Chapter 2: Examples of Mathematical Models for Chemical Processes

In this chapter we develop mathematical models for a number of elementary chemical processes that are commonly encountered in practice. We will apply the methodology discussed in the previous chapter to guide the reader through various examples. The goal is to give the reader a methodology to tackle more complicated processes that are not covered in this chapter and that can be found in books listed in the reference. The organization of this chapter includes examples of systems that can be described by ordinary differential equations (ODE), i.e. lumped parameter systems followed by examples of distributed parameters systems, i..e those described by partial differential equations (PDE). The examples cover both homogeneous and heterogeneous systems. Ordinary differential equations (ODE) are easier to solve and are reduced to simple algebraic equations at steady state. The solution of partial differential equations (PDE) on the other hand is a more difficult task. But we will be interested in the cases were PDE's are reduced to ODE's. This is naturally the case where under appropriate assumptions, the PDE's is a one-dimensional equation at steady state conditions. It is worth to recall, as noted in the previous chapters, that the distinction between lumped and distributed parameter models depends sometimes on the assumptions put forward by the modeler. Systems that are normally distributed parameter can be modeled under appropriate assumptions as lumped parameter systems. This chapter includes some examples of this situation.

2.1 Examples of Lumped Parameter Systems

2.1.1 Liquid Storage Tank

Consider the perfectly mixed storage tank shown in figure 2.1. Liquid stream with volumetric rate F_f (m^3/s) and density ρ_f flow into the tank. The outlet stream has volumetric rate F_o and density ρ_o. Our objective is to develop a model for the variations of the tank holdup, i.e. volume of the tank. The system is therefore the liquid in the tank. We will assume that it is perfectly mixed and that the density of the effluent is the same as that of tank content. We will also assume that the tank is isothermal, i.e. no variations in the temperature. To model the tank we need only to write a mass balance equation.

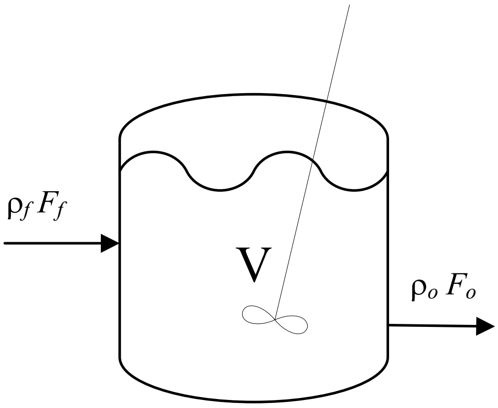

Figure 2-1 Liquid Storage Tank

Since the system is perfectly mixed, the system properties do not vary with position inside the tank. The only variations are with time. The mass balance equation can be written then on the whole system and not only on a differential element of it. This leads to therefore to a macroscopic model.

We apply the general balance equation (Eq. 1.2), to the total mass $m = \rho V$. This yields:

Mass flow in:

$$\rho_f F_f \tag{2.1}$$

Mass flow out:

$$\rho_o F_o \tag{2.2}$$

Accumulation:

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} \tag{2.3}$$

The generation term is zero since the mass is conserved. The balance equation yields:

$$\rho_f F_f = \rho_o F_o + \frac{d(\rho V)}{dt} \tag{2.4}$$

For consistency we can check that all the terms in the equation have the SI unit of *kg/s*. The resulting model (Eq. 2.4) is an ordinary differential equation (ODE) of first order where time *(t)* is the only independent variable. This is therefore a lumped parameter model. To solve it we need one initial condition that gives the value of the volume at initial time t_i, i.e.

$$V(t_i) = V_i \tag{2.5}$$

Under isothermal conditions we can further assume that the density of the liquid is constant i.e. $\rho_f = \rho_o = \rho$. In this case Eq. 2.4 is reduced to:

$$\frac{dV}{dt} = F_f - F_o \tag{2.6}$$

The volume V is related to the height of the tank L and to the cross sectional area A by:

$$V = AL \tag{2.7}$$

Since (A) is constant then we obtain the equation in terms of the state variable L:

$$A\frac{dL}{dt} = F_f - F_o \tag{2.8}$$

with initial condition:

$$L(t_i) = L_i \tag{2.9}$$

Degree of freedom analysis

For the system described by Eq. 2.8 we have the following information:

