Supplementary Notes for Catalytic Engineering

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Contents

1 Earliness and Lateness of Mixing

Assume that the reaction kinetic is dominated by the power rule, that is, $-r_A = \frac{dC_A}{dt} = kC_A^n$ for reaction $A \to R$. Then, consider the case only that $k = 1[\mathbf{L}^{n-1} \cdot \mathbf{min}^{-1} \cdot \mathbf{mol}^{1-n}]$, $C_{A0} = 1[\mathbf{mol} \cdot \mathbf{L}^{-1}]$, and $F_{A0} = 1[\mathbf{mol} \cdot \mathbf{s}^{-1}]$. Also, for the convenience of analyzing, let the volume of each reactors be equal to $1[\mathbf{L}]$.

1.1 Case 1: $n > 1$.

For this case, $-r_A = kC_A^n = kC_{A0}^n(1 - X_A)^n$. For our case, let $n = 2$. Then, $-r_A = (1 - X_A)^2$.

Subcase 1: Early Mixing. First, reactant passes the MFR reactor, and then passes the PFR reactor. Let X_M, X_P be a conversion fraction for **MFR** and **PFR** reactor. Then, the performance of **MFR** would be :

$$\begin{aligned} (X_M) \cdot \left(-\frac{1}{r_A}\right)_{X_M} &= 1 \\ \frac{X_M}{(1 - X_M)^2} &= 1 \\ X_M &= X_M^2 - 2X_M + 1 \\ X_M &= \frac{3 - \sqrt{5}}{2} (\because X_M < 1) \end{aligned}$$

Thus, $X_M \simeq 0.382$. After that, the performance of **PFR** would be :

$$\begin{aligned} \int_{X_M}^{X_P} \frac{dX_A}{-r_A} &= 1 \\ \int_{X_M}^{X_P} \frac{dX_A}{(1 - X_A)^2} &= 1 \\ \frac{1}{1 - X_A}\Big|_{X_M}^{X_P} &= 1 \\ \frac{1}{1 - X_P} - \frac{1}{1 - X_M} &= 1 \\ X_P &= \frac{1}{2 - X_M} \end{aligned}$$

Thus, $X_P \simeq 0.618$. That is, the conversion fraction of final product is 0.618 in this case.

Subcase 2: Late Mixing. First, reactant passes the PFR reactor and then passes the MFR reactor. The performance of **PFR** would be :

$$\int_0^{X_P} \frac{dX_A}{-r_A} = 1$$
$$\int_0^{X_P} \frac{dX_A}{(1-X_A)^2} = 1$$
$$\frac{1}{1-X_P} - 1 = 1$$
$$X_P = 0.5$$

After that, the performance of **MFR** would be :

$$(X_M - X_P) \cdot \left(\frac{1}{-r_A}\right)_{X_M} = 1$$
$$\frac{X_M - X_P}{(1-X_M)^2} = 1$$
$$2X_M^2 - 6X_M + 3 = 0$$
$$X_M = \frac{3-\sqrt{3}}{2}$$

Thus, $X_M \simeq 0.634$. That is, the conversion fraction of final product is 0.634 in this case. Finally, it implies that the Late Mixing is favorable in the case $n > 1$.

1.2 Case 2: $n < 1$.

For our case, let $n = 0.5$. Then, $-r_A = (1-X_A)^{0.5}$.

Subcase 1: Early Mixing. The performance of **MFR** would be :

$$X_M \cdot \left(\frac{1}{-r_A}\right)_{X_M} = 1$$
$$\frac{X_M}{(1-X_M)^0.5} = 1$$
$$X_M^2 = X_M - 1$$
$$X_M = \frac{-1+\sqrt{5}}{2}$$

Thus, $X_M \simeq 0.618$. After that, the performance of **PFR** would be :

$$\int_{X_M}^{X_P} \frac{dX_A}{-r_A} = 1$$
$$\int_{X_M}^{X_P} \frac{dX_A}{(1-X_A)^{0.5}} = 1$$
$$-2(1-X-A)^{0.5}|_{X_M}^{X_P} = 1$$
$$X_P = X_M + \sqrt{1-X_M} - \frac{1}{4}$$

Thus, $X_P \simeq 0.986$. That is, the conversion fraction of final product is 0.986 in this case.

Subcase 2: Late Mixing. The performance of **PFR** would be :

$$\int_0^{X_P} \frac{dX_A}{-r_A} = 1$$
$$\int_0^{X_P} \frac{dX_A}{(1-X_A)^{0.5}} = 1$$
$$(1-X_P)^{0.5} = \frac{1}{2}$$

Thus, $X_P = 0.75$. After that, the performance of **MFR** would be :

$$(X_M - X_P) \cdot \left(\frac{1}{-r_A}\right)_{X_M} = 1$$
$$(X_M - X_P) \cdot \frac{1}{(1 - X_M)^{0.5}} = 1$$
$$X_M - X_P = (1 - X_M)^{0.5}$$
$$X_M^2 - (2X_P - 1)X_M + (X_P^2 - 1) = 0$$

Thus, $X_M = 0.957$. That is, the conversion fraction of final product is 0.957 in this case. Finally, it implies that the Early Mixing is favorable in the case $n < 1$.

1.3 Case 3: $n = 1$.

For our case, $-r_A = 1 - X_A$.

Subcase 1: Early Mixing. The performance of **MFR** :

$$X_M \cdot \frac{1}{1 - X_M} = 1$$
$$X_M = 0.5$$

Then,

$$\int_{X_M}^{X_P} \frac{dX_A}{1 - X_A} = 1$$
$$-\ln(1 - X_A)|_{X_M}^{X_P} = 1$$
$$X_P = 1 - \frac{1}{2e}$$

Subcase 2: Late Mixing. The performace :

$$\int_{0}^{X_P} \frac{dX_A}{1 - X_A} = 1$$
$$1 - X_P = \frac{1}{e}$$

Then,

$$(X_M - X_P)\frac{1}{1 - X_M} = 1$$
$$X_M - X_P = 1 - X_M$$
$$X_M = \frac{1}{2}(1 + X_P)$$

Thus, $X_M = 1 - \frac{1}{2e}$. That is, Early Mixing and Late Mixing have the equal conversion rate for $n = 1$.