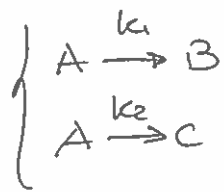


PRACTICAL SESSION 3.1

Ex. 1

PARALLEL REACTIONS IN A LIQUID CSTR



B is the desired product

$$k_1 = 0.5 \text{ min}^{-1}$$

$$k_2 = 0.1 \text{ min}^{-1}$$

$$Q = 4 \frac{\text{l}}{\text{min}}$$

$$C_A^0 = 2 \frac{\text{mol}}{\text{l}}$$

SELECTIVITY

$$S_B = \frac{C_B}{C_A^0 - C_A}$$

YIELD

$$Y_B = \frac{C_B}{C_A^0}$$

$$\dot{F}_A^0 - \dot{F}_A + R_A V = 0$$

$$Q(C_A^0 - C_A) + (-k_1 C_A - k_2 C_A)V = 0$$

$$Q(C_A^0 - C_A^0(1-X)) - C_A^0(1-X)(k_1 + k_2)V = 0 \quad k_1 + k_2 \stackrel{\text{def}}{=} K$$

$$QX - (1-X)KV = 0 \quad \tau \stackrel{\text{def}}{=} \frac{V}{Q}$$

$$\tau = \frac{1}{K} \frac{X}{1-X}$$

$$\tau(95\%) = 31.67 \text{ min}$$

$$C_A^0 - C_A - K\tau C_A \Rightarrow C_A(\tau) = \frac{C_A^0}{1+K\tau}$$

$$C_B^0 - C_B + k_1 \tau C_A \Rightarrow C_B(\tau) = k_1 \tau C_A(\tau) = \frac{k_1 \tau C_A^0}{1+K\tau}$$

$$C_B(\tau) = k_2 \tau C_A(\tau) = \frac{k_2 \tau C_A^0}{1+K\tau}$$

$$S_B = \frac{C_B}{C_A^0 - C_A} = \dots = \frac{k_1}{K_{\text{tot}}} \quad S_C = \frac{k_2}{K_{\text{tot}}}$$

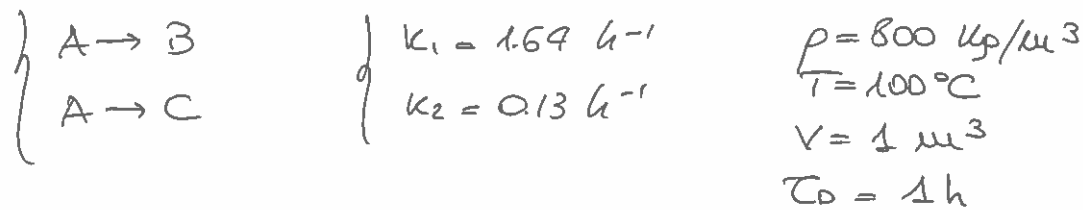
$$Y_B = \frac{C_B}{C_A^0} = \frac{k_1 \tau}{1+K\tau} \quad Y_C = \frac{k_2 \tau}{1+K\tau}$$

$$\frac{dY_B}{d\tau} = \frac{k_1(1+K\tau) - k_1 \tau K}{(1+K\tau)^2} = \frac{k_1 + k_1 K \tau - k_1 \tau K}{(1+K\tau)^2} = \frac{k_1}{(1+K\tau)^2} \quad \text{no max}$$

II-①

EX. 2

PARALLEL REACTIONS IN A BATCH REACTOR (constant density)



$$\left\{ \begin{array}{l} C_F(\tau) = C_1 \tau_0 + C_2 \tau + C_3 \\ I(\tau) = 15 \$/\text{kg}_B \end{array} \right.$$

$$\left\{ \begin{array}{l} \frac{dC_A}{dt} = -k_1 C_A - k_2 C_A \\ \frac{dC_B}{dt} = k_1 C_A \\ \frac{dC_C}{dt} = k_2 C_A \end{array} \right.$$

$$\frac{dC_A}{dt} = -(k_1 + k_2) C_A = -K C_A \quad \text{with } k_1 + k_2 \stackrel{\text{def}}{=} K$$