- Parameter of constant values: A
- Variables which values can be externally fixed (Forced variable): F_f
- Remaining variables: L and F_o
- Number of equations: 1 (Eq. 2.8)

Therefore the degree of freedom is:

Number of remaining variables – Number of equations = 2 – 1 = 1

For the system to be exactly specified we need therefore one more equations. This extra relation is obtained from practical engineering considerations. If the system is operated without control (at open loop) then the outlet flow rate F_o is a function of the liquid level L. Generally a relation of the form:

$$F_o = \alpha\sqrt{L} \tag{2.10}$$

could be used, where α is the discharge coefficient.

If on the other hand the liquid level is under control, then its value is kept constant at certain desired value L_s. If F_o is used to control the height then a control law relates F_o to L and L_s:

$$F_o = F_o(L,L_s) \tag{2.11}$$

For instant, if a proportional controller K_c is used then the control law is given by:

$$F_o = K_c(L - L_s) + F_{ob} \tag{2.12}$$

Where F_{ob} the bias, i.e. the constant value of F_o when the level is at the desired value i.e., $L = L_s$.

Note that at steady state, the accumulation term is zero (height does not change with time), i.e., $dL/dt = 0$. The model of the tank is reduced to the simple algebraic equation:

$$F_0 = F_f \tag{2.13}$$

2.1.2 Stirred Tank Heater

We consider the liquid tank of the last example but at non-isothermal conditions. The liquid enters the tank with a flow rate F_f (m^3/s), density ρ_f (kg/m^3) and temperature T_f (K). It is heated with an external heat supply of temperature T_{st} (K), assumed constant. The effluent stream is of flow rate F_o (m^3/s), density ρ_o (kg/m^3) and temperature T(K) (Fig. 2.2). Our objective is to model both the variation of liquid level and its temperature. As in the previous example we carry out a macroscopic model over the whole system. Assuming that the variations of temperature are not as large as to affect the density then the mass balance of Eq. 2.8 remains valid.

To describe the variations of the temperature we need to write an energy balance equation. In the following we develop the energy balance for any macroscopic system (Fig. 2.3) and then we apply it to our example of stirred tank heater.

The energy E(J) of any system of (Fig. 2.3) is the sum of its internal U(J), kinetic K(J) and potential energy ϕ(J):

$$E = U + K + \phi \tag{2.14}$$

Consequently, the flow of energy into the system is:

$$\rho_f F_f(\tilde{U}_f + \tilde{K}_f + \tilde{\phi}_f) \tag{2.15}$$

where the ($\tilde{\bullet}$) denotes the specific energy (*J/kg*).

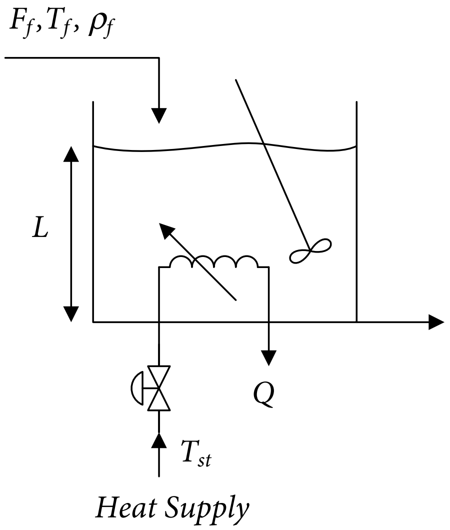

Figure 2-2 Stirred Tank Heater

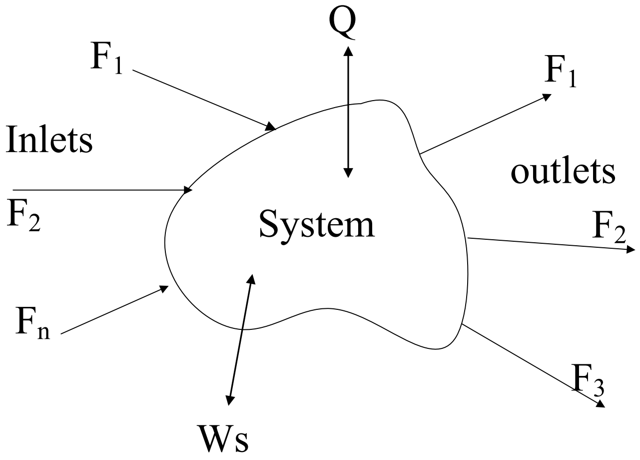

Figure 2-3 General Macroscopic System

The flow of energy out of the system is:

$$\rho_o F_o(\tilde{U}_o + \tilde{K}_o + \tilde{\phi}_o) \tag{2.16}$$

The rate of accumulation of energy is:

$$\frac{d\left(\rho V(\tilde{U}+\tilde{K}+\tilde{\phi})\right)}{dt} \tag{2.17}$$

As for the rate of generation of energy, it was mentioned in Section 1.8.4, that the energy exchanged between the system and the surroundings may include heat of reaction Q_r (*J/s*), heat exchanged with surroundings Q_e (*J/s*) and the rate of work done against pressure forces (flow work) W_{pv} (*J/s*), in addition to any other work W_o.

The flow of work W_{pv} done by the system is given by:

$$W_{pv} = F_o P_o - F_f P_f \tag{2.18}$$

where P_o and P_f are the inlet and outlet pressure, respectively.

In this case, the rate of energy generation is:

$$Q_e + Q_r - (W_o + F_o P_o - F_f P_f) \tag{2.19}$$

Substituting all these terms in the general balance equation (Eq. 1.7) yields:

$$\begin{aligned}\frac{d\left(\rho V(\tilde{U}+\tilde{K}+\tilde{\phi})\right)}{dt} &= \rho_f F_f\left(\tilde{U}_f+\tilde{K}_f+\tilde{\phi}_f\right)-\rho_o F_o\left(\tilde{U}_o+\tilde{K}_o+\tilde{\phi}_o\right)\\ &\quad + Q_e + Q_r - (W_o + F_o P_o - F_f P_f)\end{aligned} \tag{2.20}$$

We can check that all terms of this equation have the SI unit of (J/s). Equation (2.20) can be also written as:

$$\begin{aligned}\frac{d\left(\rho V(\tilde{U}+\tilde{K}+\tilde{\phi})\right)}{dt} &= \rho_f F_f\left(\tilde{U}_f+\tilde{K}_f+\tilde{\phi}_f\right)-\rho_o F_o\left(\tilde{U}_o+\tilde{K}_o+\tilde{\phi}_o\right)\\ &\quad + Q_e + Q_r - W_o - F_o\rho_o\frac{P_o}{\rho_o} + F_f\rho_f\frac{P_f}{\rho_f}\end{aligned} \tag{2.21}$$

The term $\widetilde{V} = 1/\rho$ is the specific volume (m^3/kg). Thus Eq. 2.21 can be written as:

$$\frac{d\left(\rho V(\widetilde{U} + \widetilde{K} + \widetilde{\phi})\right)}{dt} = \rho_f F_f\left(\widetilde{U}_f + P_f \widetilde{V}_f + \widetilde{K}_f + \widetilde{\phi}_f\right) - \rho_o F_o\left(\widetilde{U}_o + P_o \widetilde{V}_o + \widetilde{K}_o + \widetilde{\phi}_o\right) + Q_e + Q_r - W_o \tag{2.22}$$

The term $\widetilde{U} + P\widetilde{V}$ that appears in the equation is the specific enthalpy $\widetilde{h}$. Therefore, the general energy balance equation for a macroscopic system can be written as:

$$\frac{d\left(\rho V(\widetilde{U} + \widetilde{K} + \widetilde{\phi})\right)}{dt} = \rho_f F_f\left(\widetilde{h}_f + \widetilde{K}_f + \widetilde{\phi}_f\right) - \rho_o F_o\left(\widetilde{h}_o + \widetilde{K}_o + \widetilde{\phi}_o\right) + Q_e + Q_r - W_o \tag{2.23}$$

We return now to the liquid stirred tank heater. A number of simplifying assumptions can be introduced:

- We can neglect kinetic energy unless the flow velocities are high.
- We can neglect the potential energy unless the flow difference between the inlet and outlet elevation is large.
- All the work other than flow work is neglected, i.e. $W_o = 0$.
- There is no reaction involved, i.e. $Q_r = 0$.

