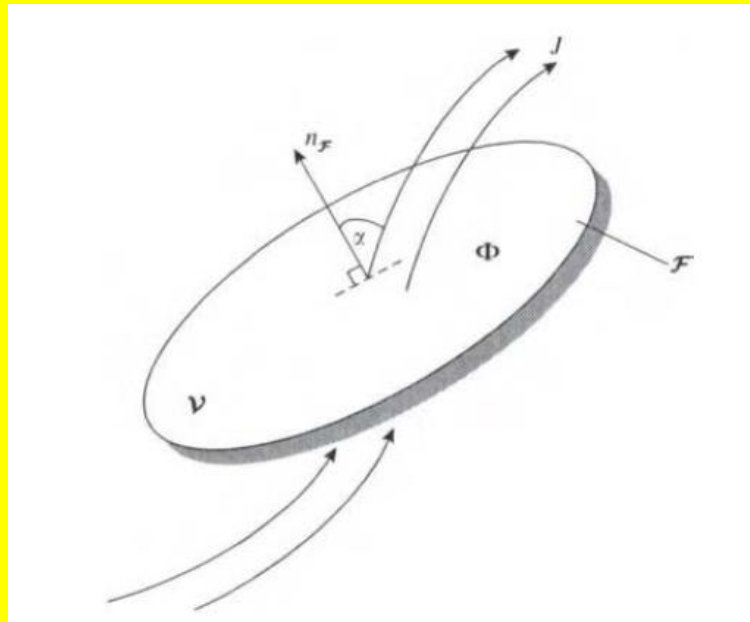
- The lumped parameter dynamic models result in **systems of ODEs often coupled with many nonlinear and linear algebraic constraints.**
- The total system is referred to as a **differential-algebraic equation (DAE) set.** The equations need to have a specified set of consistent initial conditions for all states.
- This can be a challenging problem due to the effects of the nonlinear constraints which can impose **extra conditions on the choice of initial values.**



Classification of Models

PRINCIPLE OF CONSERVATION

- As a result of the first law of thermodynamics, energy is conserved within a system, although it may change its form.
- Also, both mass and momentum in the system will be conserved quantities in any space. In most process systems, we deal with **open systems where mass, energy and momentum can flow across the boundary surface.**
- As such, we can consider a space with volume V and boundary surface T *as shown* in Fig.



General balance volume V

$$\left\{ \begin{array}{l} \text{net change} \\ \text{of quantity in time} \end{array} \right\} = \left\{ \begin{array}{l} \text{flow in} \\ \text{through boundary} \end{array} \right\} - \left\{ \begin{array}{l} \text{flow out} \\ \text{through boundary} \end{array} \right\} \\ + \left\{ \begin{array}{l} \text{net} \\ \text{generation} \end{array} \right\} - \left\{ \begin{array}{l} \text{net} \\ \text{consumption} \end{array} \right\}.$$

Lumped Conservation Balances

- Lumped parameter models **do *not incorporate the spatial variation of states within*** the balance volume; therefore, the scalar field of the intensive quantities (most often concentrations or temperature) is a **function of time only**.
- What this means is that the application of the general conservation equations leads to models which are **represented by ODEs in time**.
- Moreover, the closed boundary surface encapsulating the balance volume is also **homogeneous in space**.

Total Mass Balance

- The general expression for a *total mass balance* can be written in word form as:

$$\left\{ \begin{array}{c} \text{rate of accumulation} \\ \text{of mass} \end{array} \right\} = \left\{ \begin{array}{c} \text{mass flow} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{c} \text{mass flow} \\ \text{out} \end{array} \right\}$$

- or in the case of a lumped parameter system, the equation form for *p input streams* and *q output streams* is

$$\frac{dM}{dt} = \sum_{j=1}^p F_j - \sum_{k=1}^q F_k$$

Component Mass Balances

$$\left\{ \begin{array}{l} \text{rate of mass accumulation} \\ \text{of component } i \end{array} \right\} = \left\{ \begin{array}{l} \text{mass flow in of} \\ \text{component } i \end{array} \right\} - \left\{ \begin{array}{l} \text{mass flow out of} \\ \text{component } i \end{array} \right\} + \left\{ \begin{array}{l} \text{rate of formation or consumption} \\ \text{of component } i \end{array} \right\}$$

- Where the last term accounts for the creation or disappearance of component i via chemical reaction.
- In the case of an LPS, we have the general equation in the form

$$\frac{dm_i}{dt} = \sum_{j=1}^p f_{i,j} - \sum_{k=1}^q f_{i,k} + g_i, \quad i = 1, \dots, n,$$

- Where m_i is the mass holdup of component i within the balance volume V , j is the stream number and g_i is the mass rate of generation or consumption of species i in the balance volume due to reaction.

