

Homework 7 – Due 12/4/20 @ 11:59 PM (Midnight)

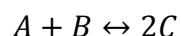
- 1.** 1-hexene (H) is used as a precursor in the production of polyethylene, and it can be produced by the dehydration reaction of hexanol (A). Water (W) is the second product of the reaction. This reaction is catalyzed by amorphous silica alumina at high temperatures. The following experimental data provides the reaction rate at various initial partial pressures of hexanol when the feed is pure hexanol.

P_{A0} (atm)	0	8	30	60	106	210
$-r'_{A0}$ (mol/hr/kg-cat)	0	0.31	0.55	0.82	0.82	0.5

- a.** Suggest a possible mechanism for this reaction? What is the most likely rate-limiting step? From your mechanism, choice of rate limiting step, and site balance determine a form of the rate law of disappearance of hexanol (A).
- b.** What are the values of the parameters of the rate law of disappearance of hexanol?
- c.** Given the data above, at the partial pressure associated with the largest reaction rate of disappearance of A, what fraction of surface sites are vacant? What fraction are occupied by A and H?
- 2.** Decide whether you agree or disagree with the following statements and justify your answers.

Statement	Agree	Disagree	Justification
When a heterogeneous reaction occurs in the liquid phase, you can ignore the desorption step.			
When the rate of adsorption is approximated to be zero, that means the adsorption step is not occurring.			
An effective catalyst makes the rate limiting step slower, allowing for the rate limiting step to be isolated and better studied.			
The distance between adjacent adsorption sites is important for reactions involving dissociative adsorption.			

- 3.** You were lucky enough to be selected for a Summer REU position at Hogwarts School of Witchcraft and Wizardry in the Potion Engineering Department. Upon arrival, you immediately are pulled aside by one of the Cauldron Design TAs, Ron Weasley. He is freaking out because he has no idea what he's doing. He begs for your help in sizing non-isothermal, adiabatic cauldrons (similar to the reactors that muggles use). He says that the liquid-phase, reversible reaction has the chemical equation



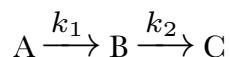
and follows an elementary rate law. The class instructor, Prof. Snape, said the reactor should have an inlet flow rate of $100 \text{ m}^3/\text{hr}$ and equimolar concentrations of A and B equal to 8 mol/L , or else there will be “consequences,” whatever that means.

You also know the following information:

$$\begin{array}{lll} C_{P,A} = 140 \text{ cal}/(\text{mol K}) & k_f(30^\circ\text{C}) = 1.8 \text{ L}/(\text{mol hr}) & E_a = 25.3 \text{ kcal/mol} \\ C_{P,B} = 100 \text{ cal}/(\text{mol K}) & K_C(30^\circ\text{C}) = 25.0 & T_{inlet} = 20^\circ\text{C} \\ C_{P,C} = 120 \text{ cal}/(\text{mol K}) & H_{rxn}^\circ(30^\circ\text{C}) = -9.6 \text{ kcal/mol} & \end{array}$$

X	0.1	0.2	0.3	0.4	0.5	0.6
$F_{A0}/-r_A [\text{m}^3]$						

- a.** Calculate and tabulate $F_{A0}/-r_A$ values for the conversions in the table above and generate a Levenspiel plot. Be sure to label axes appropriately. (Note: deriving each relationship and then using Python to calculate all values at once probably makes life easier)
- b.** Assuming the data generated in part (a) sufficiently approximates the Levenspiel plot and that a continuously stirred tank cauldron will be used first, followed by a plug-flow cauldron, what are the volumes of each cauldron such that the total volume is minimized?
- c.** Ron was originally going to assume a single plug-flow cauldron would give the smallest volume. How much bigger would a single plug-flow cauldron be compared to the volume of cauldrons in series from your answer in part (b)?

