LIQUID FLOW IN A PIPE

Consider a fluid flowing inside a pipe of constant cross sectional area (A) as shown in Figure 4.8. We would like to develop a mathematical model for the change in the fluid mass inside the pipe. Let v be the velocity of the fluid. Clearly the velocity changes with time (t), along the pipe length (z) and also with the radial direction (r). In order to simplify the problem, we assume that there are no changes in the radial direction. We also assume isothermal conditions, so only the mass balance is needed. Since the velocity changes with both time and space, the mass balance is to be carried out on microscopic scale. We consider therefore a shell element of width Δz and constant cross section area (A) as shown in Fig. 4.8.

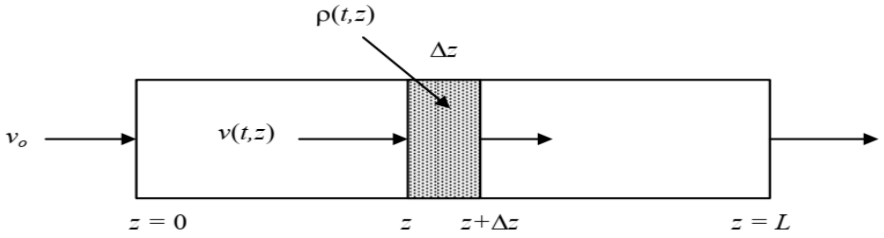

Figure 4.8 Liquid flow in a pipe

Mass into the shell:

$$\rho v A \Delta t|_z \tag{4.58}$$

where the subscript ($.|_z$) indicates that the quantity (.) is evaluated at the distance z.

Mass out of the shell:

$$\rho v A \Delta t|_{z+\Delta z} \tag{4.59}$$

Accumulation:

$$\rho A \Delta z|_{t+\Delta t} - \rho A \Delta z|_t \tag{4.60}$$

Similarly the subscript ($.|_t$) indicates that the quantity (.) is evaluated at the time t.

The mass balance equation is therefore:

$$\rho v A \Delta t|_z = \rho v A \Delta t|_{z+\Delta z} + \rho A \Delta z|_{t+\Delta t} - \rho A \Delta z|_t \tag{4.61}$$

We can check for consistency that the units in each term are in (*kg*). Dividing Eq. 4.61 by $\Delta t\ \Delta z$ and rearranging yields:

$$\frac{(\rho A)\ \big|_{t+\Delta t}-(\rho A)\ \big|_{t}}{\Delta t}=\frac{(\rho v A)\ \big|_{z}-(\rho v A)\ \big|_{z+\Delta z}}{\Delta z} \tag{4.62}$$

Taking the limit as $\Delta t \rightarrow 0$ and $\Delta z \rightarrow 0$ gives:

$$\frac{\partial(\rho A)}{\partial t}=-\frac{\partial(\rho v A)}{\partial z} \tag{4.63}$$

Since the cross section area *(A)* is constant, Eq. 4.63 yields:

$$\frac{\partial \rho}{\partial t}=-\frac{\partial(\rho v)}{\partial z} \tag{4.64}$$

or

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho v)}{\partial z}=0 \tag{4.65}$$

The ensuing equation is a partial differential equation (PDE) that defines the variation of ρ and v with the two independent variables t and z. This equation is known as the one-dimensional continuity equation. For incompressible fluids for which the density is constant, the last equation can also be written as:

$$\frac{\partial v}{\partial z}=0 \tag{4.66}$$

This indicates that the velocity is independent of axial direction for one dimensional incompressible flow.

DIFFUSION WITH CHEMICAL REACTION IN A SLAB CATALYST

We consider the diffusion of a component A coupled with the following chemical reaction A → B in a slab of catalyst shown in figure 4.9. Our objective is to determine the variation of the concentration at steady state. The concentration inside the slab varies with both the position z and time t. The differential element is a shell element of thickness Δz.

