PLUG-FLOW REACTOR

Assumptions

A plug-flow reactor represents an ideal reactor that has the following attributes:

1. Steady-state, steady flow.
2. No mixing in the axial direction. This implies that molecular and/or turbulent mass diffusion is negligible in the flow direction.
3. Uniform properties in the direction perpendicular to the flow, i.e., one-dimensional flow. This means that at any cross section, a single velocity, temperature, composition, etc., completely characterize the flow.
4. Ideal frictionless flow. This assumption allows the use of the simple Euler equation to relate pressure and velocity.
5. Ideal-gas behavior. This assumption allows simple state relations to be employed to relate T, P, ρ, Y_i, and h.

Application of Conservation Laws

Our goal here is to develop a system of first-order ODEs whose solution describes the reactor flow properties, including composition, as functions of distance, x. The geometry and coordinate definition are schematically illustrated at the top of Fig. 6.11. Table 6.1 provides an overview of the analysis listing the physical and chemical principles that generate $6 + 2N$ equations and a like number of unknown variables and functions. The number of unknowns could be easily reduced by N, by recognizing that the species production rates, $\dot{\omega}_i$, can be immediately expressed in terms of the mass fractions (see Appendix 6A) without the need to explicitly involve the $\dot{\omega}_i$. Explicitly

Table 6.1 Overview of relationships and variables for plug-flow reactor with N species

Source of Equations	Number of Equations	Variables or Derivatives Involved
Fundamental conservation principles: mass, x-momentum, energy, species	$3+N$	$\frac{d\rho}{dx}, \frac{dv_x}{dx}, \frac{dP}{dx}, \frac{dh}{dx}, \frac{dY_i}{dx} (i=1,2,\ldots,N), \dot{\omega}_i (i=1,2,\ldots,N)$
Mass action laws	N	$\dot{\omega}_i (i=1,2,\ldots,N)$
Equation of state	1	$\frac{d\rho}{dx}, \frac{dP}{dx}, \frac{dT}{dx}, \frac{dMW_{mix}}{dx}$
Calorific equation of state	1	$\frac{dh}{dx}, \frac{dT}{dx}, \frac{dY_i}{dx} (i=1,2,\ldots,N)$
Definition of mixture molecular weight	1	$\frac{dMW_{mix}}{dx}, \frac{dY_i}{dx} (i=1,2,\ldots,N)$

