Supplementary note for reactor analysis

1. Tracer response to an ideal PFR

Mass balance equation:

$$\Delta V\frac{\partial C}{\partial t}=QC-Q(C+\Delta C)$$

$$\Delta V\frac{\partial C}{\partial t}=-Q\Delta C$$

$$\frac{\partial C}{\partial t}=-Q\frac{\Delta C}{\Delta V}=-\frac{Q}{A}\cdot\frac{\Delta C}{\Delta x}=-v\cdot\frac{\Delta C}{\Delta x}$$ (v = velocity of flow)

$\Delta x\to 0$

$$\frac{\partial C}{\partial t}=-v\cdot\frac{\partial C}{\partial x}$$

let $u=t-\frac{x}{v}$

apply chain rule:

$$\frac{\partial C}{\partial t}=\frac{\partial C}{\partial u}\cdot\frac{\partial u}{\partial t}=\frac{\partial C}{\partial u}$$

$$\frac{\partial C}{\partial x}=\frac{\partial C}{\partial u}\cdot\frac{\partial u}{\partial x}=-\frac{1}{v}\cdot\frac{\partial C}{\partial u}$$

therefore, equation $\frac{\partial C}{\partial t}=-v\cdot\frac{\partial C}{\partial x}$ holds for any $C=F(u)$

$$C(x,t)=F\left(t-\frac{x}{v}\right)$$

$$C_0=C(x=0,t)=F(t)$$

$$C_e=C(x=L,t)=F\left(t-\frac{L}{v}\right)$$

$$\frac{L}{v}=\frac{A\cdot L}{A\cdot v}=\frac{V}{Q}=\tau$$

$\therefore$ when $C_0=F(t)$, $C_e=F(t-\tau)$

2. General solution for CSTR, 1st order reaction

Mass balance equation:

$$V\frac{dC}{dt}=QC_0-QC-kCV$$

$$\frac{dC}{dt}=\frac{1}{\tau}C_0-\left(\frac{1}{\tau}+k\right)C$$

let $\beta=\frac{1}{\tau}+k$

$$C'+\beta C=\frac{1}{\tau}C_0$$

multiply both sides of the equation by an integrating factor $e^{\beta t}$

$$e^{\beta t}(C'+\beta C)=\frac{1}{\tau}C_0e^{\beta t}$$

$$\left(Ce^{\beta t}\right)'=\frac{1}{\tau}C_0e^{\beta t}$$

$$Ce^{\beta t}=\frac{C_0}{\tau}\int e^{\beta t}dt=\frac{1}{\tau}\cdot\frac{C_0}{\beta}e^{\beta t}+K \qquad (K = \text{constant})$$

$$C=\frac{1}{\tau}\cdot\frac{C_0}{\beta}+Ke^{-\beta t}$$

initial condition: when $t=0$, $C=C_0$

$$K=C_0-\frac{1}{\tau}\cdot\frac{C_0}{\beta}$$

applying K to the equation,

$$C=\frac{1}{\tau}\cdot\frac{C_0}{\beta}+\left(C_0-\frac{1}{\tau}\cdot\frac{C_0}{\beta}\right)e^{-\beta t}$$

$$\frac{C}{C_0}=\frac{1}{1+k\tau}\left\{1+e^{-(k+1/\tau)t}\right\}+e^{-(k+1/\tau)t}$$

for steady state solution, $t\to\infty$

$$\frac{C}{C_0}=\frac{1}{1+k\tau}$$