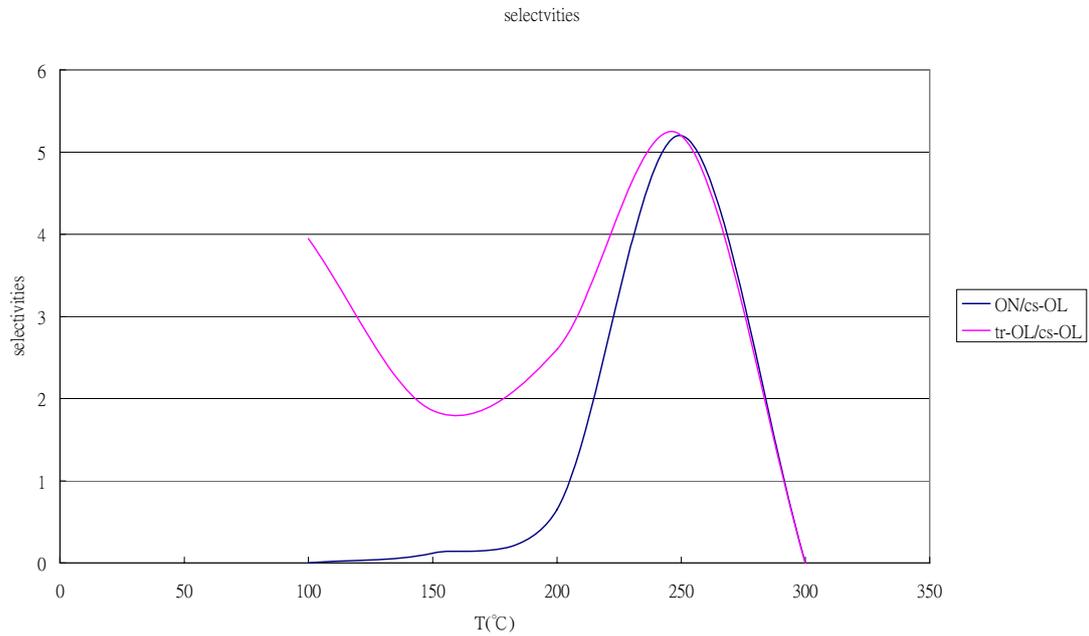


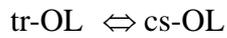
1

(a)



(b)

The equilibrium constant for the reaction



can be estimated from as a function of temperature from the mole fraction data below 100°C

$$K_P = \frac{y_{cs}}{y_{tr}}$$

$$\frac{d \ln K_P}{d(T)} = \frac{\Delta H_R}{RT^2}$$

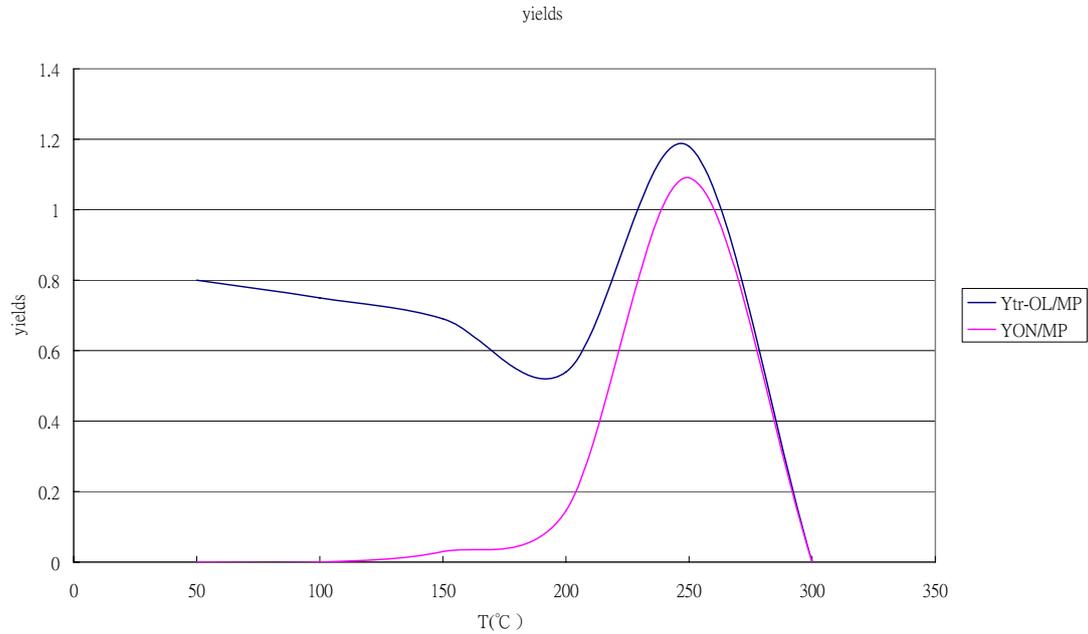
$$\ln \frac{K_{P2}}{K_{P1}} = -\frac{\Delta H_R}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

