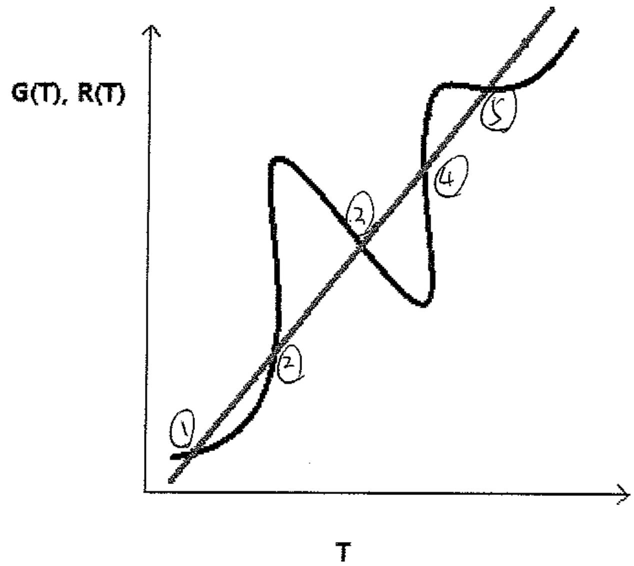
problem 1

A non-ideal steady state, wall-cooled reactor is described by the G(T) and R(T) curves below.

(a) Indicate the steady state by clearly numbering each one. Determine the stability of each steady state and justify your choices in one sentence. Assume that the heat of reaction and heat capacities are independent of temperature.



1 stable steady state

2 unstable steady state

3 stable steady state

4 unstable steady state

5 stable steady state

2.

(a) α=UA/(F_{A0}*C_{Pa})=$\frac{1500 \text{ cal/(K*h)}}{300\frac{mol}{h}*5\ cal/(K*mol)} = 1$

$T^*=\frac{T_0+\alpha T_{am}}{1+\alpha} = \frac{460+260}{1+1} = 360K$

R(T)=C_{pA}*(1+ α)*(T-T^*)= 5 cal/(mol*K)*(1+1)*(T-360)=10*(T-360)

(b) $T^{*\prime}=\frac{T_0'+\alpha T_{am}}{1+\alpha} = \frac{1020+260}{1+1} = 640K$

R(T)=C_{pA}*(1+ α)*(T-T^*)= 5 cal/(mol*K)*(1+1)*(T-640)=10*(T-640)

(c) at the highest conversion, we have G(T)=R(T), dG/dT=0

From the plot, we know the highest point would be (550K, 1.45E+04 cal/mol)