- We can also write the general mass balance in molar terms n_i by introducing the molar flowrates instead of the mass flowrates of species i in stream j .
- *The general molar balance is written as*

$$\frac{dn_i}{dt} = \sum_{j=1}^p \tilde{f}_{i,j} - \sum_{k=1}^q \tilde{f}_{i,k} + \tilde{g}_i, \quad i = 1, \dots, n.$$

Total Energy Balance

- The general conservation balance for total energy over the balance volume V with surface is given by

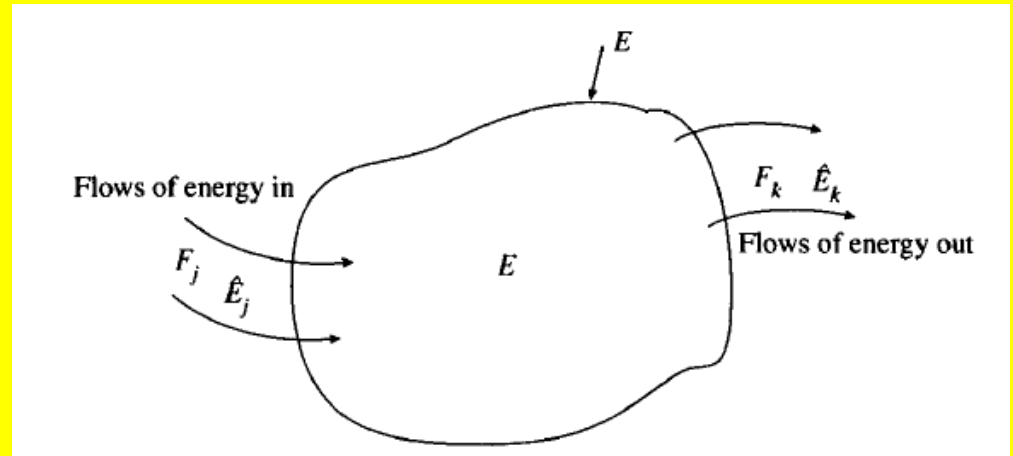
$$\left\{ \begin{array}{l} \text{rate of change} \\ \text{of total energy} \end{array} \right\} = \left\{ \begin{array}{l} \text{flow of energy} \\ \text{into the system} \end{array} \right\} - \left\{ \begin{array}{l} \text{flow of energy} \\ \text{out of system} \end{array} \right\}$$

- The total energy E [J] of the system comprises three principal components in process systems:

- internal energy U
- kinetic energy K_E
- potential energy P_E

- Hence, we can write

$$E = U + K_E + P_E$$



- The conservation balance for energy over the balance volume V can also be written as

$$\frac{dE}{dt} = \sum_{j=1}^p F_j \hat{E}_j - \sum_{k=1}^q F_k \hat{E}_k + Q + W$$

- Where Q is the heat transfer to the surrounding and W is the work done
- Using the thermodynamic relationship for enthalpy H given by $H = U + PV$, it is possible to write the general energy balance using mass specific enthalpy H [J/kg] as

$$\frac{dE}{dt} = \sum_{j=1}^p F_j (\hat{H} + \hat{K}_E + \hat{P}_E)_j - \sum_{k=1}^q F_k (\hat{H} + \hat{K}_E + \hat{P}_E)_k + Q + \hat{W}$$

Simplifications and Modifications of the General Energy Balance

- **Assumption 1 : In many cases, the kinetic and potential energy components can be neglected**
- This is a common representation in **chemical process systems** where internal energy content often **dominates the total energy** content of the system. The equation will be simplified to :

$$\frac{dU}{dt} = \sum_{j=1}^p F_j \hat{H}_j - \sum_{k=1}^q F_k \hat{H}_k + Q + \hat{W}$$

- Computation of the specific enthalpies for all inlet and outlet streams is usually done **using thermodynamic prediction packages** which can take into account fluid phase non-idealities.