T(K)	323	373
y_{tr}	0.8	0.75
y_{cs}	0.2	0.25
K_P	0.25	0.33

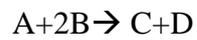
$$\ln \frac{0.25}{0.33} = -\frac{\Delta H_R}{8.314} \left(\frac{1}{323} - \frac{1}{373} \right)$$

$$\Delta H_R = 5562 \frac{J}{mole}$$

(c)



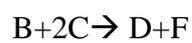
2.



$$r_{D1} = k_{D1} C_A C_B^2$$



$$r_{E2} = k_{E2} C_A C_D$$



$$r_{F3} = k_{F3} C_B C_C^2$$

$$k_{D1} = 0.25 \text{ dm}^6/\text{mol}^2 \cdot \text{min}$$

$$v_0 = 10 \text{ dm}^3/\text{min}$$

$$k_{E2} = 0.1 \text{ dm}^3/\text{mol} \cdot \text{min}$$

$$C_{A0} = 1.5 \text{ mol}/\text{dm}^3$$

$$k_{F3} = 5.0 \text{ dm}^6/\text{mol}^2 \cdot \text{min}$$

$$C_{B0} = 2.0 \text{ mol}/\text{dm}^3$$

$$r_{A,net} = -k_{D1} C_A C_B^2 - 3k_{E2} C_A C_D$$

$$r_{B,net} = -2k_{D1} C_A C_B^2 - k_{F3} C_B C_C^2$$

$$r_{C,net} = k_{D1} C_A C_B^2 + k_{E2} C_A C_D - 2k_{F3} C_B C_C^2$$

$$r_{D,net} = k_{D1} C_A C_B^2 - 2k_{E2} C_A C_D + k_{F3} C_B C_C^2$$

$$r_{E,net} = k_{E2} C_A C_D$$

$$r_{F,net} = k_{F3} C_B C_C^2$$

For isothermal, liquid phase $T=T_0$, $P=P_0$

$$\begin{aligned} v &= v_0 \\ F_A &= C_A v_0 \end{aligned}$$

For PFR

$$\begin{aligned} \frac{dF_j}{dV} &= r_j = v_0 \frac{dC_j}{dV} \\ v_0 \frac{dC_A}{dV} &= -k_{D1} C_A C_B^2 - 3k_{E2} C_A C_D \\ v_0 \frac{dC_B}{dV} &= -2k_{D1} C_A C_B^2 - k_{F3} C_B C_C^2 \\ v_0 \frac{dC_C}{dV} &= k_{D1} C_A C_B^2 + k_{E2} C_A C_D - 2k_{F3} C_B C_C^2 \\ v_0 \frac{dC_D}{dV} &= k_{D1} C_A C_B^2 - 2k_{E2} C_A C_D + k_{F3} C_B C_C^2 \\ v_0 \frac{dC_E}{dV} &= k_{E2} C_A C_D \\ v_0 \frac{dC_F}{dV} &= k_{F3} C_B C_C^2 \end{aligned}$$

