CEN416
PROCESS DESIGN II

Selectivity in Reactions in Series (Consecutive Reactions)

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

$$r_A = -k_1 C_A$$

$$r_R = k_1 C_A - k_2 C_R$$

$$r_S = k_2 C_R$$

For irreversible reactions in series the mixing of fluid of different composition is the key to the formation of intermediate.

The maximum possible amount of any and all intermediates is obtained if fluids of different compositions and at different stages of conversion are not allowed to mix.

Quantitative Analysis

Batch Reactor

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

$$C_R = C_{A0} k_1 \left(\frac{e^{-k_1 t}}{k_2 - k_1} + \frac{e^{-k_2 t}}{k_1 - k_2} \right)$$

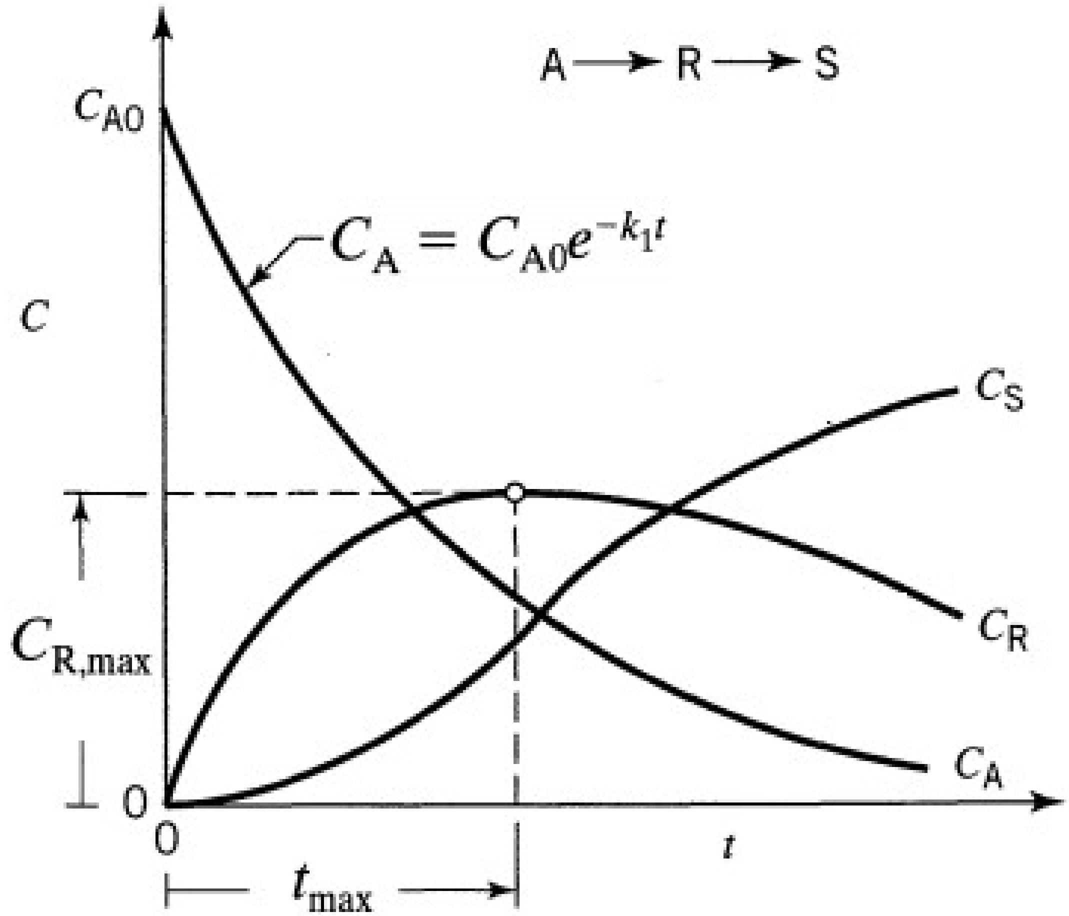
$$C_S = \frac{C_{A0}}{k_2 - k_1} \left[k_2 \left[1 - e^{-k_1 t} \right] - k_1 \left[1 - e^{-k_2 t} \right] \right]$$