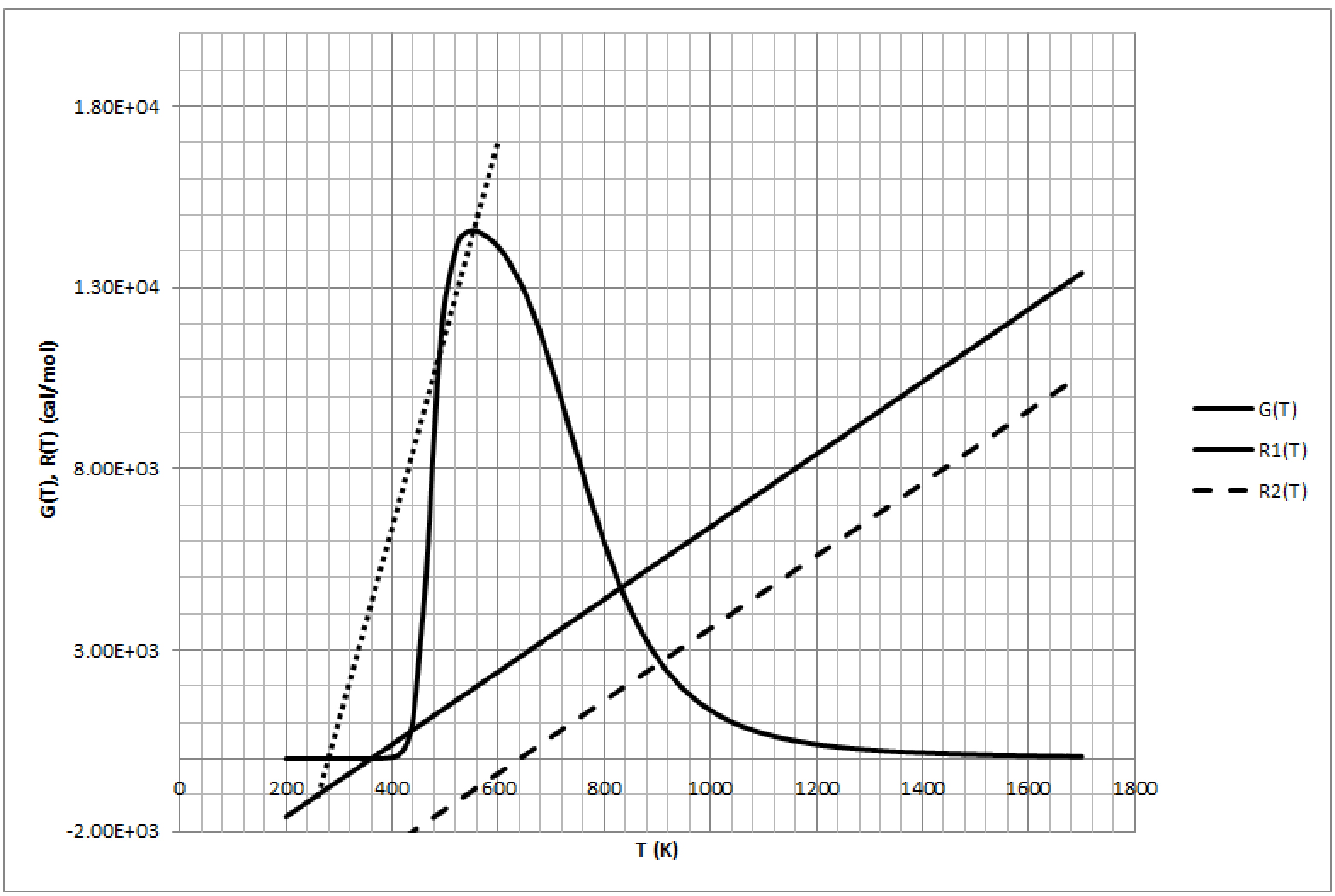
X=G_{max} (T)/ (-ΔH_{RX})= $\frac{1.45\text{E+04 cal/mol}}{15000 \text{ cal/mol}}$ =0.97

R(T) should pass the point which is (550K, 1.45E+04 cal/mol)

R(T)=-[C_{pA}*UA/(F_{A0}*C_{pA})*T_{am}+ C_{pA} *T_o-C_{pA}*(UA/(F_{A0}*C_{pA})+1)*T] $T^*=\frac{T_0+\alpha T_{am}}{1+\alpha}$ α=UA/(F_{A0}*C_{Pa})

R(550)=1.45e+04

UA = 14590 cal/(K * h)



3.a) X_A from mole balance:

$$\frac{F_{A0} X_A}{-r_A} = V$$

or, $$\frac{1000\, X_A}{C_A^2} = V$$

or $$\frac{1000\, X_A}{C_{A0}^2 (1-X_A)^2} = 500$$ [liquid phase, $C_A = C_{A0}(1-X_A)$]

or, $X_A^2 - 4X_A + 1 = 0$

or, $$X_A = \frac{4 \pm \sqrt{16-4}}{2}$$

$= 0.268$ (Other value neglected as $X_A < 1$).