- **Assumption 2** We normally do not deal directly with the internal energy U , in the general energy balance but prefer to use alternate properties.
- Using the definition of enthalpy we can write the above equation as

$$\frac{dU}{dt} = \frac{d(H - PV)}{dt} = \sum_{j=1}^p F_j \hat{H}_j - \sum_{k=1}^q F_k \hat{H}_k + Q + \hat{W},$$

$$\frac{dH}{dt} - \frac{d(PV)}{dt} = \sum_{j=1}^p F_j \hat{H}_j - \sum_{k=1}^q F_k \hat{H}_k + Q + \hat{W}.$$

- If P and V are constant, then we can write,

$$\frac{dH}{dt} = \sum_{j=1}^p F_j \hat{H}_j - \sum_{k=1}^q F_k \hat{H}_k + Q + \hat{W}$$

- **Assumption 3** In the above equation, the specific enthalpy of the balance volume and the **specific enthalpy at the outlet** are not necessarily equal.
- In the case where **pressure variations within the balance volume are small, such as in liquid systems or where enthalpy variations due to pressure are small**, we can **assume that the specific enthalpies are equal** and hence:

$$\hat{H} = \hat{H}_k \quad k = 1, \dots, q.$$

- We can then write the energy balance as

$$\frac{dH}{dt} = \sum_{j=1}^p F_j \hat{H}_j - \sum_{k=1}^q F_k \hat{H} + Q + \hat{W}.$$

- *This is the most common form of the **energy balance for a liquid system***

- **Assumption 4** We know that in the above Eq. , the enthalpies are evaluated at the temperature conditions of the feeds (T_j) and also at the system temperature (T).
- *By making certain assumptions about the enthalpy representation, we can make further simplifications. In particular, we note that the enthalpy of the feed H_j can be written in terms of the system temperature T .*

$$\hat{H}_j(T_j) = \hat{H}_j(T) + \int_T^{T_j} c_{p_j}(T) dT$$

- If we assume that C_p is a constant, then

$$\hat{H}_j(T_j) = \hat{H}_j(T) + c_{p_j}(T_j - T)$$

- Hence, we can write our modified energy balance as

$$\frac{dH}{dt} = \sum_{j=1}^p F_j \left[\hat{H}_j(T) + c_{p_j}(T_j - T) \right] - \sum_{k=1}^q F_k \hat{H}(T) + Q + \hat{W}$$

- **Assumption 5:** It has already been mentioned that when considering reacting systems no explicit appearance of the heat of reaction is seen in the general energy balance.
- This is because the energy gain or loss is seen in the value of the outlet enthalpy evaluated at the system temperature T .
- *We can now develop the energy balance in a way which makes the reaction term explicit in the energy balance.*

$$V\rho c_p \frac{dT}{dt} = \sum_{j=1}^P F_j c_{p_j} (T_j - T) + rV(-\Delta H_R) + Q + \hat{W}$$

- *This is the most **common form of energy balance for reacting systems***

- The first term on the right-hand side **represents the energy needed to adjust all feeds to the reactor conditions.**
- The second represents **the energy generation or consumption at the reactor temperature.**
- The last two terms are the relevant **heat and work terms**

CONSERVATION BALANCES FOR MOMENTUM

- In many systems it is also important to consider the conservation of momentum.
- This is particularly the case **in mechanical systems and in flow systems where various forces act.**
- These can include **pressure forces, viscous forces, shear forces and gravitational forces.** Momentum is the product of mass and velocity. We can thus write the general form of the balance applied to a similar balance volume as

$$\left\{ \begin{array}{l} \text{rate of change} \\ \text{of momentum} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of momentum} \\ \text{into system} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of momentum} \\ \text{out of system} \end{array} \right\} \\ + \left\{ \begin{array}{l} \text{rate of momentum} \\ \text{generation} \end{array} \right\}.$$