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

$$t_{max} = \frac{1}{k_{log\ mean}} = \frac{\ln (k_2/k_1)}{k_2 - k_1}$$

Quantitative Analysis

Batch Reactor



Quantitative Analysis

PFR

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

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

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

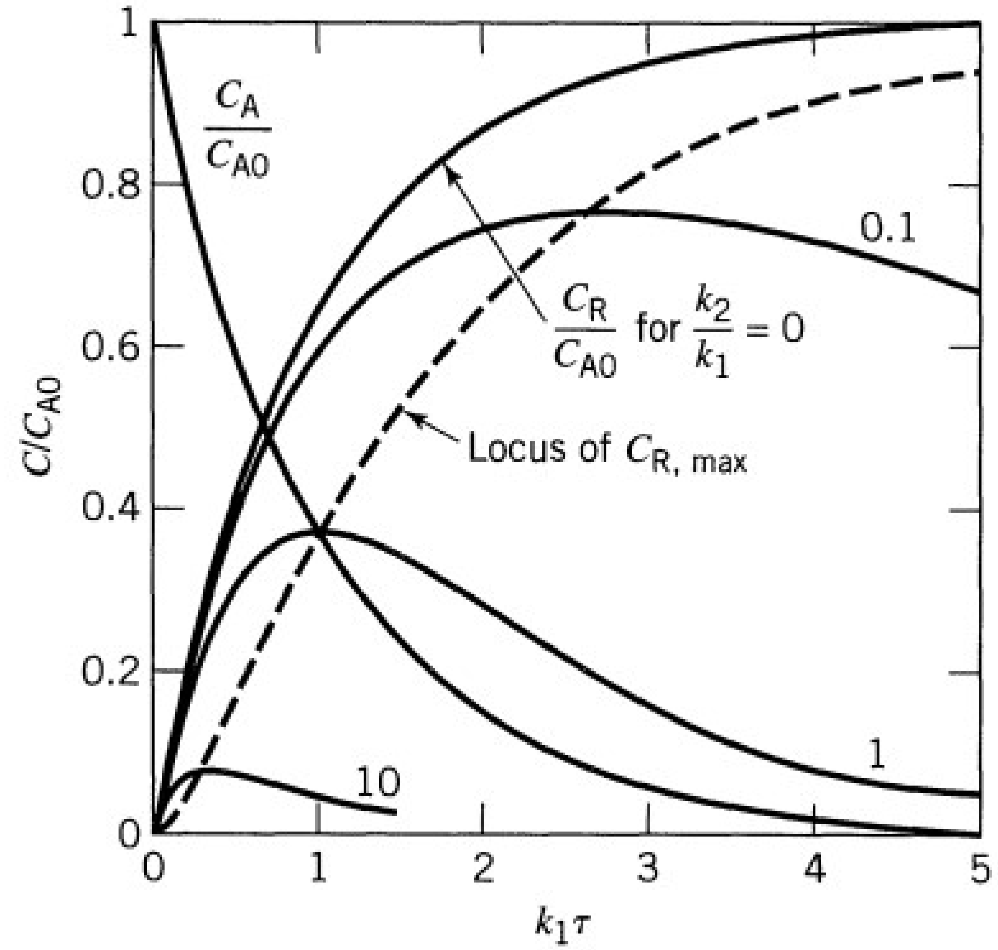
$$C_S = \frac{C_{A0}}{k_2 - k_1}\left[k_2\left[1 - e^{-k_1 \tau}\right] - k_1\left[1 - e^{-k_2 \tau}\right]\right]$$

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

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

Quantitative Analysis

PFR



REFERENCES

1. Sinnot, R.K. 1999, Coulson's & Richardson's Chemical Engineering, Volume 6, Chemical Engineering Design, ButterWorth Heinemann, Oxford.

2. Turton R., Bailie R.C., Whitin W.C., Shaeiwitz J.A. 1998, Analysis, Synthesis and Design of Chemical Processes, Prentice Hall, New Jersey.