

**CEN416**  
**PROCESS DESIGN II**

## Quantitative Analysis

MFR

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

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

$$vC_{A0} = vC_A + k_1C_AV$$

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

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



$$0 = vC_R + (-k_1C_A + k_2C_R)V$$



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

## Quantitative Analysis

MFR

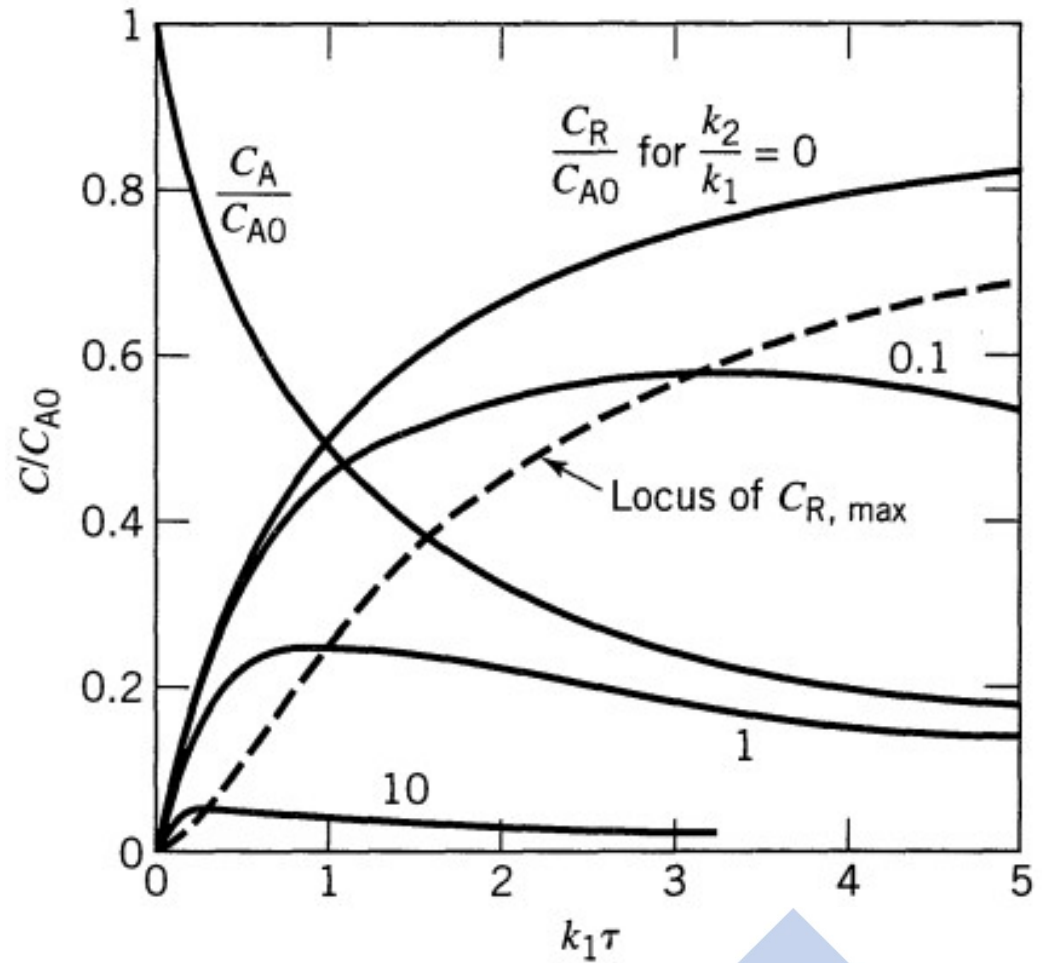
$$C_A + C_R + C_S = C_{A0} = \text{constant} \rightarrow \frac{C_S}{C_{A0}} = \frac{k_1 k_2 \tau_m^2}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}$$