- The last term is the **summation of all the forces acting on the system**. In considering momentum, it is important to consider all components of the forces acting on the system under study.
- This means that the problem is basically a 3D problem. In reality we often simplify this to a 1D problem. This alternative expression of the momentum balance is given by:

$$\left\{ \begin{array}{l} \text{rate of change} \\ \text{of momentum} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of momentum} \\ \text{into system} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of momentum} \\ \text{out of system} \end{array} \right\} + \left\{ \begin{array}{l} \text{sum of all forces} \\ \text{on the system} \end{array} \right\}.$$

- We can write the general momentum balance equation as

$$\frac{d\mathcal{M}}{dt} = \mathcal{M}^{(i)} - \mathcal{M}^{(o)} + \sum_{k=1}^p \mathcal{F}_k$$

- Momentum balances in models for lumped parameter systems appear most often in equations relating **convective flows to forces generated by pressure, viscous and gravity gradients**.
- These are typically expressed by some form of the general **Bernoulli equation** which incorporates various simplifications.

THE SET OF CONSERVATION BALANCES FOR LUMPED SYSTEMS

- The process model of an LPS consists of a set of conservation balance equations that are **ODEs equipped with suitable constitutive equations.**
- The balance equations are usually **coupled through reaction rate and transfer terms.**

STEADY-STATE LUMPED PARAMETER SYSTEMS

- In some circumstances we might be interested only in the steady state of the process.
- The general mass and energy balances can be modified to give the steady-state balances by simply **setting all derivative (time varying) terms to zero**.
- Hence, we arrive at the equivalent steady-state mass, component mass and total energy balances.
- Steady-state total mass balance

$$0 = \sum_{j=1}^p F_j - \sum_{k=1}^q F_k$$

- *Steady-state component mass balance*

$$0 = \sum_{j=1}^p f_{i,j} - \sum_{k=1}^q f_{i,k} + g_i, \quad i = 1, \dots, n;$$

- *Steady-State energy balance*

$$0 = \sum_{j=1}^p F_j (\hat{U} + P_1 \hat{V}_1 + \hat{K}_E + \hat{P}_E)_j \\ - \sum_{k=1}^q F_k (\hat{U} + P_2 \hat{V}_2 + \hat{K}_E + \hat{P}_E)_k + Q + \hat{W}$$

- These equations are typically solved using some form of iterative numerical solver such as Newton's method.
- Steady-state balances **form the basis for the substantial number of process flowsheeting programs** which are routinely used in the process industries. These include **ASPEN PLUS , HYSIM and PRO II.**

ANALYSIS OF LUMPED PARAMETER MODELS

Degrees of Freedom Analysis

- In the same way that algebraic equations require a degree of freedom analysis **to ensure they are properly posed and solvable**, dynamic models also require a similar analysis.
- The basis concept of DOF analysis is **to determine the difference between the number of variables (unknowns) in a given problem, and the number of equations** that describe a mathematical representation of the problem.
- Thus,

$$N_{DF} = N_u - N_e$$

- Where N_{DF} is the number of DOF, N_u the number of independent variables (unknowns) and N_e the number of independent equations.
- There are three possible values for NDF to take:
 - (a) **NDF = 0** This implies that the number of independent unknowns and independent equations is the same.
 - **A unique solution exists.**

(b) $N_{DF} > 0$

- This implies that the number of **independent variables** is **greater than the number of independent equations**.
 - The problem is *underspecified* and a solution is possible only if **some of the independent variables are "fixed"** (i.e. held constant) **by some external considerations in order that N_{DF} be reduced to zero**. Some thought must be given to which system variables are chosen as fixed. In the case of optimization these DOF will be adjusted to give a "best" solution to the problem.