$$C_A = C_A^0 \exp(-Kt)$$

$$\frac{dC_B}{dt} = k_1 C_A = k_1 C_A^0 \exp(-Kt)$$

$$C_B - C_B^0 = k_1 C_A^0 \int_0^\tau \exp(-Kt) dt = \dots = \frac{k_1 C_A^0}{K} (1 - \exp(-K\tau))$$

$$\text{solution} \quad \left\{ \begin{array}{l} C_A(\tau) = C_A^0 \exp(-K\tau) \\ C_B(\tau) = \frac{k_1 C_A^0}{K} (1 - \exp(-K\tau)) \\ C_C(\tau) = \frac{k_2 C_A^0}{K} (1 - \exp(-K\tau)) \end{array} \right.$$

$$C_A(\tau) = C_A^0 \exp(-K\tau) \Rightarrow \ln \frac{C_A}{C_A^0} = -K\tau \quad \tau = -\frac{1}{K} \ln \frac{C_A}{C_A^0}$$

$$\tau = -\frac{1}{K} \ln \frac{C_A^0(1-X)}{C_A^0} = -\frac{1}{K} \ln(1-X)$$

$$\tau(98\%) = -\frac{\ln(1-X)}{K} = 2.18 \text{ h} \quad \frac{M_{\text{cydes}}}{\text{day}} = \frac{24}{\tau + \tau_0} = 7.52$$

$$P_{\pi B} = C_B V \frac{M_{\text{cydes}}}{\text{day}} = \dots = 155.5 \frac{\mu\text{mol}}{\text{day}}$$

Optimal economical conditions

$$\text{MARGIN} = \text{INCOMES} - \text{COSTS}$$

$$M = I - C \quad \text{to be maximized}$$

$$I = I(t) = P_B \cdot \text{Price}_B \cdot \text{MW}_B =$$

$$= \frac{24 \text{ h}}{\tau + \tau_0} \cdot C_B V \cdot \underset{\text{Tagg}}{15 \$} \cdot \text{MW}_B$$

$$\stackrel{!}{=} \frac{24 \cdot V \cdot 15 \text{ MW}_B}{\tau + \tau_0} C_B = 24 \cdot V \cdot 15 \cdot \text{MW}_B \frac{C_B}{\tau + \tau_0}$$

$$I(\tau) = 24 V \cdot 15 \cdot \text{MW}_B \cdot \frac{k_1 G_0}{k} \cdot \frac{1 - \exp(-k_1 \tau)}{\tau + \tau_0} = \beta \frac{1 - \exp(-k_1 \tau)}{\tau + \tau_0}$$

$$C(\tau) = (C_1 \tau_0 + C_2 \tau + C_3) \cdot \frac{\text{M cycles}}{\text{day}} = \frac{24}{\tau + \tau_0} (C_1 \tau_0 + C_2 \tau + C_3)$$

$$M = I - C = \beta \frac{1 - \exp(-k_1 \tau)}{\tau + \tau_0} - 24 \frac{(C_1 \tau_0 + C_2 \tau + C_3)}{\tau + \tau_0}$$

$$\stackrel{!}{=} \frac{\beta (1 - \exp(-k_1 \tau)) - 24 (C_1 \tau_0 + C_2 \tau + C_3)}{\tau + \tau_0}$$

$$\frac{dM}{d\tau} = \frac{(\beta k_1 \exp(-k_1 \tau) - 24 C_2)(\tau + \tau_0) - (\beta (1 - \exp(-k_1 \tau)) - 24 (C_1 \tau_0 + C_2 \tau + C_3))}{(\tau + \tau_0)^2}$$