4. The elementary liquid-phase reactions

take place in a non-isothermal 100-L CSTR with heat effects. The volumetric feed rate is 1000 L/min at a concentration of A of 0.3 mol/L with an inlet temperature of 20 °C.

Additional Information

$$C_{P,A} = C_{P,B} = C_{P,C} = 200 \text{ J/mol}\cdot\text{K}$$

$$k_1 = 1.3 \text{ min}^{-1} \text{ at } 300 \text{ K, with } E_1 = 11.9 \text{ kcal/mol}$$

$$k_2 = 3.5 \text{ min}^{-1} \text{ at } 500 \text{ K, with } E_2 = 23.0 \text{ kcal/mol}$$

$$\Delta H_{Rx1A} = -38.0 \text{ kJ/mol A}$$

$$\Delta H_{Rx1B} = -65.0 \text{ kJ/mol B}$$

$$UA = 30.0 \text{ kJ/mol}\cdot\text{K} \text{ with } T_a = 57 \text{ °C}$$

- a.** At what temperatures are the different steady states and what are the effluent concentrations for each species at each steady state? Be sure to include your plot of $G(T)$, $R(T)$ vs T with properly labeled axes and a legend. (Note: you do not need Polymath to plot $G(T)$ and $R(T)$ vs T , Python can be used to plot them)
- b.** By comparing the selectivities of B/C, which steady state would you choose if you wanted to maximize formation of B?

Note: Include all code used in this homework, clearly labeled for the problem it belongs to.

- 1.** 1-hexene (H) is used as a precursor in the production of polyethylene, and it can be produced by the dehydration reaction of hexanol (A). Water (W) is the second product of the reaction. This reaction is catalyzed by amorphous silica alumina at high temperatures. The following experimental data provides the reaction rate at various initial partial pressures of hexanol when the feed is pure hexanol.

P_{A0} (atm)	0	8	30	60	106	210
$-r'_{A0}$ (mol/hr/kg-cat)	0	0.31	0.55	0.82	0.82	0.5

- a.** Suggest a possible mechanism for this reaction? What is the most likely rate-limiting step? From your mechanism, choice of rate limiting step, and site balance determine a form of the rate law of disappearance of hexanol (A).
- b.** What are the values of the parameters of the rate law of disappearance of hexanol?
- c.** Given the data above, at the partial pressure associated with the largest reaction rate of disappearance of A, what fraction of surface sites are vacant? What fraction are occupied by A and H?

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```
In [330]: import numpy as np
import matplotlib.pyplot as plt
```

#1.

1-hexene (H) is used as a precursor in the production of polyethylene, and it can be produced by the dehydration reaction of hexanol (A).

Water (W) is the second product of the reaction.

This reaction is catalyzed by amorphous silica alumina at high temperatures.

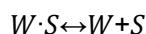
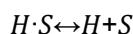
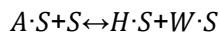
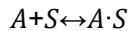
The following experimental data provides the reaction rate at various initial partial pressures of hexanol when the feed is pure hexanol.

P_{A0} (atm) 0 8 30 60 106 210

$-r_{A0}$ (mol/hr/kg-cat) 0 0.31 0.55 0.82 0.82 0.5