(c) $N_{DF} < 0$

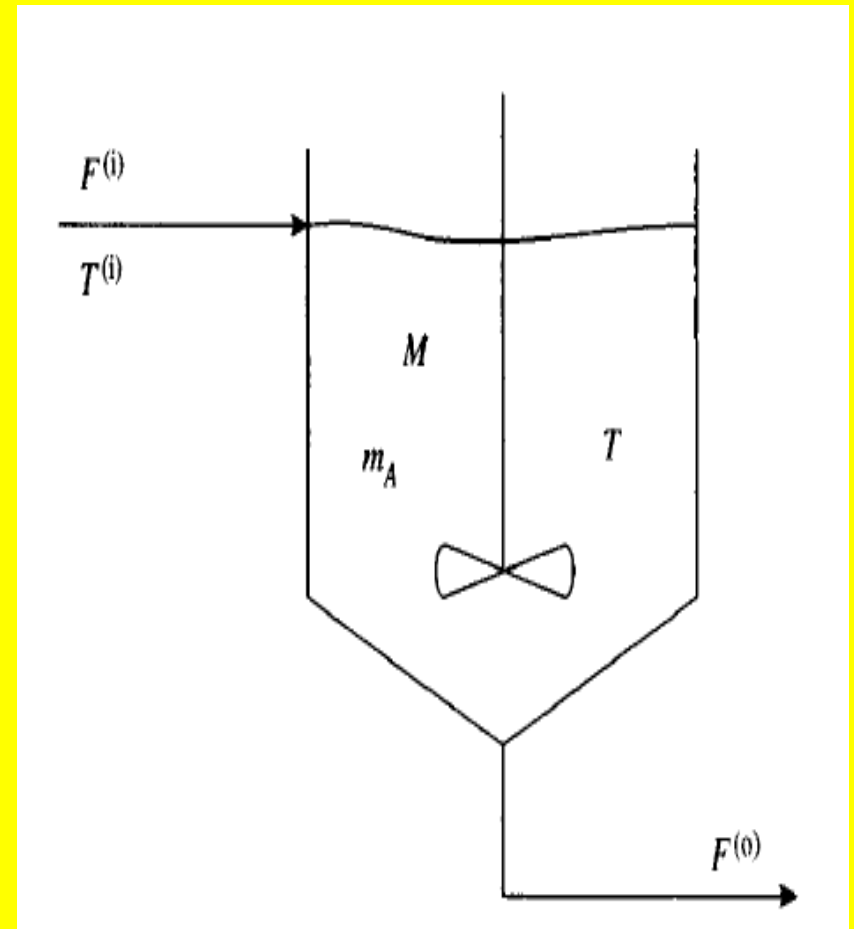
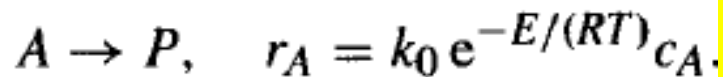
- This implies that the number of **variables** is **less than the number of equations**.

The problem is *overspecified*, meaning that there are **less variables than equations**. If this occurs it is necessary to check and make sure that you have included all relevant variables.

- **EXAMPLE** (Lumped parameter modelling of a CSTR).
- A CSTR is shown in Fig. below with reactant volume V , component mass holdup M_A for component A , feed flowrate F_i [m^3/s] at temperature T^i , Feed concentration of component A is c_A^i . Outlet flowrate F^o is in units [m^3/s].

Assumptions

- A1. perfect mixing implying no spatial variations,
- A2. incompressible fluid phase,
- A3, constant physical properties,
- A4. all flows and properties given in mole units,
- A5 . equal molar densities,
- A6. reactions and reaction rates given by



Model equations

- The following state the overall mass balance, the component balance for A and the total energy balance.

accumulation-rate = in-flow - out-flow + source,

$$\frac{d(\rho V)}{dt} = F^{(i)} \rho^{(i)} - F^{(o)} \rho,$$

$$\frac{d(m_A)}{dt} = f_A^{(i)} - f_A^{(o)} - Vr_A,$$

$$V \rho c_p \frac{d(T)}{dt} = F^{(i)} \bar{H}^{(i)} \rho - F^{(o)} \bar{H} \rho - Vr_A \Delta H_R.$$

- A set of constitutive equations accompanies the conservation balances. These include:
- The model equations above have to be solved for the following set of state variables:

$$\underline{x} = [V \quad m_A \quad T]^T$$

$$f_A^{(i)} = F^{(i)} c_A^{(i)}, \quad f_A^{(o)} = F^{(o)} c_A, \quad M = V \rho, \quad m_A = c_A V,$$
$$r_A = k_0 e^{-E/(RT)} c_A, \quad H = M c_p T, \quad \bar{H} = \frac{H}{M}, \quad \bar{H}^{(i)} = c_p^{(i)} T^{(i)}.$$