The energy balance (Eq. 2.23) is reduced to:

$$\frac{d\left(\rho V\widetilde{U}\right)}{dt} = \rho_f F_f \widetilde{h}_f - \rho_o F_o \widetilde{h}_o + Q_e \tag{2.24}$$

Here Q_e is the heat (J/s) supplied by the external source. Furthermore, as mentioned in Section 1.12, the internal energy $\widetilde{U}$ for liquids can be approximated by enthalpy, $\widetilde{h}$. The enthalpy is generally a function of temperature, pressure and composition. However, it can be safely estimated from heat capacity relations as follows:

$$\tilde{h} = \tilde{C}p(T - T_{ref}) \tag{2.25}$$

where $\tilde{C}p$ is the average heat capacity.

Furthermore since the tank is well mixed the effluent temperature T_o is equal to process temperature T. The energy balance equation can be written, assuming constant density $\rho_f = \rho_o = \rho$, as follows:

$$\rho\tilde{C}_p \frac{d\left(V(T - T_{ref})\right)}{dt} = \rho F_f \tilde{C}_p (T_f - T_{ref}) - \rho F_o \tilde{C}_p (T - T_{ref}) + Q_e \tag{2.26}$$

Taking $T_{\mathrm{ref}} = 0$ for simplicity and since $V = AL$ result in:

$$\rho\tilde{C}_p A \frac{d\left(LT\right)}{dt} = \rho F_f \tilde{C}_p T_f - \rho F_o \tilde{C}_p T + Q_e \tag{2.27}$$

or equivalently:

$$A \frac{d\left(LT\right)}{dt} = F_f T_f - F_o T + \frac{Q_e}{\rho\tilde{C}_p} \tag{2.28}$$

Since

$$A \frac{d\left(LT\right)}{dt} = AT \frac{d\left(L\right)}{dt} + AL \frac{d\left(T\right)}{dt} \tag{2.29}$$

and using the mass balance (Eq. 2.8) we get:

$$AL \frac{dT}{dt} + T(F_f - F_o) = F_f T_f - F_o T + \frac{Q_e}{\rho\tilde{C}_p} \tag{2.30}$$

or equivalently:

$$AL\frac{dT}{dt} = F_f(T_f - T) + \frac{Q_e}{\rho\tilde{C}_p} \tag{2.31}$$

The stirred tank heater is modeled, then by the following coupled ODE's:

$$A\frac{dL}{dt} = F_f - F_o \tag{2.32}$$

$$AL\frac{dT}{dt} = F_f(T_f - T) + \frac{Q_e}{\rho\tilde{C}_p} \tag{2.33}$$

This system of ODE's can be solved if it is exactly specified and if conditions at initial time are known,

$$L(t_i) = L_i \qquad \text{and } T(t_i) = T_i \tag{2.34}$$

Degree of freedoms analysis

For this system we can make the following simple analysis:

- Parameter of constant values: A, ρ *and* C_p
- (Forced variable): F_f and T_f
- Remaining variables: L, F_o, T, Q_e
- Number of equations: 2 (Eq. 2.32 and Eq. 2.33)

The degree of freedom is therefore, 4 − 2 = 2. We still need two relations for our problem to be exactly specified. Similarly to the previous example, if the system is operated without control then F_o is related to L through (Eq. 2.10). One additional relation is obtained from the heat transfer relation that specifies the amount of heat supplied:

$$Q_e = UA_H\,(T_{st} - T) \tag{2.35}$$

U and A_H are heat transfer coefficient and heat transfer area. The source temperature T_{st} was assumed to be known. If on the other hand both the height and temperature are under control, i.e. kept constant at desired values of L_s and T_s then there are two control laws that relate respectively F_o to L and L_s and Q_e to T and T_s:

$$F_o = F_o(L, L_s), \text{ and } Q_e = Q_e(T, T_s) \tag{2.36}$$

2.1.3 Isothermal CSTR

We revisit the perfectly mixed tank of the first example but where a liquid phase chemical reactions taking place:

$$A \xrightarrow{k} B \tag{2.37}$$

The reaction is assumed to be irreversible and of first order. As shown in figure 2.4, the feed enters the reactor with volumetric rate F_f (m^3/s), density ρ_f (kg/m^3) and concentration C_{Af} ($mole/m^3$). The output comes out of the reactor at volumetric rate F_o, density ρ_0 and concentration C_{Ao} ($mole/m^3$) and C_{Bo} ($mole/m^3$). We assume isothermal conditions.

Our objective is to develop a model for the variation of the volume of the reactor and the concentration of species A and B. The assumptions of example 2.1.1 still hold and the total mass balance equation (Eq. 2.6) is therefore unchanged

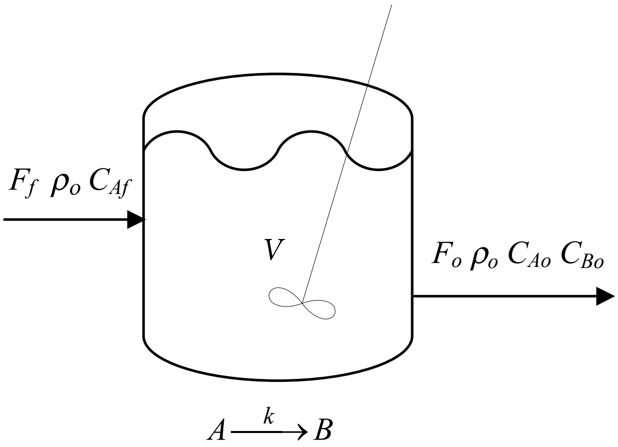

Figure 2.4 Isothermal CSTR

The component balance on species A is obtained by the application of (Eq. 1.3) to the number of moles ($n_A = C_A V$). Since the system is well mixed the effluent concentration $C_{A\mathrm{o}}$ and $C_{B\mathrm{o}}$ are equal to the process concentration C_A and C_B.

Flow of moles of A in:

$$F_f\, C_{Af} \tag{2.38}$$

Flow of moles of A out:

$$F_o\, C_{Ao} \tag{2.39}$$

Rate of accumulation:

$$\frac{dn}{dt} = \frac{d(VC_A)}{dt} \tag{2.40}$$

Rate of generation: $-rV$

where r ($moles/m^3 s$) is the rate of reaction.

Substituting these terms in the general equation (Eq. 1.3) yields:

$$\frac{d(VC_A)}{dt} = F_f\ C_{Af} - F_o\ C_A - rV \tag{2.41}$$

We can check that all terms in the equation have the unit (*mole/s*).

We could write a similar component balance on species B but it is not needed since it will not represent an independent equation. In fact, as a general rule, a system of n species is exactly specified by n independent equations. We can write either the total mass balance along with $(n - 1)$ component balance equations, or we can write n component balance equations.

Using the differential principles, equation (2.41) can be written as follows:

$$\frac{d(VC_A)}{dt} = V\frac{d(C_A)}{dt} + C_A\frac{d(V)}{dt} = F_f\ C_{Af} - F_o\ C_A - rV \tag{2.42}$$

Substituting Equation (2.6) into (2.42) and with some algebraic manipulations we obtain:

$$V\frac{d(C_A)}{dt} = F_f(\ C_{Af} - C_A) - rV \tag{2.43}$$

In order to fully define the model, we need to define the reaction rate which is for a first-order irreversible reaction:

$$r = k\ C_A \tag{2.44}$$

Equations 2.6 and 2.43 define the dynamic behavior of the reactor. They can be solved if the system is exactly specified and if the initial conditions are given:

$$V(t_i) = V_i \text{ and } C_A(t_i) = C_{Ai} \tag{2.45}$$

Degrees of freedom analysis

- Parameter of constant values: A
- (Forced variable): F_f and C_{Af}
- Remaining variables: V, F_o, and C_A
- Number of equations: 2 (Eq. 2.6 and Eq. 2.43)

The degree of freedom is therefore 3 − 2 =1. The extra relation is obtained by the relation between the effluent flow F_o and the level in open loop operation (Eq. 2.10) or in closed loop operation (Eq. 2.11).