Total heat generated in the reactor due to reaction per unit time,

$$\dot{Q}_{gen} = -\Delta H_{Rx}(T)\, F_{A0} X_A$$

$$\Delta C_p = \frac{1}{2} C_{P,B} - C_{PA} = 0$$

$$\Delta H_{Rx} = \frac{1}{2} H_B - H_A = -10 \text{ kJ/mol. at } 298\text{K}.$$

$$\Delta H_{Rx}(T) = \Delta H_{Rx}(T_R) + \Delta C_p (T - T_R)$$

$\because \quad \Delta C_P = 0,$

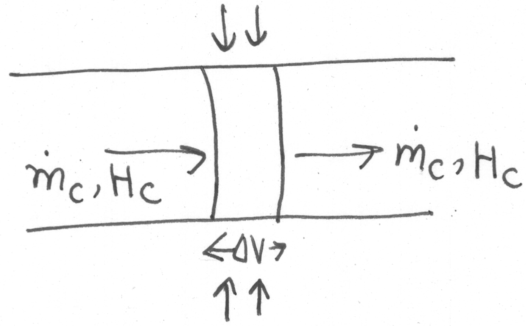
$$\Delta H_{Rx}(T) = \Delta H_{RX}(T_R) = -10 \text{ kJ/mol}.$$

$$\dot{Q}_{gen} = 10 \times 10^3 \times 0.268 \text{ kJ/hr}$$

$$= 2.68 \times 10^6 \text{ J/hr}$$

$$= 2680 \text{ kJ/hr}.$$

b)



Heat in − Heat out + Heat added from the surrounding $= 0$

$$\dot{m}_c H_c \big|_V - \dot{m}_c H_c \big|_{V+\Delta V} + Ua(T - T_{am})\Delta V = 0$$

T = temp of reactor $= 900\text{K}$.

or, $$\frac{\dot{m}_c H_c \big|_{V+\Delta V} - \dot{m}_c H_c \big|_V}{\Delta V} = Ua(T - T_{am})$$

As $\Delta V \to 0$, $$\frac{d}{dV}(\dot{m}_c H_c) = Ua(T - T_{am})$$

$dH_c = C_{pc}\, dT_{am}$, $dV = A_c\, dz$. , $\dot{m}_c$ is constant since no rxn in cooling coil

or, $$\dot{m}_c C_{pc} \frac{dT_{am}}{dV} = Ua(T - T_{am})$$

or, $$\boxed{\frac{dT_{am}}{dz} = \frac{Ua\, A_c}{\dot{m}_c C_{pc}} (T - T_{am})}$$

c) $$\int_{300}^{T_{am}} \frac{dT_{am}}{T - T_{am}} = \frac{Ua A_c}{\dot{m}_c C_{pc}} \int_0^z dz$$

[Note: Look at the bounds of the integration]

$$-\ln \frac{T - T_{am}}{T - 300} = \frac{Ua A_c}{\dot{m}_c C_{pc}} \cdot z$$

or, $$\frac{900 - T_{am}}{900 - 300} = e^{-\frac{z}{210}}$$ $\left[\frac{Ua A_c}{\dot{m}_c C_{pc}} = \frac{1}{210}\right]$

or, $$\boxed{T_{am} = 900 - 600\, e^{-\frac{z}{210}}}$$

d) Heat balance on the whole cooling tube:

Heat in − Heat out + Heat removed from reactor

= 0 (at steady state).

$$\dot{m}_c H_c|_{in} - \dot{m}_c H_c|_{out} + \dot{Q}_{gen} = 0$$

or, $\dot{m}_c C_{pc} (T_{am,in} - T_{am,out}) + \dot{Q}_{gen} = 0.$

or, $T_{c,out} = \dfrac{\dot{Q}_{gen}}{\dot{m}_c C_{pc}} + T_{co}$

or, $900 - 600 e^{-z/210} = \dfrac{2680}{30 \times 4.2} + 300$

$\Rightarrow z = 7.58$ metres

e) $\overline{T}_{am} = \dfrac{1}{z} \displaystyle\int_0^z T_{am}\, dz$

$$= \frac{1}{z} \int_0^z \left[T + (T_{am,o} - T) e^{-\frac{U_a A_c z}{\dot{m}_c C_{pc}}} \right] dz$$