```
In [331]: PA0 = np.array([ 0 , 8 , 30 , 60 , 106, 210]) #ATM
rA0 = np.array([0 ,0.31 , 0.55 , 0.82 , 0.82 , 0.5]) #rA0 = -rA0 and (mol/h
r/kg-cat)
```

Mechanism:



A. You know that the rate limiting step is the surface reaction. Given this information, determine a form of the rate law of disappearance of hexanol (A).

Rate limiting Step = $A \cdot S + S \rightleftharpoons H \cdot S + W \cdot S$

$$r_{AA} = k_A P_A C_S - k_A C_{AS} = k_A (P_A C_S - C_{AS} / K_{AA})$$

where $C_s = C_v$ (vacant sites)

$$r_S = k_S C_{AS} C_S - k_S C_{HS} C_{WS} = k_S (C_{AS} C_S - C_{HS} C_{WS} / K_S)$$

= approximately 0

$$r_{DH} = k_{DH} C_{HS} - k_{DH} P_H C_S = k_{DH} (C_{HS} - P_H C_S / K_{DH})$$

= approximately 0

$$C_{AS} = K_{AA} P_A * C_S$$

$$C_{HS} = P_H C_S / K_{DH}$$

$$C_{WS} = P_W C_S / K_{DW}$$

$$= C_S (1 + (K_{AA} P_A) + (P_H / K_{DH}) + (P_W / K_{DW}))$$

$$C_S = C_T / (1 + (K_{AA} * P_A) + (P_H / K_{DH}) + (P_W / K_{DW}))$$

$$r_S = k_{SC} T^2 ((K_{AA} P_A) - (P_H P_W / (K_{DH} K_{DW} K_S)) / (1 + (K_{AAP_A}) + (P_H^*/K_{DH}) + (P_W/K_{DC}))^2$$

$$r_S = k_S (C_{AS} C_S - C_{HS} C_{WS} / K_S)$$

$$= k_S ((K_{AA} P_A C_S^2) - (P_H C_S / K_{DH}) (P_W * C_S / K_{DW}) / K_S)$$

$$= k_S ((K_{AA} P_A C_S^2) - (P_H P_W C_S^2 / (K_{DH} K_{DW} K_S)))$$

$$= k_{SC} S^2 ((K_{AA} P_A) - (P_H P_W / (K_{DH} K_{DW} * K_S)))$$

$$C_T = C_S + C_{AS} + C_{HS} + C_{WS}$$

$$= C_S + K_{AA} P_A C_S + P_H C_S / K_{DH} + P_W C_S / K_{DW}$$

$$= C_S (1 + (K_{AAP_A}) + (P_H / K_{DH}) + (P_W / K_{DW}))$$

$$C_S = C_T / (1 + (K_{AAP_A}) + (P_H / K_{DH}) + (P_W / K_{DW}))$$

$$r_S = k_{SC} T^2 ((K_{AA} P_A) - (P_H P_W / (K_{DH} K_{DW} K_S)) / (1 + (K_{AAP_A}) + (P_H^*/K_{DH}) + (P_W/K_{DC}))^2$$

$$-r_A = r_S$$

Part A)

$$-r_A = [k_S C T^2 [(KAA PA) - (PH PW / (KAA KDH KDW KS))] / (1 + (KAA PA) + (PH / KDH) + (PW / KDC))^2]$$

$$-r_A = k_S C T^2 ((K_AA P_A) - (P_H P_W / (K_AA K_DH K_DW K_S))) / (1 + (K_AAP_A) + (P_H^*/K_DH) + (P_W/K_DC))^2$$

$$P_{H0} = 0$$

$$P_{W0} = 0$$

$$-r_{A0} = k_S C T^2 K_AA P_{A0} / (1 + (K_AAP_{A0}))^2$$

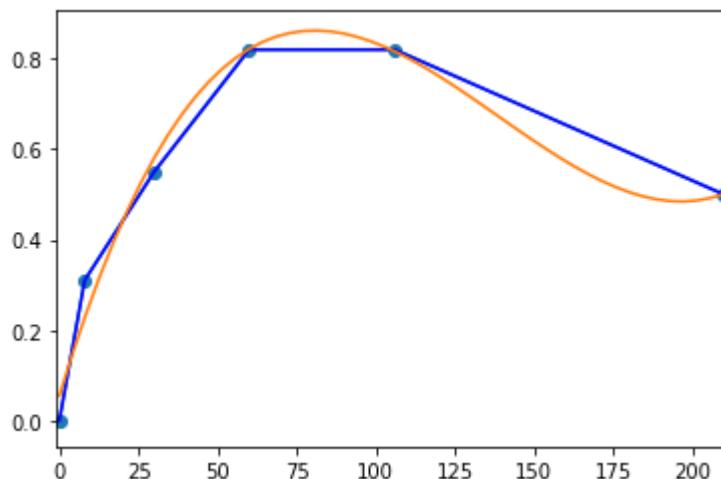
```
In [332]: plt.scatter(PA0,rA0)
plt.plot(PA0,rA0)
np.polyfit(PA0,rA0,1)