The steady state behavior can be simply obtained by setting the accumulation terms to zero. Equation 2.6 and 2.43 become:

$$F_0 = F_f \tag{2.46}$$

$$F_f(\ C_{Af} - C_A) = rV \tag{2.47}$$

More complex situations can also be modeled in the same fashion. Consider the catalytic hydrogenation of ethylene:

$$A + B \rightarrow P \tag{2.48}$$

where A represents hydrogen, B represents ethylene and P is the product (ethane). The reaction takes place in the CSTR shown in figure 2.5. Two streams are feeding the reactor. One concentrated feed with flow rate F_1 (m^3/s) and concentration C_{B1} ($mole/m^3$) and another dilute stream with flow rate F_2 (m^3/s) and concentration C_{B2} ($mole/m^3$). The effluent has flow rate F_o (m^3/s) and concentration C_B ($mole/m^3$). The reactant A is assumed to be in excess.

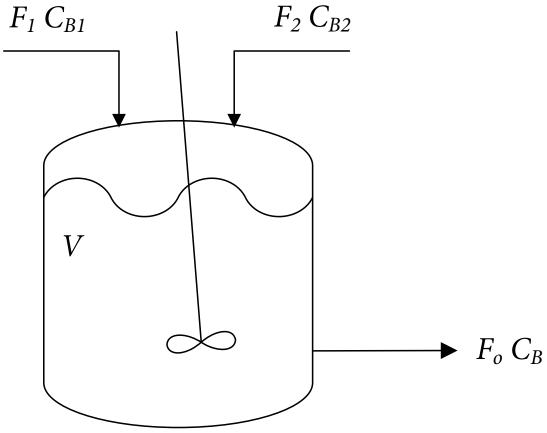

Figure 2-5 Reaction in a CSTR

The reaction rate is assumed to be:

$$r = \frac{k_1 C_B}{(1 + k_2 C_B)^2} \qquad (mole/m^3.s) \tag{2.49}$$

where k_1 is the reaction rate constant and k_2 is the adsorption equilibrium constant. Assuming the operation to be isothermal and the density is constant, and following the same procedure of the previous example we get the following model:

Total mass balance:

$$A\frac{dL}{dt} = F_1 + F_2 - F_o \tag{2.50}$$

Component *B* balance:

$$V\frac{d(C_A)}{dt} = F_1(\ C_{B1} - C_B) + F_2(\ C_{B2} - C_B) - rV \tag{2.51}$$

Degrees of freedom analysis

- Parameter of constant values: A, k_1 *and* k_1
- (Forced variable): F_1 F_2 C_{B1} and C_{B2}
- Remaining variables: V, F_o, and C_B
- Number of equations: 2 (Eq. 2.50 and Eq. 2.51)

The degree of freedom is therefore 3 − 2 =1. The extra relation is between the effluent flow F_o and the level L as in the previous example.

2.1.4 Gas-Phase Pressurized CSTR

So far we have considered only liquid-phase reaction where density can be taken constant. To illustrate the effect of gas-phase chemical reaction on mass balance equation, we consider the following elementary reversible reaction:

$$A \leftrightarrow 2B \tag{2.52}$$

taking place in perfectly mixed vessel sketched in figure 2.6. The influent to the vessel has volumetric rate F_f (m^3/s), density ρ_f (kg/m^3), and mole fraction y_f. Product comes out of the reactor with volumetric rate F_o, density ρ_o, and mole fraction y_o. The temperature and volume inside the vessel are constant. The reactor effluent passes through control valve which regulate the gas pressure at constant pressure P_g.