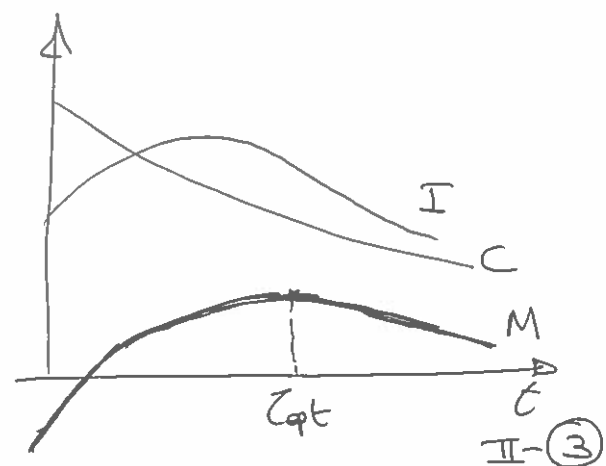
$$\stackrel{!}{=} 0$$

algebraic non linear equations $0 = (\beta k_1 \exp(-k_1 \tau) - 24 C_2)(\tau + \tau_0) - (\beta (1 - \exp(-k_1 \tau)) - 24 (C_1 \tau_0 + C_2 \tau + C_3))$

must be solved numerically

Alternatively, the I , C and M functions can be plotted and the maximum of M can be read directly

$$\tau_{\text{opt}} = 1.72 \text{ h}$$



EX 3.

NON ISOTHERMAL CSTR at constant density

$$V = 1135 \text{ l}$$



M does not participate
to the reaction
(it behaves like an inert species)

$$\begin{cases} \dot{Q}_A^0 = 1360 \text{ l/h} \\ \dot{Q}_H^0 = 1320 \text{ l/h} \\ \dot{Q}_B^0 = 6600 \text{ l/h} \\ \dot{Q}_C^0 = 0 \end{cases}$$

$$\begin{cases} \dot{F}_A^0 = 18.50 \text{ kmol/h} \\ \dot{F}_H^0 = 32.60 \text{ kmol/h} \\ \dot{F}_B^0 = 364 \text{ kmol/h} \end{cases}$$

$$T_{in} = 29^\circ\text{C}$$



$$T_{max} = 53^\circ\text{C}$$

$$\begin{cases} A = 16.96 \cdot 10^{12} \text{ h}^{-1} \\ E = 72000 \text{ J/mol} \end{cases} \quad \left\{ K = A \exp(-E/RT) \right.$$

Specific heats

$$\widetilde{C}_{PA} = 146 \text{ J/mol K}$$

$$\widetilde{C}_{PB} = 75 \text{ "}$$

$$\widetilde{C}_{PC} = 182 \text{ "}$$

$$\widetilde{C}_{PD} = 82 \text{ "}$$

Formation enthalpies

$$\widetilde{H}_A^0(T_0 = 20^\circ\text{C}) = -148918 \text{ J/mol}$$

$$\widetilde{H}_B^0 = -275000 \text{ "}$$

$$\widetilde{H}_C^0 = -505360 \text{ "}$$

$$\text{MASS BALANCE} \quad \dot{Q}(C_A^0 - C_A) + R_A V = 0$$

$$\text{ENERGY BALANCE} \quad X(T) = - \frac{\int_{T_{in}}^T \widetilde{C}_{Pim} dT}{\Delta \widetilde{H}_R(T)}$$

$$\begin{cases} C_A^0 = \frac{\dot{F}_A^0}{Q_{tot}} = 2.11 \frac{\text{mol}}{\text{l}} \\ C_B^0 = \frac{\dot{F}_B^0}{Q_{tot}} = 38.9 \text{ "} \\ C_H^0 = \frac{\dot{F}_H^0}{Q_{tot}} = 3.53 \text{ "} \end{cases}$$

$$\tau = \frac{V}{Q_{tot}} = 0.123 \text{ h}$$

$$C_A^0 X = K C_A^0 (1-X) \tau$$

$$\widetilde{C}_{Pim} = \sum_{j=1}^4 C_{Pj} \vartheta_j^0 =$$

$$= \widetilde{C}_{PA} \vartheta_A^0 + \widetilde{C}_{PB} \vartheta_B^0 + \widetilde{C}_{PH} \vartheta_H^0$$

$$X(T) = \frac{-\widetilde{C}_{Pim} (T - T_{in})}{\Delta \widetilde{U}_R^0 + \Delta \widetilde{C}_P (T - T_0)}$$