Note that a set of *initial conditions is needed for the solution.*

Initial conditions:

$$V(0) = V_0; \quad m_A(0) = m_{A_0}; \quad T(0) = T_0.$$

- As shown in the example above, the general form of the lumped parameter model equations is an initial value problem for a set of ODEs with algebraic constraints and initial conditions $X(0)$. This is called a **DAE-IVP problem**:

$$\begin{aligned}\frac{dx}{dt} &= f(x, y, t), \\ 0 &= g(x, y, t), \\ x(0) &= x_0.\end{aligned}$$

High-Index Differential-Algebraic Equations

- The index is the **minimum number of differentiations with respect to time that the algebraic system of equations has to undergo to convert the system into a set of ODEs,**
- The index of a pure ODE system is **zero** by definition. If the index of a DAE is one (1), then **the initial values of the differential variables can be selected arbitrarily,** and **easily solved by conventional methods such as Runge-Kutta and Backward Differentiation methods.**
- If, however, **the index is higher than 1, special care should be taken in assigning the initial values of the variables,** since some "hidden" constraints lie behind the problem specifications.

- The requirement of index-1 for a DAE set is equivalent to the requirement that the algebraic equation set should have Jacobian of full rank with respect to the algebraic variables.
- That is

$$g_z = \left(\frac{\partial g}{\partial z} \right)$$

must be non-singular.

- EXAMPLE (A linear DAE system). Consider a simple linear DAE system given by

$$\dot{x}_1 = x_1 + x_2 + z_1, \quad (f_1)$$

$$\dot{x}_2 = x_1 - x_2 - z_1, \quad (f_2)$$

$$0 = x_1 + 2x_2 - z_1; \quad (g_1)$$

- let us investigate the index of this system. To do so, we differentiate the algebraic constraint g_1 to get

$$0 = \dot{x}_1 + 2\dot{x}_2 - \dot{z}_1$$

$$\dot{z}_1 = \dot{x}_1 + 2\dot{x}_2.$$

- Substitute for x'_1 and X'_2 from $f1$ and $f2$ to get

$$\dot{z}_1 = 3x_1 - x_2 - z_1$$

- Hence, this algebraic constraint has been converted to an ODE after 1 differentiation. This system is INDEX = 1
- As an alternative, consider a change in the algebraic constraint g_1 to

$$0 = x_1 + 2x_2.$$

- Differentiate this for the first time to get

$$0 = \dot{x}_1 + 2\dot{x}_2$$

- and substitute from $(f1)$ and $(f2)$ to get

$$0 = 3x_1 - x_2 - z_1$$

- Clearly, this first differentiation has not produced a differential equation in z_1 , hence we differentiate once more to get

$$0 = 3\dot{x}_1 - \dot{x}_2 - \dot{z}_1,$$

$$\dot{z}_1 = 3\dot{x}_1 - \dot{x}_2$$

and

$$\dot{z}_1 = 2x_1 + 4x_2 + 4z_1$$

- This result shows that the DAE set is **INDEX = 2**

- It might be asked why the index is of importance in DAE systems. It is not an issue for pure ODE systems but when the $\text{INDEX} > 1$ the numerical techniques which are used to solve such problems fail to control the solution error and can fail completely.

Factors Leading to High-Index Problems

- It has been seen that inappropriate specifications lead to problems with high index.
- There are at least three main reasons why high-index problems arise. These include:
 - (i) Choice of specified (design) variables,
 - (ii) The use of forcing functions on the system,
 - (iii) Modelling issues.
- It must be said that in all the above situations there may be inappropriate cases which lead to a high-index problem. Other situations are valid and truly lead to high-index problems.
- However, numerical routines are generally incapable of handling these high index situations. **We prefer to model in such a way that we obtain an index-one (1) problem.**

STABILITY OF THE MATHEMATICAL PROBLEM

- The propagation of errors is not only dependent on the type of method used but is influenced dramatically by the **behaviour of the problem** notably by the integral curves, which represent the family of solutions to the problem.
- This is clearly dependent on the **individual problem**.