Flow of moles A in:

$$(SN_A)|_z \tag{4.67}$$

where S (m^2) is the surface area and N_A ($moles\ A/s\ m^2$) is the molar flux.

Flow of moles A out:

$$(SN_A)|_{z+\Delta z} \tag{4.68}$$

Rate of generation of A:

$$-(S\Delta z)r \tag{4.69}$$

where $r = kC_A$ is the rate of reaction, assumed to be of first order. There is no accumulation term since the system is assumed at steady state. The mass balance equation is therefore,

$$(SN_A)|_z - (SN_A)|_{z+\Delta z} - (S\Delta z)kC_A = 0 \tag{4.70}$$

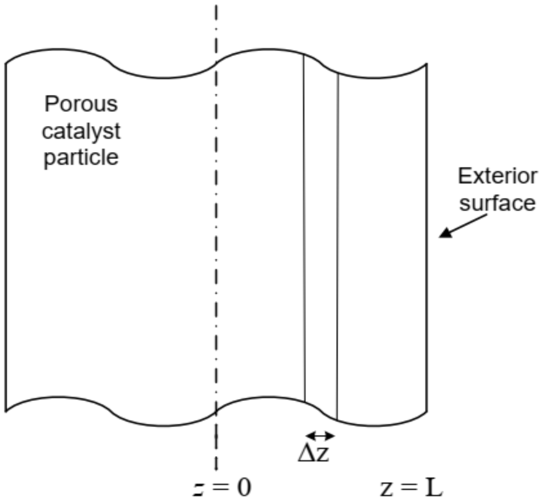

Figure 4.9 diffusion with chemical reaction inside a slab catalyst

Dividing equation (4.70) by $S\Delta z$ results in:

$$\frac{(N_A)|_z - (N_A)|_{z+\Delta z}}{\Delta z} - kC_A = 0 \tag{4.71}$$

Taking the limit when $\Delta z \rightarrow 0$, the last equation becomes:

$$\frac{dN_A}{dz} - kC_A = 0 \tag{4.72}$$

The molar flux is given by Fick's law as follows:

$$N_A = -D_A \frac{dC_A}{dz} \tag{4.73}$$

where D_A is diffusivity coefficient of *(A)* inside the catalyst particle. Equation (4.73) can be then written as follows:

$$D_A \frac{d^2 C_A}{dz^2} - kC_A = 0 \tag{4.74}$$

This is also another example where a one-dimensional distributed system is reduced to a lumped parameter system at steady state. In order to solve this second-order ODE, the following boundary conditions could be used:

$$\text{at } z = L,\ C_A = C_{Ao} \tag{4.75}$$

$$\text{at } z = 0,\ dC_A/dr = 0 \tag{4.76}$$

The first condition imposes the bulk flow concentration C_{Ao} at the end length of the slab. The second condition implies that the concentration is finite at the center of the slab.

HEAT EXCHANGER: DISTRIBUTED PARAMETER MODEL

Steam of known temperature T_s flowing around the tube is heating a liquid L of density ρ_L and constant velocity v from temperature T_{L1} to T_{L2}. The temperature in the tube varies obviously with axial direction z, radial direction r and time t. To simplify the problem we will assume that there are no change in the radial direction. This assumption is valid if the radius is small and no large amount of heat is transferred. The heat transfer from the steam to the liquid depends on the heat transfer coefficient on the steam side, h_{to} and on the transfer on the liquid side h_{ti}. We also neglect the thermal capacity of the metal wall separating the steam and the liquid and assume that the exchange between the steam and liquid occurs with an overall heat transfer coefficient U. We also assume constant heat capacity for the liquid. An energy balance on a differential element of the exchanger of length Δz and cross-sectional area A, yields:

Flow of energy in:

$$(vA\rho\,\overline{C}p\,)\Delta t|_z \tag{4.77}$$

Flow of energy out:

$$(vA\rho\,\overline{C}p\,)\Delta t|_{z+\Delta z} \tag{4.78}$$

Energy accumulation:

$$(A\rho\,\widetilde{h}\,\Delta z)|_{t+\Delta t} - (A\rho\,\widetilde{h}\,\Delta z)|_{t} \tag{4.79}$$

Energy generated:

$$U(\pi D\Delta z)(T - T_s)\Delta t \tag{4.80}$$

Using the expression for specific enthalpy and dividing by $A\Delta t\Delta z$, the energy balance yields:

$$\frac{\left(\rho A\overline{C}p(T-T_{ref})\Delta z\right)|_{t+\Delta t} - \left(\rho A\overline{C}p(T-T_{ref})\Delta z\right)|\,t}{\Delta t} = \frac{(vA\rho\overline{C}pT)\,|_{z} - (vA\rho\overline{C}pT)\,|_{z+\Delta z}}{\Delta z} - U(\frac{\pi D}{A})(T-T_s) \tag{4.81}$$

Taking the limit as Δt an Δz goes to zero gives:

$$\frac{\partial(\rho A\overline{C}pT)}{\partial t} = -\frac{\partial(vA\rho\overline{C}pT)}{\partial z} - U(\frac{\pi D}{A})(T-T_s) \tag{4.82}$$

Since $A = \pi D^2/4$ and dividing by $\rho\,\overline{C}p$ Eq. (4.82) is equivalent to:

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial z} - (\frac{4U}{\rho\overline{C}pD})(T-T_s) \tag{4.83}$$

At steady state the PDE becomes the following ODE,

$$0 = -v\frac{dT}{dz} - (\frac{4U}{\rho\overline{C}pD})(T-T_s) \tag{4.84}$$

With the following condition:

$$T(z=0) = T_0 \tag{4.85}$$

MASS EXCHANGE IN PACKED COLUMN

In previous section we presented some examples of mass transfer units that can be described by simple ODE's. This includes all the operations that can occur in tray or spray-tray towers. In this section we present an example of modeling a mass transfer operation that occurs in packed tower. Absorption is a mass transfer process in which a vapor solute (A) in a gas mixture is absorbed by contact with a liquid phase in which the solute is more or less soluble. The gas phase consists usually of an inert gas and the solute. This process involves flow transfer of the solute A through a stagnant non diffusive gas B into a stagnant liquid C. The liquid is mainly immiscible in the gas phase. An example is the absorption of ammonia (A) from air (B) by liquid water (C). The operation can be carried out either in tray (plate) towers or in packed towers. The operation in tray towers can be modeled similarly to the liquid-liquid extraction process. We consider here the absorption taking place in a packed tower.

Consider the binary absorption tower shown in Figure 4.10. A liquid stream flow downward with molar flow rate L and feed composition (X_{Af}). Vapor stream flows upward with molar flow rate (G) and feed composition (Y_{Af}). A simple vapor-liquid equilibrium relation of the form of:

$$Y_A = HX_A \tag{4.86}$$

is used, where H (mole fraction gas/mole fraction liquid) is the Henry's law constant. This assumption is valid for dilute streams. The molar rates can be considered constants, i.e. not changing from one stage to another, thus the total mass balance need not be written. To establish the model equations we need to write equations for liquid and vapor phase. To simplify the problem we assume constant liquid and vapor holdup in each stage. We also assume isothermal conditions. An energy balance therefore is not needed.

The flux N_A transferred from bulk liquid to bulk gas is given by:

$$N_A = K_Y\,(Y_A - Y_A{}^*) \tag{4.87}$$

Where K_Y is the overall mass transfer in the gas-phase (*kgmole/m*^{2}*s mole fraction*) and Y_A^* is the value that would be in equilibrium with X_A. The flux can also be expressed as:

$$N_A = K_X\,(X_A - X_A^*) \tag{4.88}$$

Where K_X is the overall mass transfer coefficient in the liquid-phase and X_A^* is the value that would be in equilibrium with Y_A.

