

Chap 8.

8.1 가 1

$A \rightarrow R \rightarrow S, \quad k_1, k_2$

8.1 8.2

8.2

A 가 R R S 가

가 . R

가

PFR() MFR()

8.1

PFR 가

PFR,

Chap. 3

가

PFR

t τ

$$\frac{C_A}{C_{A0}} = e^{-k_1\tau}$$

$$\frac{C_R}{C_{A0}} = \frac{k_1}{k_2 - k_1} (e^{-k_1\tau} - e^{-k_2\tau})$$

$$C_S = C_{A0} - C_A - C_R$$

$$\frac{C_{R,max}}{C_{A0}} = \left(\frac{k_1}{k_2} \right)^{k_2/(k_2-k_1)}$$

$$\tau_{p,opt} = \frac{1}{k_{\log mean}} = \frac{\ln(k_2/k_1)}{k_2 - k_1}$$

MFR

8.4

A

$$F_{A0} = F_A + (-r_A)V$$

$$vC_{A0} = vC_A + k_1 C_A V$$

$$\tau_m = \frac{V}{v}$$

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + k_1 \tau_m}$$

R

$$vC_{R0} = vC_R + (-r_R)V$$

$$0 = vC_R + (-k_1 C_A + k_2 C_R)V$$

$$C_R = \frac{k_1 C_A}{1 + k_2 \tau_m}$$

$$C_R = \frac{k_1 \tau_m C_{A0}}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}$$

C_S

$$C_{A0} = C_A + C_R + C_S$$

R 가 가

$$\frac{dC_R}{d\tau_m} = 0$$

$$\tau_{m,opt} = \frac{1}{\sqrt{k_1 k_2}}$$

R

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{\left[\left(k_2/k_1\right)^{1/2} + 1\right]^2}$$

$k_1 = k_2$

,

R

가

가

PFR

MFR

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$k_2/k_1 > 1$

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R PFR 가 MFR
 8.4 (b) 8.5(b) k_2/k_1
 8.6 R PFR 가

8.2 1 0



$$-r_A = k_1 C_A$$

$$r_R = k_1 C_A - k_2$$

$$t=0 \quad C_A = C_{A0}, \quad C_{R0} = C_{S0} = 0$$

$$\frac{dC_A}{dt} = -k_1 C_A$$

$$C_A = C_{A0} \exp(-k_1 t)$$

$$\frac{dC_R}{dt} = k_1 C_A - k_2$$

$$\frac{dC_R}{dt} = k_1 C_{A0} \exp(-k_1 t) - k_2$$

$$C_R = C_{A0} - C_{A0} \exp(-k_1 t) - k_2 t$$

R 가 가

$$\frac{dC_R}{dt} = k_1 C_{A0} \exp(-k_1 t) - k_2 = 0$$

$$t_{R,max} = \frac{1}{k_1} \ln \frac{1}{K}$$

8.7

8.3 0 1



$$-r_A = k_1$$

$$r_R = \begin{cases} k_1 - k_2 C_R & A \text{ present} \\ -k_2 C_R & A \text{ absent} \end{cases}$$

$$t=0 \quad C_A = C_{A0}, \quad C_{R0} = C_{S0} = 0$$

$$\frac{dC_A}{dt} = -k_1$$

$$C_A = C_{A0} - k_1 t$$

A 가 $t < \frac{C_{A0}}{k_1}$

$$\frac{dC_R}{dt} = k_1 - k_2 C_R$$

Laplace transform

$$\bar{C}_R - C_{R0} = \frac{k_1}{s} - k_2 \bar{C}_R$$

$$\bar{C}_R = \frac{k_1}{s(s+k_2)}$$

$$\bar{C}_R = \frac{k_1}{k_2} \left(\frac{1}{s} - \frac{1}{s+k_2} \right)$$

$$C_R = \frac{k_1}{k_2} (1 - \exp(-k_2 t))$$

$t = \frac{C_{A0}}{k_1}$ R

$$C_R = \frac{k_1}{k_2} \left(1 - \exp\left(-\frac{k_2 C_{A0}}{k_1}\right) \right)$$