- **EXAMPLE** (Stability of a simple linear ordinary differential system). Before addressing the general nonlinear ODE system, let us look at a simple 2 variable problem to illustrate some basic characteristics
- Consider the problem

$$\frac{dy}{dt} = y' = \mathbf{A}y + \phi,$$

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} -2000 & 999.75 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 1000.25 \\ 0 \end{pmatrix},$$

where $y_1(0) = 0$; $y_2(0) = -2$

- The *exact solution* is given by

$$y_1(t) = -1.499e^{-0.5t} + 0.499e^{-20005t} + 1,$$
$$y_2(t) = -2.999e^{-0.5t} - 0.0025e^{-20005t} + 1.$$

- Note that the first terms in each equation represent the **slow transients in the solution** whilst the second terms are the **fast transients** (see the exponential terms). Finally, the **constant terms represent the steady state values**. The **slow transients determine just how long it takes to reach steady state**.
- We can note that the fast transient is over at $t = 0.002$ whilst the slow transient is over at $t = 10$.
- If we solved this with a classical Runge-Kutta method, we would need about 7000 steps to reach steady state. Even though the fast transient has died out quickly, the **eigenvalue** associated with this component still controls the steplength of the method when the method has a finite limit on the solution errors.

- Now let us consider the general nonlinear set of ODEs given by

$$y' = f(t, y) \quad y(a) = y_0, \quad t \in (a, b).$$

- The behaviour of the solution to the **problem near a particular solution $g(t)$** can be qualitatively assessed by the linearized variational equations given by:

$$y' = \mathbf{J}(t, g(t))[y - g(t)] + f(t, g(t)),$$

where $\mathbf{J} = \partial f_i / \partial y_j$ is evaluated at $(t, g(t))$.

- Since the local behaviour is being considered, the Jacobian could be replaced by a constant matrix A provided the variation of J in an interval of t is small.
- Assuming that the matrix A has distinct eigenvalues, λ_i , $i = 1, 2, \dots, n$ and that the eigenvectors are v_i , $i = 1, 2, \dots, n$ the general solution of the variational equation has the form

$$y(t) = \sum_{i=1}^n c_i e^{\lambda_i t} v_i + g(t).$$

- There are *three important cases related to the eigenvalues, which illustrate the three major classes of problems to be encountered.*

Unstable Case

- Here, some of the **eigenvalues are positive and large**, hence the solution curves spread out. A very difficult problem for any ODE method. This is inherent instability in the mathematical problem.
- Consider the solution of the following ordinary differential equation (ODE-IVP):

$$y' = y - t, \quad y(0) = 1.$$

- This is an inherently unstable problem with a positive eigenvalue = 1. It is clear that as this problem is integrated numerically, the solution will continue to grow without bound as time heads for infinity.
- Some process engineering problems have this type of characteristic.
- Some catalytic reactor problems can exhibit **thermal runaway** which leads to an unstable situation when a critical temperature in the reactor is reached.
- Certain processes which have a control system installed can also exhibit instability due to **unsatisfactory controller tuning or design.**

Stable Case

- Here the eigenvalues have **negative real parts and are small in magnitude** and hence the solution curves are roughly parallel to $g(t)$.
- *These are reasonably easy problems to solve, using conventional explicit techniques like Euler or Runge-Kutta methods. Stable problems are also common in process engineering.*

Ultra Stable Case

- Here, some **eigenvalues are large and negative** (there are others that are small and negative) and the solution curves quickly converge to $g(t)$. This behaviour is **good for propagation of error in the ODE but not for a numerical method**. This class of problems is called "stiff".
- When inappropriate numerical methods such as Euler's method is applied to an ultra stable problem then there is bound to be difficulties.
- It should be noted that stiffness is a **property of the mathematical problem** not the numerical method.

- Consider the problem given by

$$\frac{dy}{dt} = Ay, \quad y(0) = [2, 1]^T, \quad t \in [0, 10],$$

- where the matrix A is given by

$$A = \begin{pmatrix} -500.5 & 499.5 \\ 499.5 & -500.5 \end{pmatrix}$$

- The exact solution to this linear ODE is

$$\begin{aligned} y_1 &= 1.5e^{-t} + 0.5e^{-1000t}, \\ y_2 &= 1.5e^{-t} - 0.5e^{-1000t}. \end{aligned}$$

- Eigen values of the Jacobian of A are

$$\lambda_1 = -1000; \lambda_2 = -1$$

- Hence, the problem has the initial transient followed by the integration of the slower transient as seen in the analytic solutions.