A mass balance on the liquid phase for a differential volume (Fig. 4.10) of the column length z and cross sectional area S yields:

Flow of mole in:

$$[(SLX_A)\Delta t|_z + (N_A S\Delta t)\,|_z]\Delta z \tag{4.89}$$

Flow of moles out:

$$(SLX_A)\Delta t|_{z+\Delta z} \tag{4.90}$$

Rate of accumulation:

$$(SH_LX_A\square z)|_{t+\square t} - (SH_LX_A\square z)|_t \tag{4.91}$$

where X_A is the liquid fraction of A and H_L the liquid holdup (*mole/m*^{3}).

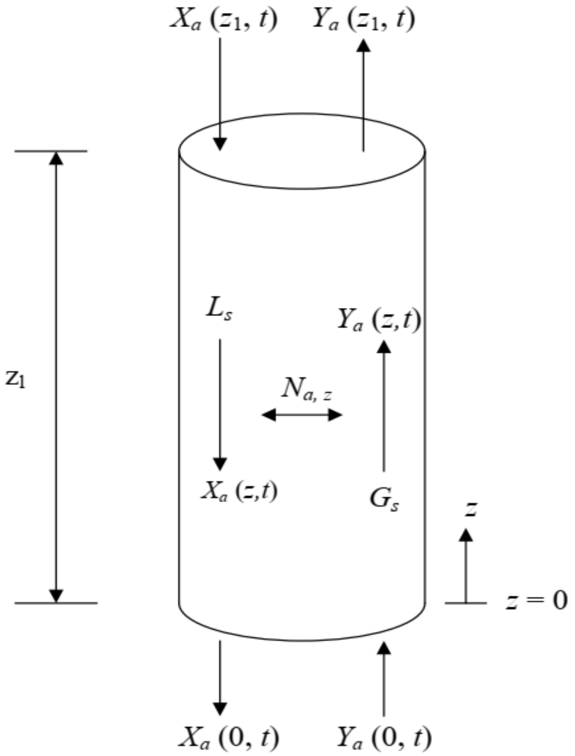

Figure 4.10 Packed column

The balance equation yields:

$$(SH_L X_A \Delta z)|_{t+\Delta t} - (SH_L X_A \Delta z)|_t = (SLX_A)\Delta t|_{z+\Delta z} - [(SLX_A)\Delta t|_z + (N_A S\Delta t)\Delta t|_z]\Delta z \qquad (4.92)$$

Dividing by $S\Delta t\Delta z$ and taking the limits as Δz and Δt goes to zero yield:

$$H_L \frac{\partial X_A}{\partial t} = L\frac{\partial X_A}{\partial z} + N_A \qquad (4.93)$$

which is equivalent to

$$H_L \frac{\partial X_A}{\partial t} = L\frac{\partial X_A}{\partial z} + K_Y(Y_A - Y_A^*) \qquad (4.94)$$

We could also use the expression of flux (Eq. 4.92):

$$H_L \frac{\partial X_A}{\partial t} = L \frac{\partial X_A}{\partial z} + K_X (X_a^* - X_A) \tag{4.95}$$

We can develop material balances for the gas phase that are similar to Eq. 4.95. This gives:

$$H_G \frac{\partial X_A}{\partial t} = -G \frac{\partial Y_A}{\partial z} + K_Y (Y_A - Y_A^*) \tag{4.96}$$

or alternatively:

$$H_G \frac{\partial Y_A}{\partial t} = -G \frac{\partial Y_A}{\partial z} + K_X (X_a^* - X_A) \tag{4.97}$$

It should be noted that the analysis carried here can be used for a number of operations where packed columns are used. This includes liquid-liquid extraction, gas-liquid absorption and gas-solid drying. In each of these operations an equilibrium relation of the type:

$$Y_A = f(X_A) \tag{4.98}$$

is generally available