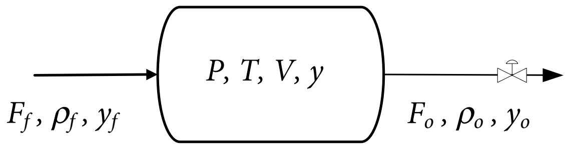

Figure 2-6 Gas Pressurized Reactor

Writing the macroscopic total mass balance around the vessel gives:

$$\frac{d(\rho V)}{dt} = \rho_f F_f - \rho_o F_o \tag{2.53}$$

Since V is constant we have:

$$V\frac{d\rho}{dt} = \rho_f F_f - \rho_o F_o \tag{2.54}$$

Writing the component balance, for fixed V, results in:

$$V\frac{dC_A}{dt} = F_f C_{Af} - F_o C_{A0} - r_1 V + r_2 V \tag{2.55}$$

The reaction rates for the reversible reaction are assumed to be:

$$r_1 = k_1\, C_A \tag{2.56}$$

$$r_2 = k_2 {C_B}^2 \tag{2.57}$$

Equations (2.54) and (2.55) define the variations of density and molar concentration. One can also rewrite the equation to define the behavior of the pressure *(P)* and mole fraction *(y)*. The concentration can be expressed in term of the density through ideal gas law:

$$C_A = yP/RT \tag{2.58}$$

$$C_B = (1 - y)P/RT \tag{2.59}$$

Similarly, the density can be related to the pressure using ideal gas law:

$$\rho = MP/RT = [M_A y + M_B (1 - y)]P/RT \tag{2.60}$$

Where M_A and M_B are the molecular weight of A and B respectively. Therefore one can substitute equations (2.58) to (2.60) into equations (2.54 & 2.55) in order to explicitly write the latter two equations in terms of y and P. Or, alternatively, one can solve all equations simultaneously.

Degrees of freedom analysis:

- Parameters: V, k_1, k_2, R, T, M_A and M_B
- Forcing function: F_f, C_{Af}, y_f
- Variables: C_A, C_B, y, P, ρ, F
- Number of equations: 5 (Eqs. 2.54, 2.55, 2.58, 2.59, 2.60)

The degree of freedom is therefore 6 − 5 =1. The extra relation relates the outlet flow to the pressure as follows:

$$F_o = C_v \sqrt{\frac{P - P_g}{\rho}} \tag{2.61}$$

where C_v is the valve-sizing coefficient. Recall also that P_g is assumed to be constant.

2.1.5 Non-Isothermal CSTR

We reconsider the previous CSTR example (Sec 2.1.3), but for non-isothermal conditions. The reaction A → B is exothermic and the heat generated in the reactor is removed via a cooling system as shown in figure 2.7. The effluent temperature is different from the inlet temperature due to heat generation by the exothermic reaction.

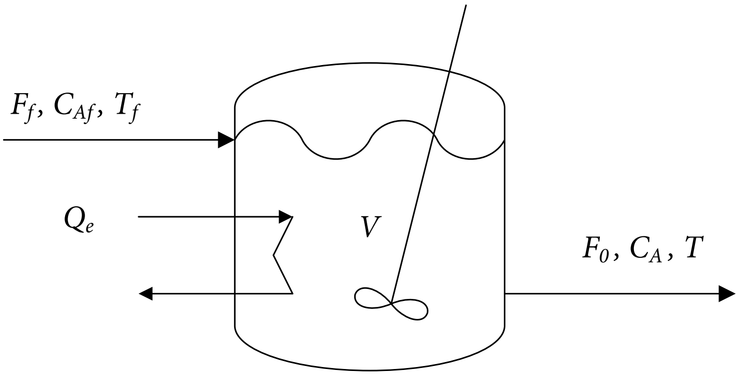

Figure 2-7 Non-isothermal CSTR

Assuming constant density, the macroscopic total mass balance (Eq. 2.6) and mass component balance (Eq. 2.43) remain the same as before. However, one more ODE will be produced from the applying the conservation law (equation 2.23) for total energy balance. The dependence of the rate constant on the temperature:

$$k = k_o e^{-E/RT} \tag{2.62}$$

should be emphasized.