$$= \frac{1}{z} \left[Tz + (T_{am,o} - T) \cdot -\frac{\dot{m}_c C_{pc}}{U_a A_c} \left[e^{-\frac{U_a A_c z}{\dot{m}_c C_{pc}}} - 1 \right] \right]$$

$$= T + \frac{1}{z} (T - T_{am,o}) \cdot \frac{\dot{m}_c C_{pc}}{U_a A_c} \left(e^{-\frac{U_a A_c z}{\dot{m}_c C_{pc}}} - 1 \right)$$

Problem 4

a) general mol balance:

$$F_{A0} - F_A + \int_V r_A \, dV = \cancel{\frac{dN_A}{dt}}^{\,0} \text{; steady state}$$

$$r_A = -k = -A\exp\left(\frac{-E_a}{RT}\right)$$

if $E_a \ll RT$ then $\exp\left(\frac{-E_a}{RT}\right) \sim \exp(0) = 1$

$$r_A = -A$$

$$F_{A0} - F_A - \int_V A \, dV = 0$$

$k \neq f(V)$

$$F_{A0} - F_A - AV = 0$$

$$F_{A0} - F_{A0}(1-X) = AV$$

$$\boxed{X = \frac{AV}{F_{A0}}}$$

steady-state energy balance:

$$\dot{Q} - \cancel{\dot{W}_s}^{\,0} - F_{A0}\sum_i \Theta_i C_{pi}(T-T_0) - \Delta H_{Rx}(T) F_{A0} X = 0$$

$$X = \frac{\dot{Q} - F_{A0}\sum_i \Theta_i C_{pi}(T-T_0)}{\Delta H_{Rx}(T) F_{A0}}$$

$$= \boxed{\frac{-\dot{Q} + F_{A0}C_{pA}(T-T_0)}{-F_{A0}\left(\Delta H^\circ_{Rx}(T_R) + \Delta C_p(T-T_R)\right)}}$$

b)