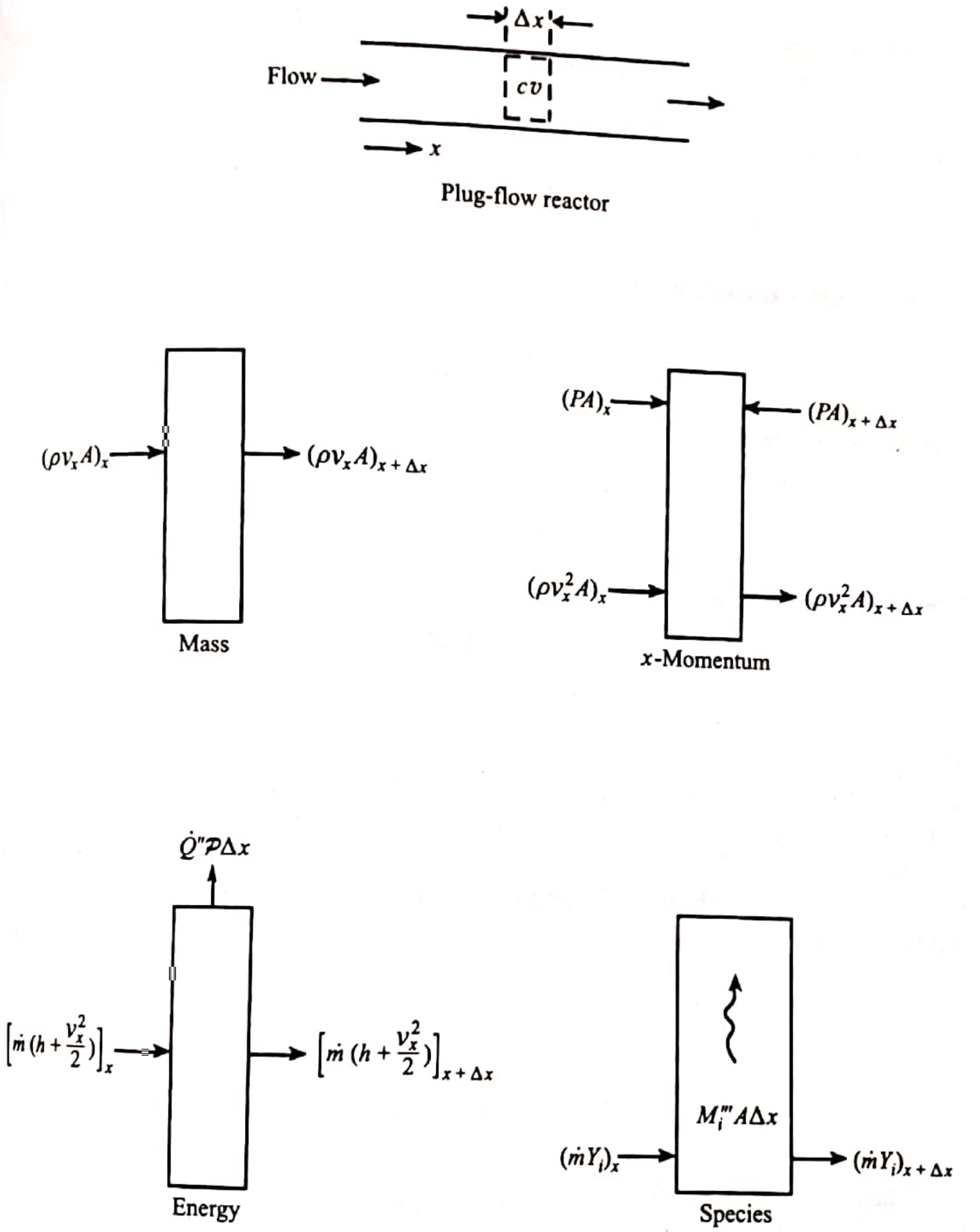

Figure 6.11 Control volumes showing fluxes of mass, x-momentum, energy, and species for a plug-flow reactor.

retaining them, however, clearly reminds us of the importance of chemical reactions in our analysis. Although not shown in Table 6.1, the following parameters are treated as known quantities, or functions, and are necessary to obtain a solution: $\dot{m}$, $k_i(T)$, $A(x)$, and $\dot{Q}''(x)$. The area function $A(x)$ defines the cross-sectional area of the reactor as a function of x; thus, our model reactor could represent a nozzle, or a diffuser, or any particular one-dimensional geometry, and not just a constant cross-sectional device as suggested by the top sketch in Fig. 6.11. The heat flux function $\dot{Q}''(x)$, although explicitly indicating that the wall heat flux is known, is also intended to indicate that the heat flux may be calculated from a given wall-temperature distribution.

With reference to the fluxes and control volumes illustrated in Fig. 6.11, we can easily derive the following conservation relationships:

Mass Conservation

$$\frac{d(\rho v_x A)}{dx} = 0. \quad (6.39)$$

x-Momentum Conservation

$$\frac{dP}{dx} + \rho v_x \frac{dv_x}{dx} = 0. \quad (6.40)$$

Energy Conservation

$$\frac{d(h + v_x^2/2)}{dx} + \frac{\dot{Q}''\mathcal{P}}{\dot{m}} = 0. \quad (6.41)$$

Species Conservation

$$\frac{dY_i}{dx} - \frac{\dot{\omega}_i MW_i}{\rho v_x} = 0. \quad (6.42)$$

The symbols v_x and $\mathcal{P}$ represent the axial velocity and local perimeter of the reactor, respectively. All of the other quantities have been defined previously. The derivation of these equations is left as an exercise for the reader (see problem 6.1).