$$\Delta \widetilde{C}_P = \sum_{j=1}^3 \widetilde{C}_{Pj} \nu_j =$$

$$= -\widetilde{C}_{PA} - \widetilde{C}_{PB} + \widetilde{C}_{PC}$$

$$\Delta \widetilde{U}_R^0 = \sum_{j=1}^3 \widetilde{H}_R^0 \nu_j =$$

$$= -\widetilde{H}_A^0 - \widetilde{H}_B^0 + \widetilde{H}_C^0$$

$$\left\{ \begin{array}{l} X = \frac{kT}{1+kT} \\ X = \frac{-\varphi^{im}(T-T_{im})}{\widetilde{\Delta H_R^0} + \widetilde{\Delta C_P}(T-T_0)} \end{array} \right.$$

$$\left\{ \begin{array}{l} X = \frac{A \exp(-E/RT) \tau}{1 + A \exp(-E/RT) \tau} \\ X = \frac{-\varphi^{im}(T-T_{im})}{\widetilde{\Delta H_R^0} + \widetilde{\Delta C_P}(T-T_0)} \end{array} \right.$$

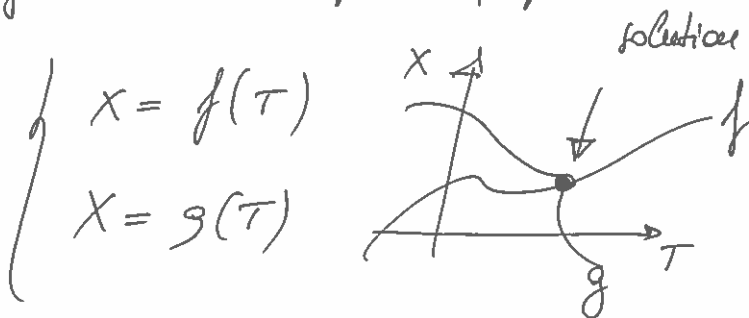
NLS of 2 equations (non linear)

$$\underline{\text{NLS}} \left\{ \begin{array}{l} X - \frac{A \exp(-E/RT) \tau}{1 + A \exp(-E/RT) \tau} = 0 \\ X + \frac{\varphi^{im}(T-T_{im})}{\widetilde{\Delta H_R^0} + \widetilde{\Delta C_P}(T-T_0)} = 0 \end{array} \right. \left\{ \begin{array}{l} f_1(X, T) = 0 \\ f_2(X, T) = 0 \end{array} \right.$$

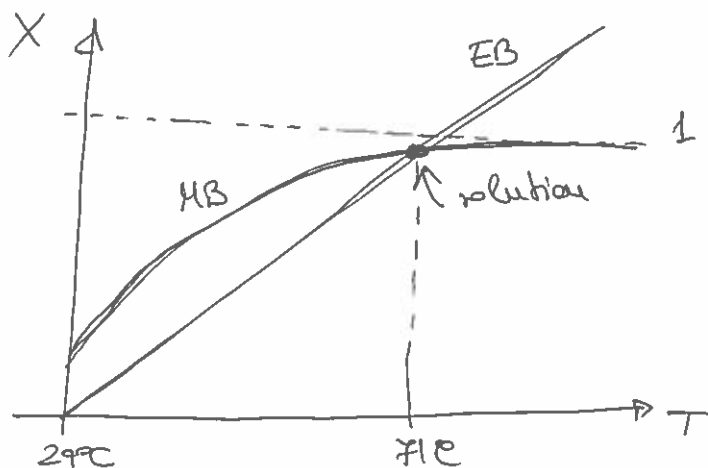
It can be written as a single NL equation in T

$$\frac{A \exp(-E/RT) \tau}{1 + A \exp(-E/RT) \tau} = - \frac{\varphi^{im}(T-T_{im})}{\widetilde{\Delta H_R^0} + \widetilde{\Delta C_P}(T-T_0)}$$

Also a graphical procedure is possible, directly on the equations of the NLS in the following form:



SOLUTION
 $T = 71.9^\circ\text{C}$
 $X = 96.1\%$



EX 4

PLUG FLOW REACTOR with constant density
REACTIONS IN SERIES $A \xrightarrow{k_1} B \xrightarrow{k_2} C$

exactly same exercise PC 1-6

$$\text{solutions} \left\{ \begin{array}{l} C_A(\tau) = C_A^0 \exp(-k_1 \tau) \\ C_B(\tau) = \frac{k_1 C_A^0}{k_2 - k_1} (\exp(-k_1 \tau) - \exp(-k_2 \tau)) \\ C_C(\tau) = C_A^0 - C_A(\tau) - C_B(\tau) \end{array} \right.$$

$$\left\{ \begin{array}{l} k_1 = 1.99 \text{ s}^{-1} \\ k_2 = 1.86 \text{ s}^{-1} \end{array} \right.$$

$$C_{A0} = 35.7 \frac{\text{mol}}{\text{m}^3}$$

$$\tau = 3.23 \text{ s}$$

$$\eta_c = \frac{C_C(\tau)}{C_{A0}(\tau)} = 96.8 \%$$

EX 5

Same exercise above, only different numbers

- same analytical solution
- same MATLAB code
- quasi-steady state hypothesis for species B

if we look at the kinetic
constants we see that
the second reaction is
more than 1000 times
FASTER than the first one

$$k_1 = 0.57 \text{ s}^{-1}$$

$$k_2 = 1114 \text{ s}^{-1}$$

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

this means that B disappears as
soon as it is produced

we can assume it is in quasi steady
state

$$\frac{k_2}{k_1} \gg 1 \Rightarrow \frac{dC_B}{dt} \sim 0 \Rightarrow k_1 C_A(\tau) = k_2 C_B(\tau)$$

$$\Rightarrow C_B(\tau) = \frac{k_1}{k_2} C_A^0 \exp(-k_1 \tau)$$

Thus the problem is simplified because we have $C_B(\tau)$ explicitly and we do not have to solve the corresponding ODE equations

$$\left\{ \begin{array}{l} \frac{dA}{d\tau} = -k_1 A \\ \frac{dC_C}{d\tau} = k_2 \cdot C_B = \frac{k_2 k_1}{k_2} A^0 \exp(-k_1 \tau) \end{array} \right.$$

$$\left\{ \begin{array}{l} \frac{dA}{d\tau} = -k_1 A \\ \frac{dC_C}{d\tau} = k_1 A^0 \exp(-k_1 \tau) \end{array} \right.$$

2 equations

it is interesting to observe that k_2 does not appear explicitly

Indeed, if $k_2 \gg k_1$, the RDS (RATE DETERMINING STEP) is the first reaction

$$\left\{ \begin{array}{l} A(\tau) = A^0 \exp(-k_1 \tau) \\ C_C(\tau) = A^0 (1 - \exp(-k_1 \tau)) \\ C_B(\tau) = \frac{k_1}{k_2} A^0 \exp(-k_1 \tau) \end{array} \right.$$

← since $\frac{k_1}{k_2} \ll 1$ it is always expected to be very small

EX 6

SERIES REACTION IN A CONSTANT VOLUME BATCH REACTOR



$$T = 500 \text{ K}$$

$$V = 0.50 \text{ m}^3$$

$$N_A^0 = 20 \text{ kmol}$$

$$\tau_D = 1 \text{ h}$$

$$C_{A0} = \frac{N_A^0}{V} = 40 \frac{\text{kmol}}{\text{m}^3}$$

$$\left\{ \begin{array}{l} k_1 = 1.75 \text{ h}^{-1} \\ k_2 = 0.0297 \text{ h}^{-1} \end{array} \right.$$

$$\left\{ \begin{array}{l} \frac{dC_A}{dt} = -k_1 C_A \\ \frac{dC_B}{dt} = k_1 C_A - k_2 C_B \\ \frac{dC_C}{dt} = k_2 C_B \end{array} \right. \Rightarrow \left\{ \begin{array}{l} C_A(t) = C_A^0 \exp(-k_1 t) \\ C_B(t) = \frac{k_1 C_A^0}{k_2 - k_1} (\exp(-k_1 t) - \exp(-k_2 t)) \\ C_C(t) = C_A^0 - C_B - C_A \end{array} \right.$$