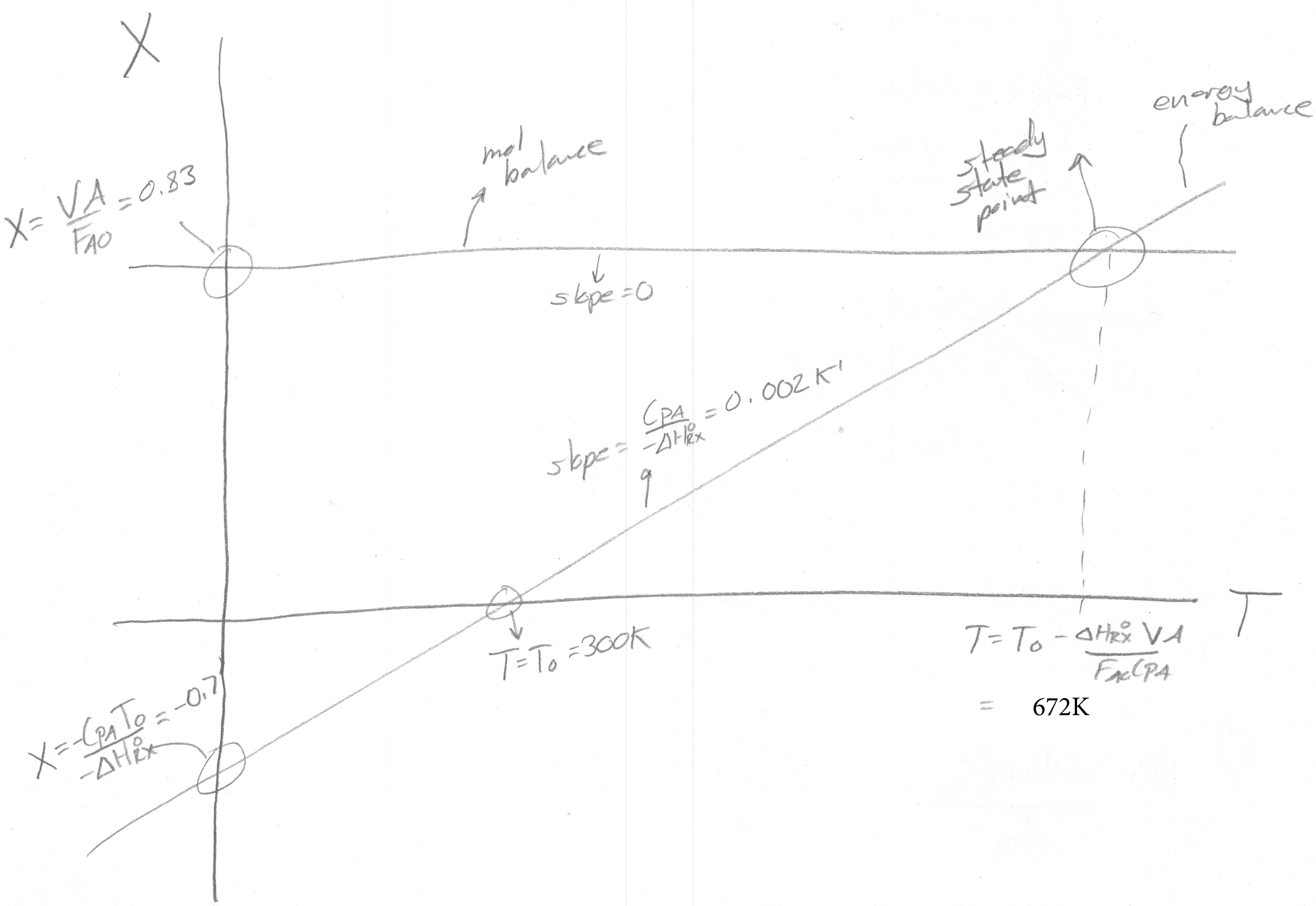
mol balance $X = \frac{AV}{F_{A0}} = \frac{\left(0.25 \frac{mol}{L\,min}\right)(100 L)}{30 \frac{mol}{min}} = \boxed{0.83}$

energy balance $X = \frac{-\cancel{\dot{Q}}^{\,0} + F_{A0}C_{pA}(T-T_0)}{-F_{A0}\left(\Delta H^\circ_{Rx}(T_R) + \cancel{\Delta C_p}(T-T_R)^{\,0}\right)} \Rightarrow T = T_0 + \frac{-\Delta H^\circ_{Rx} X}{C_{pA}}$

$C_{pA} = C_{pB} \rightarrow \Delta C_p = 0$

$$= 300K + \frac{\left(6700 \frac{J}{mol}\right)(0.83)}{15\ J/mol \cdot K} = \boxed{672}$$

C)



X
$X = \frac{VA}{F_{A0}} = 0.83$
mol balance
slope = 0
steady state point
energy balance
slope = $\frac{C_{PA}}{-\Delta H^{\circ}_{Rx}} = 0.002\ K^{-1}$
T
$T = T_0 = 300K$
$T = T_0 - \frac{\Delta H^{\circ}_{Rx} VA}{F_{A0} C_{PA}}$
= 672K
$X = \frac{-C_{PA} T_0}{-\Delta H^{\circ}_{Rx}} = -0.7$

d) The reaction is 0^{th} order so concentration (mixing) is unimportant and in the $E_a \ll RT$ limit temperature doesn't matter either (mixing unimportant).

Basically the rate is completely independent of the concentration and the temperature so the conditions within the reactor don't make any difference and all reactors of a given volume will give the same conversion.