The general energy balance (Eq. 2.23) for macroscopic systems applied to the CSTR yields, assuming constant density and average heat capacity:

$$\rho \widetilde{C}_p \frac{d\left(V(T - T_{ref})\right)}{dt} = \rho F_f \widetilde{C}_p (T_f - T_{ref}) - \rho F_o \widetilde{C}_p (T - T_{ref}) + Q_r - Q_e \tag{2.63}$$

where Q_r (J/s) is the heat generated by the reaction, and Q_e (J/s) the rate of heat removed by the cooling system. Assuming $T_{\text{ref}} = 0$ for simplicity and using the differentiation principles, equation 2.63 can be written as follows:

$$\rho \widetilde{C}_p V \frac{dT}{dt} + \rho \widetilde{C}_p T \frac{dV}{dt} = \rho F_f \widetilde{C}_p T_f - \rho F_o \widetilde{C}_p T + Q_r - Q_e \tag{2.64}$$

Substituting Equation 2.6 into the last equation and rearranging yields:

$$\rho\widetilde{C}_p V\frac{dT}{dt} = \rho F_f \widetilde{C}_p (T_f - T) + Q_r - Q_e \tag{2.65}$$

The rate of heat exchanged Q_r due to reaction is given by:

$$Q_r = -(\Delta H_r) Vr \tag{2.66}$$

where ΔH_r (J/mole) is the heat of reaction (has negative value for exothermic reaction and positive value for endothermic reaction). The non-isothermal CSTR is therefore modeled by three ODE's:

$$\frac{dV}{dt} = F_f - F_o \tag{2.67}$$

$$V\frac{d(C_A)}{dt} = F_f(\ C_{Af} - C_A) - rV \tag{2.68}$$

$$\rho\widetilde{C}_p V\frac{dT}{dt} = \rho F_f \widetilde{C}_p (T_f - T) + (-\Delta H_r) Vr - Q_e \tag{2.69}$$

where the rate (r) is given by:

$$r = k_o e^{-E/RT} C_A \tag{2.70}$$

The system can be solved if the system is exactly specified and if the initial conditions are given:

$$V(t_i) = V_i \qquad T(t_i) = T_i \qquad \text{and} \qquad C_A(t_i) = C_{Ai} \tag{2.71}$$

Degrees of freedom analysis

- Parameter of constant values: ρ, E, R, C_p, ΔH_r *and* k_o
- (Forced variable): F_f, C_{Af} and T_f

- Remaining variables: V, F_o, T, C_A and Q_e
- Number of equations: 3 (Eq. 2.67. 2.68 and 2.69)

The degree of freedom is 5−3 = 2. Following the analysis of example 2.1.3, the two extra relations are between the effluent stream (F_o) and the volume (V) on one hand and between the rate of heat exchanged (Q_e) and temperature (T) on the other hand, in either open loop or closed loop operations.

A more elaborate model of the CSTR would include the dynamic of the cooling jacket (Fig. 2.8). Assuming the jacket to be perfectly mixed with constant volume V_j, density ρ_j and constant average thermal capacity Cp_j, the dynamic of the cooling jacket temperature can be modeled by simply applying the macroscopic energy balance on the whole jacket:

$$\rho_j \tilde{C}_{p_j} V_j \frac{dT_j}{dt} = \rho_j F_j \tilde{C}_{p_j} (T_{jf} - T_j) + Q_e \tag{2.72}$$

Since V_j, ρ_j, Cp_j and T_{jf} are constant or known, the addition of this equation introduces only one variable (T_j). The system is still exactly specified.

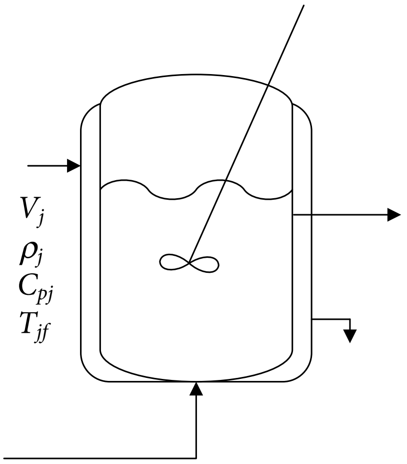

Figure 2-8 Jacketed Non-isothermal CSTR

2.1.6 Mixing Process

Consider the tank of figure 2.9 where two solutions 1 and 2 containing materials A and B are being mixed. Stream 1 has flow rate F_1 (m^3/s), density ρ_1 (kg/m^3), T_1 (K),