Max. yield of B $y_B = \frac{C_B}{C_A^0} = \frac{k_1}{k_2 - k_1} (\exp(-k_1 t) - \exp(-k_2 t))$

same position of maximum of B
see previous problem

$$\tau_{\text{yield B}}^{\text{max}} = \frac{\ln \frac{k_2}{k_1}}{k_2 - k_1}$$

$$\tau_{\text{yield B}}^{\text{max}} = 2.37 \text{ h}$$

Max. production of B

$$P_B \stackrel{\text{def}}{=} N_B(\tau) \text{ cycles/day} = C_B(\tau) V \cdot \frac{24 \text{ h}}{\tau + \tau_D}$$

$$= \frac{24 \cdot k_1 C_{A0} V}{k_2 - k_1} \frac{[\exp(-k_1 \tau) - \exp(-k_2 \tau)]}{(\tau + \tau_D)}$$

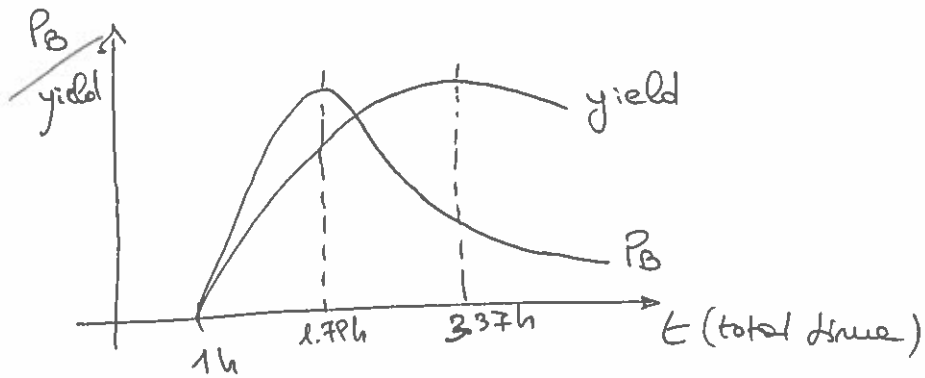
$$\propto \frac{\exp(-k_1 \tau) - \exp(-k_2 \tau)}{\tau + \tau_D}$$

$$\frac{dP_B}{d\tau} = \alpha \frac{(-k_1 \exp(-k_1 \tau) + k_2 \exp(-k_2 \tau))(\tau + \tau_D) - (\exp(-k_1 \tau) - \exp(-k_2 \tau))}{(\tau + \tau_D)^2} = 0$$

$$(-k_1 \exp(-k_1 \tau) + k_2 \exp(-k_2 \tau))(\tau + \tau_D) - (\exp(-k_1 \tau) - \exp(-k_2 \tau)) = 0$$

non linear algebraic
equation to solve in τ

$$(-k_1 \exp(-k_1 \tau) + k_2 \exp(-k_2 \tau)) (\tau + \tau_0) - (\exp(-k_1 \tau) - \exp(-k_2 \tau)) = 0$$



instead of solving the
equation above, one
can plot the PB
function and find the
maximum value
on it

$$\tau_{\text{max production}} = 0.79 \text{ h}$$

EXERCISE 8



$$\text{inlet mixture} \left\{ \begin{array}{l} T_{in} = 330 \text{ K} \\ \dot{F}_{tot}^{in} = 163 \text{ kmol/h} \\ C_A^{in} = 9.30 \text{ kmol/m}^3 \\ x_A^{in} = 0.90 \\ x_B^{in} = 0 \\ x_I^{in} = 0.10 \end{array} \right.$$

$$\text{thermodynamic data} \left\{ \begin{array}{l} \Delta H_R(T_0) = \Delta H_R^\circ = -6800 \text{ J/mol} \\ T_0 = 300 \text{ K} \\ C_{pA} = 131 \text{ J/mol/K} \\ C_{pB} = 171 \text{ J/mol/K} \\ C_{pI} = 161 \text{ J/mol/K} \end{array} \right.$$

$$\text{kinetics} \left\{ \begin{array}{l} k_f(T_f^*) = 31.1 \text{ 1/h} \\ T_f^* = 360 \text{ K} \\ E = 65700 \text{ J/mol} \end{array} \right.$$

$$\text{thermodynamic equilibrium} \left\{ \begin{array}{l} K_{eq}(T_{eq}^*) = 3.03 \\ T_{eq}^* = 60^\circ\text{C} = 333 \text{ K} \end{array} \right.$$