For CSTR

$$\begin{aligned} V &= \frac{F_{j0} - F_j}{-r_j} \\ v_0(C_{A0} - C_A) &= V(k_{D1} C_A C_B^2 + 3k_{E2} C_A C_D) \\ v_0(C_{B0} - C_B) &= V(2k_{D1} C_A C_B^2 - k_{F3} C_B C_C^2) \\ v_0 C_C &= V(k_{D1} C_A C_B^2 + k_{E2} C_A C_D - 2k_{F3} C_B C_C^2) \\ v_0 C_D &= V(k_{D1} C_A C_B^2 - 2k_{E2} C_A C_D + k_{F3} C_B C_C^2) \\ v_0 C_E &= V(k_{E2} C_A C_D) \\ v_0 C_F &= V(k_{F3} C_B C_C^2) \end{aligned}$$

For Batch

assume constant volume $V=V_0$

$$\frac{dC_j}{dt} = r_j$$

$$\frac{dC_A}{dt} = -k_{D1}C_A C_B^2 - 3k_{E2}C_A C_D$$

$$\frac{dC_B}{dt} = -2k_{D1}C_A C_B^2 - k_{F3}C_B C_C^2$$

$$\frac{dC_C}{dt} = k_{D1}C_A C_B^2 + k_{E2}C_A C_D - 2k_{F3}C_B C_C^2$$

$$\frac{dC_D}{dt} = k_{D1}C_A C_B^2 - 2k_{E2}C_A C_D + k_{F3}C_B C_C^2$$

$$\frac{dC_E}{dt} = k_{E2}C_A C_D$$

$$\frac{dC_F}{dt} = k_{F3}C_B C_C^2$$

3.

m-xylene \rightarrow benzene + methane $k_1 = 0.22 \text{ s}^{-1}$ at $673 \text{ }^\circ\text{C}$
A B C

m-xylene \rightarrow p-xylene $k_2 = 0.71 \text{ s}^{-1}$ at $673 \text{ }^\circ\text{C}$
A D

$$y_{A0} = 0.75$$

$$y_{I0} = 0.25$$

$$v_0 = 2000 \text{ dm}^3 / \text{min}$$

$$C_{T0} = 0.05 \text{ mol} / \text{dm}^3$$

$$F_{T0} = v_0 C_{T0}$$

$$C_{A0} = 0.0375 \text{ mol} / \text{dm}^3$$

$$F_{A0} = v_0 C_{A0}$$

$$C_j = C_{T0} \left(\frac{F_j}{F_{T0}} \right) \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T} \right)$$

$$r_A = -k_1 C_A - k_2 C_A = -C_A (k_1 + k_2)$$

$$r_B = k_1 C_A$$

$$r_C = k_1 C_A$$

$$r_D = k_2 C_A$$

For PFR

$$\frac{dF_A}{dV} = -(k_1 + k_2)C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$\frac{dF_B}{dV} = k_1 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$\frac{dF_C}{dV} = k_1 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$\frac{dF_D}{dV} = k_2 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$F_T = F_A + F_B + F_C + F_D$$

For CSTR

$$F_{j0} - F_j = -r_j V$$

$$F_{A0} - F_A = V(k_1 + k_2)C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$F_B = V k_1 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$F_C = V k_1 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$F_D = V k_2 C_{T0} \left(\frac{F_A}{F_T} \right)$$

$$F_T = F_A + F_B + F_C + F_D$$

For Batch

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

$$\frac{dC_B}{dt} = k_1 C_A$$

$$\frac{dC_C}{dt} = k_1 C_A$$

$$\frac{dC_D}{dt} = k_2 C_A$$

[NOTE]: When you use Matlab to solve problems, you should make each term consistent. For example, if you want to use molar flow rate (F_j), all equations should be expressed by F_j . Do not use F_j and C_j at the same time and do not have too many variables.