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

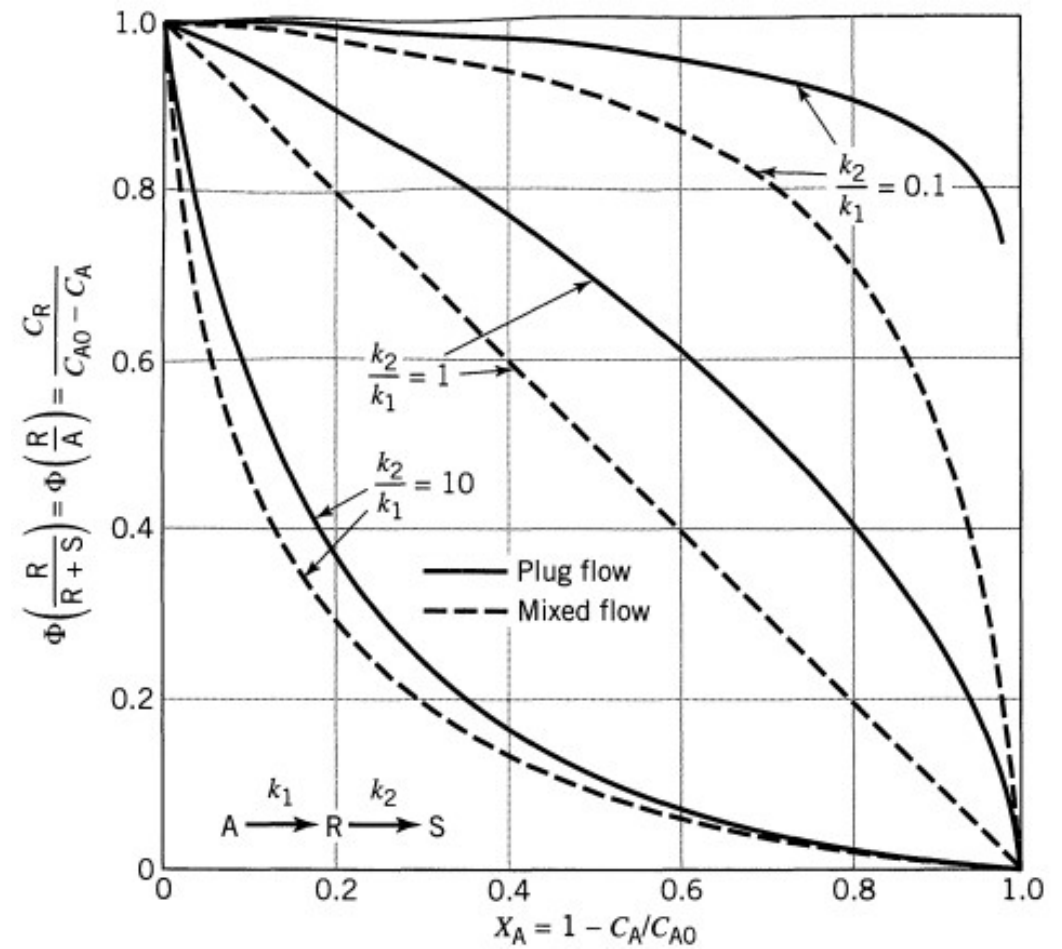
$$\frac{C_{R,\text{max}}}{C_{A0}} = \frac{1}{[(k_2/k_1)^{1/2} + 1]^2}$$

# Quantitative Analysis

MFR



- Comparison of the fractional yields of R in mixed flow and plug flow reactors for the unimolecular-type reactions



## Product Distribution and Temperature

If two competing steps in multiple reactions have rate constants  $k_1$  and  $k_2$  then the relative rates of these steps are given by

$$\frac{k_1}{k_2} = \frac{k_{10}e^{-E_1/RT}}{k_{20}e^{-E_2/RT}} = \frac{k_{10}}{k_{20}} e^{(E_2 - E_1)/RT} \propto e^{(E_2 - E_1)/RT}$$

$$\frac{k_1}{k_2} = \frac{k_{10}e^{-E_1/RT}}{k_{20}e^{-E_2/RT}} = \frac{k_{10}}{k_{20}} e^{(E_2 - E_1)/RT} \propto e^{(E_2 - E_1)/RT}$$

This ratio changes with temperature depending on whether  $E_1$  is greater or smaller than  $E_2$ , so

$$\text{when } T \text{ rises } \begin{cases} k_1/k_2 \text{ increases if } E_1 > E_2 \\ k_1/k_2 \text{ decreases if } E_1 < E_2 \end{cases}$$

## REFERENCES

1. Sinnott, 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.