SOLUTION

a) Preliminary calculations

$$\left\{ \begin{array}{l} \bar{F}_A^{in} = x_A^{in} \cdot \bar{F}_{tot}^{in} = 146.7 \text{ kmol/h} \\ \bar{F}_B^{in} = x_B^{in} \cdot \bar{F}_{tot}^{in} = 0 \\ \bar{F}_I^{in} = x_I^{in} \cdot \bar{F}_{tot}^{in} = 16.3 \text{ kmol/h} \end{array} \right. \left\{ \begin{array}{l} \vartheta_A = \frac{x_A^{in}}{x_A^{in}} = 1 \\ \vartheta_B = \frac{x_B^{in}}{x_A^{in}} = 0 \\ \vartheta_I = \frac{x_I^{in}}{x_A^{in}} = 0.111 \end{array} \right.$$

$$\bar{C}_p^{in} = \sum_j \vartheta_j \bar{C}_{pj} = 148.8 \text{ J/mol/K}$$

$$\Delta \bar{C}_p = \bar{C}_{pB} - \bar{C}_{pA} = 40 \text{ J/mol/K}$$

$$\Delta H_R^{in} = \Delta H_R^\circ + \Delta \bar{C}_p (T_{in} - T_0) = -5700 \text{ J/mol}$$

$$\Delta H^* = \Delta H(T_{eq}^*) = \Delta \bar{H}_R^0 + \Delta \bar{G}_P(T_{eq}^* - T_0) = -5580 \text{ J/mol}$$

b) Kinetics

$$K_f(T_f^*) = K_f^* = A \exp\left(-\frac{E}{RT_f^*}\right)$$

$$K_f(T) = A \exp\left(-\frac{E}{RT}\right)$$

$$K_f(T) = K_f^* \exp\left(-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_f^*}\right)\right) \quad (E1)$$

c) equilibrium constant

$$\frac{d \ln K_{eq}}{dT} = \frac{\Delta \bar{H}_R}{RT^2} \quad \Delta \bar{H}_R = \Delta \bar{H}_R^0 + \Delta \bar{G}_P(T - T_0)$$

$$\ln K_{eq} = C' + \frac{\Delta \bar{G}_P}{R} \ln T - \frac{\Delta \bar{H}_R^0 - \Delta \bar{G}_P T_0}{RT}$$

$$\ln \frac{K_{eq}}{K_{eq}^*} = -\left(\frac{\Delta \bar{H}_R^0}{R} - \frac{\Delta \bar{G}_P T^*}{R}\right)\left(\frac{1}{T} - \frac{1}{T^*}\right) + \frac{\Delta \bar{G}_P}{R} \ln \frac{T}{T^*}$$

$$K_{eq} = K_{eq}^* \exp\left[-\left(\frac{\Delta \bar{H}_R^0}{R} - \frac{\Delta \bar{G}_P T^*}{R}\right)\left(\frac{1}{T} - \frac{1}{T^*}\right) + \frac{\Delta \bar{G}_P}{R} \ln \frac{T}{T^*}\right] \quad (E2)$$

in case $\Delta \bar{G}_P = 0 \Rightarrow K_{eq} = K_{eq}^* \exp\left(-\frac{\Delta \bar{H}_R^0}{R}\left(\frac{1}{T} - \frac{1}{T^*}\right)\right)$
~~Don't use this~~ You'll fail

d) formation rate of reference species

$$R_A = -k_f \cdot A + k_b \cdot B = -k_f A^0(1-X) + k_b A^0 X$$

$$= \dots = k_f A^0 \left(-1 + X \left(1 + \frac{1}{K_{eq}}\right)\right)$$

$$k_b = \frac{k_f}{K_{eq}}$$

$$-R_A = k_f A^0 \left(1 - \left(1 + \frac{1}{K_{eq}}\right)X\right) \quad (E3)$$

e) equilibrium conversion (useful)

$$k_f \cdot C_A^{eq} = k_b \cdot C_B^{eq} \rightarrow k_f C_A^0 (1 - X_{eq}) = k_b C_A^0 X_{eq}$$

$$X_{eq} = \frac{K_{eq}}{1 + K_{eq}} \quad ! \text{ be careful } K_{eq} = K_{eq}(T) \rightarrow X_{eq} = X_{eq}(T)$$