A 가 $t > \frac{C_{A0}}{k_1}$

$$\frac{dC_R}{dt} = -k_2 C_R$$

$$t = \frac{C_{A0}}{k_1} \quad C_R = \frac{k_1}{k_2} \left(1 - \exp\left(-\frac{k_2 C_{A0}}{k_1}\right) \right)$$

$$C_R = C_1 \exp(-k_2 t)$$

$$\frac{k_1}{k_2} \left(1 - \exp\left(-\frac{k_2 C_{A0}}{k_1}\right) \right) = C_1 \exp\left(-\frac{k_2 C_{A0}}{k_1}\right)$$

$$C_1 = \frac{k_1}{k_2} \left\{ \exp\left(\frac{k_2 C_{A0}}{k_1}\right) - 1 \right\}$$

$$C_R = \frac{k_1}{k_2} \left\{ \exp\left(\frac{k_2 C_{A0}}{k_1}\right) - 1 \right\} \exp(-k_2 t)$$

R 가 가 $t = \frac{C_{A0}}{k_1}$.

: A 가 $t > \frac{C_{A0}}{k_1}$ $\frac{dC_R}{dt} = -k_2 C_R = 0$,

R 0, A 가 $t < \frac{C_{A0}}{k_1}$ $\frac{dC_R}{dt} = k_1 - k_2 C_R = 0$

가 , , $t < \frac{C_{A0}}{k_1}$. $\frac{dC_R}{dt} = 0$

8.8

$$t = \frac{C_{A0}}{k_1}$$

8.4 가 가

2 가



$$-r_A = -\frac{dC_A}{dt} = k_1 C_A^2$$

$$r_R = \frac{dC_R}{dt} = k_1 C_A^2 - k_2 C_R^2$$

$$r_S = \frac{dC_S}{dt} = k_2 C_R^2$$

$$k_1 = k_2 = 1, \quad t=0 \quad C_A = 1, \quad C_R = C_S = 0$$

Matlab m-file(ch8_4.m, ch8-4f.m) .

8.5 가



$$-r_A = -\frac{dC_A}{dt} = k_1 C_A - k_2 C_R$$

$$r_R = \frac{dC_R}{dt} = k_1 C_A - (k_2 + k_3) C_R + k_4 C_S$$

$$r_S = \frac{dC_S}{dt} = k_3 C_R - k_4 C_S$$

$$t=0 \quad C_A = C_{A0}, \quad C_R = C_S = 0$$

Laplace transform

$$s\bar{C}_A - C_{A0} = -k_1\bar{C}_A + k_2\bar{C}_R$$

$$s\bar{C}_R = k_1\bar{C}_A - (k_2 + k_3)\bar{C}_R + k_4\bar{C}_S$$

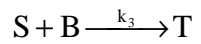
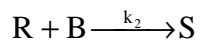
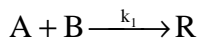
$$s\bar{C}_S = k_3\bar{C}_R - k_4\bar{C}_S$$

$$\bar{C}_A, \bar{C}_R, \bar{C}_S$$

$$k_1 = k_2 = k_3 = k_4 = 1, \quad t=0 \quad C_A = 1, \quad C_R = C_S = 0$$

Matlab m-file(ch8_5.m, ch8-5f.m)

8.6 가 -

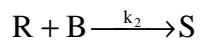
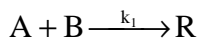


A, R, S, T

, B

:

2 가 -



가

가

$$r_A = \frac{dC_A}{dt} = -k_1 C_A C_B$$

$$r_B = \frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_R C_B$$

$$r_R = \frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$$

$$r_S = \frac{dC_S}{dt} = k_2 C_R C_B$$

PFR

$$\frac{r_R}{r_A} = \frac{dC_R}{dC_A} = -1 + \frac{k_2 C_R}{k_1 C_A}$$

$$\frac{dC_R}{dC_A} - \frac{k_2 C_R}{k_1 C_A} = -1$$

$$\frac{d(PC_R)}{dC_A} = Q$$

$$P \frac{dC_R}{dC_A} + \frac{dP}{dC_A} C_R = Q$$

$$\frac{dC_R}{dC_A} + \frac{1}{P} \frac{dP}{dC_A} C_R = \frac{Q}{P}$$

$$d(\ln P) = -\frac{k_2}{k_1} d(\ln C_A)$$

$$P = C_A^{-k_2/k_1}, \quad Q = -C_A^{-k_2/k_1}$$

$$C_R = C_A^{k_2/k_1} \int_{C_{A0}}^{C_A} -C_A^{-k_2/k_1} dC_A$$

$$\frac{k_2}{k_1} \neq 1$$

$$C_R = \frac{1}{1 - k_2/k_1} \left[C_{A0}^{1-k_2/k_1} - C_A^{1-k_2/k_1} \right] C_A^{k_2/k_1}$$

$$\frac{C_R}{C_{A0}} = \frac{1}{1 - k_2/k_1} \left[\left(\frac{C_A}{C_{A0}} \right)^{k_2/k_1} - \frac{C_A}{C_{A0}} \right]$$

$$\frac{k_2}{k_1} = 1$$

$$C_R = C_A \ln \left(\frac{C_A}{C_{A0}} \right)$$

R

$$\frac{dC_R}{dC_A} = -1 + \frac{k_2 C_R}{k_1 C_A} = 0$$

$$\frac{k_2}{k_1} \neq 1$$

$$\left(\frac{C_R}{C_{A0}} \right)_{\max} = \frac{1}{1 - k_2/k_1} \left[\left(\frac{k_2}{k_1} \frac{C_R}{C_{A0}} \right)_{\max}^{k_2/k_1} - \frac{k_2}{k_1} \left(\frac{C_R}{C_{A0}} \right)_{\max} \right]$$

$$\left(\frac{C_R}{C_{A0}} \right)_{\max} = \left(\frac{k_2}{k_1} \right)^{k_2/(k_1 - k_2)} = \left(\frac{k_1}{k_2} \right)^{k_2/(k_2 - k_1)}$$

$$\frac{k_2}{k_1} = 1$$

$$C_{R,\max} = C_{R,\max} \ln \left(\frac{C_{R,\max}}{C_{A0}} \right)$$

$$C_{R,\max} = \frac{1}{e}$$

A-R-S

$$0 = \Delta C_A + \Delta C_R + \Delta C_S$$

B

R 1 B, S 가 2 B 가

$$\Delta C_B + \Delta C_R + 2\Delta C_S = 0$$

MFR

MFR

$$\tau_m = \frac{C_{A0} - C_A}{-r_A} = \frac{-C_R}{-r_R}$$

$$\frac{C_{A0} - C_A}{k_1 C_A C_B} = \frac{-C_R}{k_2 C_R C_B - k_1 C_A C_B}$$

$$\frac{-C_R}{C_{A0} - C_A} = -1 + \frac{k_2 C_R}{k_1 C_A}$$

R

$$C_R = \frac{C_A (C_{A0} - C_A)}{C_A + (k_2/k_1)(C_{A0} - C_A)}$$

R 가 가

$$\frac{dC_R}{dC_A} = 0 \quad C_A$$

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{[1 + (k_2/k_1)^2]^{1/2}}$$

PFR

가 8.13 , MFR

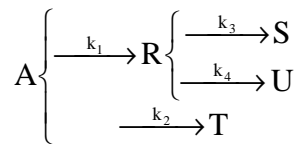
가 8.14

8.13 8.14

8.2

가

8.7 Denbigh



1

$$-r_A = -\frac{dC_A}{dt} = (k_1 + k_2)C_A$$

$$r_R = \frac{dC_R}{dt} = k_1C_A - (k_3 + k_4)C_R$$

$$r_S = \frac{dC_S}{dt} = k_3C_R$$

$$r_T = \frac{dC_T}{dt} = k_2C_A$$

$$r_U = \frac{dC_U}{dt} = k_4C_R$$

$$t=0 \quad C_A = C_{A0}, \quad C_R = C_{R0}, \quad C_S = C_{S0}, \quad C_T = C_{T0}, \quad C_U = C_{U0}$$

A-R-S

1 가