Reacting System Modeling

Monday, September 25, 2017 5:59 PM

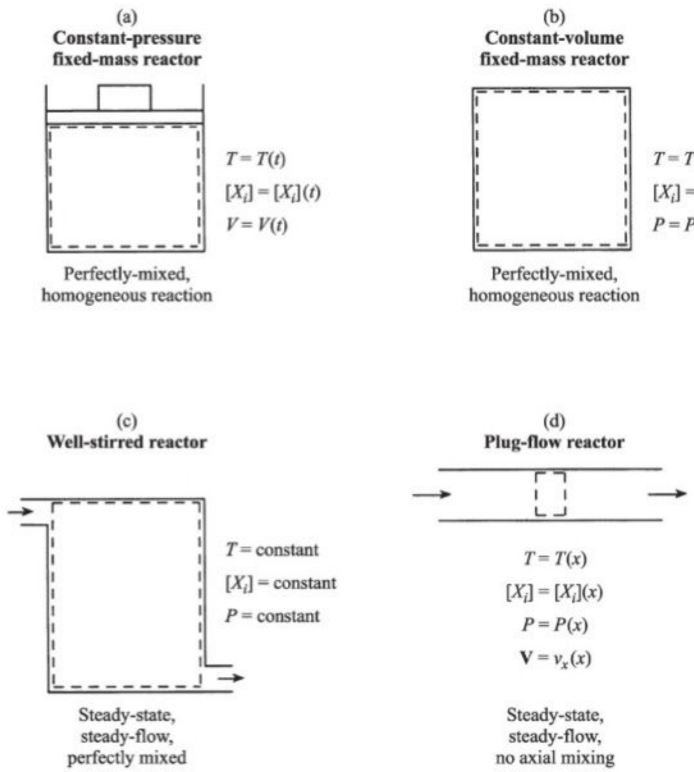

Figure 6.1 Simple chemically reacting systems: (a) constant-pressure, fixed mass; (b) constant-volume, fixed mass; (c) well-stirred reactor; (d) plug-flow reactor.

Const. P fixed mass reactor

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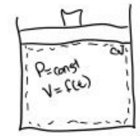

Cons. of energy

$$m\frac{du}{dt} = \cancel{\dot{E}_{in}}^{0} - \cancel{\dot{E}_{out}}^{0} + \dot{Q}_{in} - \dot{W}_{out}$$

$$\frac{dh}{dt} = \frac{du}{dt} + P\frac{dV}{dt} \Rightarrow \frac{du}{dt} = \frac{dh}{dt} - P\frac{dV}{dt}$$

$$\frac{\dot{W}}{m} = P\frac{dV}{dt}$$

$$\boxed{\frac{\dot{Q}}{m} = \frac{dh}{dt}}$$

$$h = \frac{H}{m} = \frac{\sum_{i=1}^{N} N_i \bar{h}_i}{m}$$

$$\frac{dh}{dt} = \frac{1}{m}\frac{d}{dt}\left(\sum_i N_i \bar{h}_i\right) = \frac{1}{m}\left(\sum_i\left(\bar{h}_i \frac{dN_i}{dt}\right) + \sum_i\left(N_i \frac{d\bar{h}_i}{dt}\right)\right)$$

if I.G., then $\bar{h}_i = \bar{h}_i(T \text{ only})$

$$\frac{d\bar{h}_i}{dt} = \frac{\partial \bar{h}_i}{\partial T}\frac{\partial T}{\partial t} = \bar{c}_{p_i}\frac{\partial T}{\partial t}$$

$$\frac{\dot{Q}}{\cancel{m}} = \frac{1}{\cancel{m}}\left(\sum_i\left(\bar{h}_i \frac{dN_i}{dt}\right) + \sum_i\left(N_i c_{p_i}\frac{dT}{dt}\right)\right)$$

$$N_i = V[X_i]$$

$$\frac{dN_i}{dt} = V\frac{d[X_i]}{dt} + [X_i]\frac{dV}{dt}$$

$$\frac{dN_i}{dt} = V\dot{\omega}$$

$$\dot{\omega} = \frac{d[x_i]}{dt} + \frac{[x_i]}{V}\frac{dV}{dt}$$

$$\Rightarrow \dot{Q} = \sum_i(\bar{h}_i V\dot{\omega}_i) + \sum_i\left(V[x_i]\bar{c}_{p_i}\frac{dT}{dt}\right)$$

$$\frac{\dot{Q}}{V} = \sum_i(\bar{h}_i\dot{\omega}_i) + \sum_i\left([x_i]\bar{c}_{p_i}\frac{dT}{dt}\right)$$

$$\boxed{\frac{dT}{dt} = \frac{\dot{Q}/V - \sum_i(\bar{h}_i\dot{\omega}_i)}{\sum_i([x_i]\bar{c}_{p_i})}}$$

$$\frac{dT}{dt} = f([x_i], T)$$

$$\dot{\omega}_i = \frac{d[x_i]}{dt} + \frac{[x_i]}{V}\frac{dV}{dt}$$

$$\hookrightarrow \frac{d[x_i]}{dt} = \dot{\omega}_i - \frac{[x_i]}{V}\frac{dV}{dt}$$

I.G. $PV = \sum_i N_i R_u T$

$P = \text{const}$

$$\frac{dV}{dt} = \frac{1}{P}\left(R_u T\sum_i\frac{dN_i}{dt} + \sum N_i R_u\frac{dT}{dt}\right)$$

$$\frac{d[x_i]}{dt} = \dot{\omega}_i - \frac{[x_i]\cancel{\frac{1}{P}}}{\cancel{\frac{1}{P}}\sum_i N_i \cancel{R_u} T}\left(\cancel{R_u} T\sum_i\frac{dN_i}{dt} + \sum N_i\cancel{R_u}\frac{dT}{dt}\right)$$

$$\frac{d[x_i]}{dt} = \dot{\omega}_i - \frac{[x_i]}{\sum_i N_i}\left(\sum_i\frac{dN_i}{dt}\right) - \frac{[x_i]}{T}\frac{dT}{dt}$$

$$\frac{dN_i}{dt} = V\dot{\omega}_i$$

$$N_i = V[x_i]$$

$$\boxed{\frac{d[x_i]}{dt} = \dot{\omega}_i - \frac{[x_i]}{\sum_j[x_j]}\sum_i\dot{\omega}_i - \frac{[x_i]}{T}\frac{dT}{dt}}$$

$$\frac{d[x_i]}{dt} = f([x_i], T)$$

I.C. $T(t=0) = T_0$

$[x_i](t=0) = [x_i]_0$