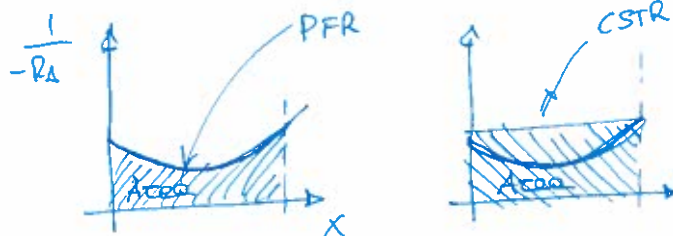
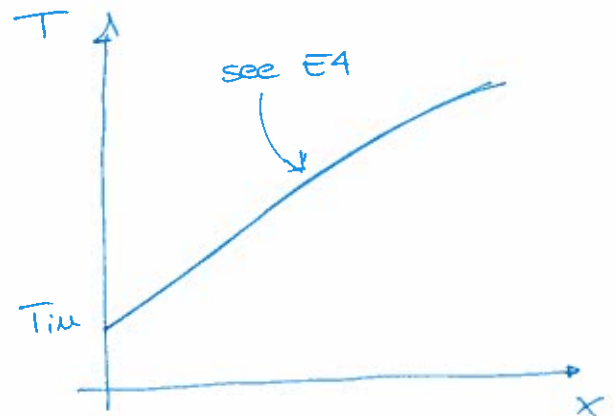
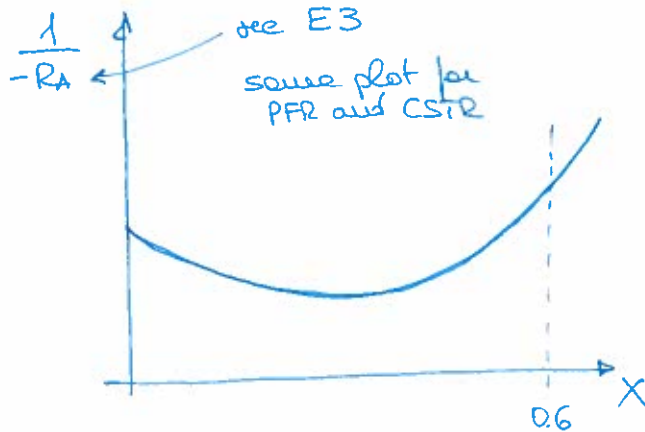
f) ENERGY BALANCE EQUATION

$$\int_{T_{in}}^T \bar{C}_p^{in} dT + \Delta H_R(T) X = 0$$

$$\bar{C}_p = \text{const} \Rightarrow T = T_{in} + \frac{-\Delta H_R^{in} X}{\bar{C}_p^{in} + \Delta \bar{C}_p X} \quad (E4)$$

this is the same for PFR and CSTR cases

g) LEVENSPHIEL'S PLOT



PFR

$$V = A_{rea} \cdot \dot{F}_A^{in}$$

CSTR

$$V = A_{rea} \cdot \dot{F}_A^{in}$$

PFR

$$A_{rea} = \int_0^{X_f} \frac{dX}{-R_A}$$

X_f = is the desired final conversion

CSTR

$$A_{rea} = \frac{1}{-R_A} \cdot X_f$$

PFR

$$V = \dot{F}_A^{\text{in}} \int_0^X \frac{dX}{-R_A}$$

$$T = T_{\text{in}} + \frac{-\Delta H_R^{\text{in}} X}{\widetilde{C}_{p,\text{in}} + \Delta \widetilde{C}_p X}$$

Alternative approach:

PFR

$$\frac{dX}{dV} = - \frac{R_A}{\dot{F}_A^{\text{in}}}$$

$$\frac{dT}{dV} = \frac{\dot{Q}_R}{\dot{F}_A^{\text{in}} (\widetilde{C}_{p,\text{in}} + \Delta \widetilde{C}_p X)}$$

+ ICs

$$\begin{cases} X(V=0) = 0 \\ T(V=0) = T_{\text{in}} \end{cases}$$

$$\dot{Q}_R = \text{heat release} = R_A \Delta \widetilde{H}_R$$