To obtain a useful form of the equations where the individual variable derivatives can be isolated, Eqns. 6.39 and 6.41 can be expanded and rearranged to yield the following:

$$\frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{v_x}\frac{dv_x}{dx} + \frac{1}{A}\frac{dA}{dx} = 0 \quad (6.43)$$

$$\frac{dh}{dx} + v_x \frac{dv_x}{dx} + \frac{\dot{Q}''\mathcal{P}}{\dot{m}} = 0. \quad (6.44)$$

The $\dot{\omega}_i$s appearing in Eqn. 6.42 can be expressed using Eqn. 4.31, with the $[X_i]$s transformed to Y_is.

The functional relationship of the ideal-gas calorific equation of state,

$$h = h(T, Y_i), \quad (6.45)$$

can be exploited using the chain rule to relate dh/dx and dT/dx, yielding

$$\frac{dh}{dx} = c_p \frac{dT}{dx} + \sum_{i=1}^{N} h_i \frac{dY_i}{dx}. \quad (6.46)$$

To complete our mathematical description of the plug-flow reactor, we differentiate the ideal-gas equation of state,

$$P = \rho R_u T / MW_{mix}, \quad (6.47)$$

to yield

$$\frac{1}{P}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{MW_{mix}}\frac{dMW_{mix}}{dx}, \tag{6.48}$$

where the mixture molecular weight derivative follows simply from its definition expressed in terms of species mass fractions, i.e.,

$$MW_{mix} = \left[\sum_{i=1}^{N} Y_i / MW_i\right]^{-1} \tag{6.49}$$

and

$$\frac{dMW_{mix}}{dx} = -MW_{mix}^2 \sum_{i=1}^{N} \frac{1}{MW_i}\frac{dY_i}{dx}. \tag{6.50}$$

Equations 6.40, 6.42, 6.43, 6.44, 6.46, 6.48, and 6.49 contain in a linear fashion the derivatives $d\rho/dx$, dv_x/dx, dP/dx, dh/dx, dY_i/dx ($i = 1, 2, \ldots, N$), dT/dx, and dMW_{mix}/dx. The number of equations can be reduced by eliminating some of the derivatives by substitution. One logical choice is to retain the derivatives dT/dx, $d\rho/dx$, and dY_i/dx ($i = 1, 2, \ldots, N$). With this choice, the following equations constitute the system of ODEs that must be integrated starting from an appropriate set of initial conditions:

$$\frac{d\rho}{dx} = \frac{\left(1 - \dfrac{R_u}{c_p MW_{mix}}\right)\rho^2 v_x^2 \left(\dfrac{1}{A}\dfrac{dA}{dx}\right) + \dfrac{\rho R_u}{v_x c_p MW_{mix}} \sum_{i=1}^{N} MW_i \dot{\omega}_i \left(h_i - \dfrac{MW_{mix}}{MW_i} c_p T\right)}{P\left(1 + \dfrac{v_x^2}{c_p T}\right) - \rho v_x^2}, \tag{6.51}$$

$$\frac{dT}{dx} = \frac{v_x^2}{\rho c_p}\frac{d\rho}{dx} + \frac{v_x^2}{c_p}\left(\frac{1}{A}\frac{dA}{dx}\right) - \frac{1}{v_x \rho c_p}\sum_{i=1}^{N} h_i \dot{\omega}_i MW_i, \tag{6.52}$$

$$\frac{dY_i}{dx} = \frac{\dot{\omega}_i MW_i}{\rho v_x} \tag{6.53}$$

Note that in Eqns. 6.41 and 6.52, $\dot{Q}''$ has been set to zero for simplicity.

A residence time, t_R, can also be defined, and one more equation added to the set:

$$\frac{dt_R}{dx} = \frac{1}{v_x}. \tag{6.54}$$