P 8-3

$$A \rightleftharpoons D$$
$$A \rightleftharpoons U$$

(a) Balance equations

$$\frac{dC_A}{dt} = -k_1\left[C_A - \frac{C_D}{K_{1A}}\right] - k_2\left[C_A - \frac{C_U}{K_{2A}}\right]$$

$$\frac{dC_D}{dt} = k_1\left[C_A - \frac{C_D}{K_{1A}}\right]$$

$$\frac{dC_C}{dt} = k_2\left[C_A - \frac{C_C}{K_{2A}}\right]$$

$k_1 = 1.0$

$k_2 = 100$

$K_{1A} = 1.0$

$K_{2A} = 1.5$

$C_{A0} = 1$

$$X = 1 - \frac{C_A}{C_{A0}}$$

⇒ Solve using ODE solver, for time profile

b) C_U is max. at $t = 0.04$ min ($C_A = 0.59$ mol/dm³)

(c) $C_{Ae} = 0.08 \ mol/dm^3$

$C_{De} = 0.8 \ mol/dm^3$

$C_{Ue} = 0.12 \ mol/dm^3$

(d) CSTR

$$\tau = \frac{C_{A0} - C_A}{-r_A)_{exit}}$$

⇒ Algebraic equations

1) $$C_{A0} - C_A - \tau\left[k_1\left(C_A - \frac{C_D}{K_{1A}}\right) + k_2\left(C_A - \frac{C_U}{K_{2A}}\right)\right] = 0$$

2) $$-C_D + \tau\left[k_1\left(C_A - \frac{C_D}{K_{1A}}\right)\right] = 0$$

3) $$-C_U + \tau\left[k_2\left(C_A - \frac{C_U}{K_{2A}}\right)\right] = 0$$

⇒ Solve simultaneously with $\tau = 1, 10, 100$ min

$\tau = 10$ min → $C_A = 0.13$; $C_D = 0.67$; $C_U = 0.2 \ \frac{mol}{dm^3}$