points = np.array([(0,0), (8,.31), (30,.55), (60,.82), (106,.82), (210,.5)])
# get x and y vectors
x = points[:,0]
y = points[:,1]

# calculate polynomial
z = np.polyfit(x, y, 3)
f = np.poly1d(z)

# calculate new x's and y's
x_new = np.linspace(x[0], x[-1], 50)
y_new = f(x_new)

plt.plot(x,y, 'b', x_new, y_new)
plt.xlim([x[0]-1, x[-1] + 1])
plt.show()
```



B. What are the values of the parameters KAA and k1

(where $K_{AA} = k_{AA}/k_{DA}$ and $k_1 = k_s C T^2$) in the rate law of disappearance of hexanol?

```
In [333]: from scipy.optimize import curve_fit

PA0 = np.array([ 0 , 8 , 30 , 60 , 106, 210]) #ATM
_rA0 = np.array([0 ,0.31 , 0.55 , 0.82 , 0.82 , 0.5])

def rate_law(P, k1, KAA):
    return k1 * KAA * P / ((1 + KAA*P)**2)

popt, pcov = curve_fit(rate_law, PA0, _rA0)

k1, KAA = popt
print('Part B')
print("k1 = {:.3e}, KAA = {:.3e}".format(k1, KAA))
```

Part B
 $k_1 = 3.084 \times 10^0$, $K_{AA} = 1.395 \times 10^{-2}$

C. Given the data above, at the partial pressure associated with the largest reaction rate of disappearance of A,

what fraction of surface sites are vacant?

What fraction are occupied by A and H?

$$C_S / C_T = 1 / (1 + (K_{AA} P_{A0}) + (P_H / K_{DH}) + (P_W / K_{DW}))$$

Initially last two terms will be zero

**ANSWER: at $P_{A0} = 60$ atm

$$C_S / C_T = 1 / (1 + (K_{AA} * P_{A0}))$$

$$= 1 / 1 + (.01395) * 60 = 0.544$$

Fraction of Surface Sites that are vacant = .544

**ALTERNATE ANSWER: at $P_{A0} = 106$ atm

$$C_S / C_T = 1 / 1 + (.01395) * 106 = .4$$

Initially the occupied A, and H sites will be = 0

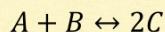
Part C at $P_{A0} = 60$ atm Fraction of Surface Sites that are vacant = .544

at $P_{A0} = 106$ atm Fraction of Surface Sites that are vacant = .4

2. Decide whether you agree or disagree with the following statements and justify your answers.

Statement	Agree	Disagree	Justification
When a heterogeneous reaction occurs in the liquid phase, you can ignore the desorption step.		X	No, Desorption is opposite of Adsorption and we need to consider all the steps
When the rate of adsorption is approximated to be zero, that means the adsorption step is not occurring.		X	No, it could mean it is not the rate limiting step
An effective catalyst makes the rate limiting step slower, allowing for the rate limiting step to be isolated and better studied.		X	No, an effective catalyst should speed up the rate limiting step
The distance between adjacent adsorption sites is important for reactions involving dissociative adsorption.		X	yes! Because if there is too large a spacing there will be failure of dissociative adsorption

- 3.** You were lucky enough to be selected for a Summer REU position at Hogwarts School of Witchcraft and Wizardry in the Potion Engineering Department. Upon arrival, you immediately are pulled aside by one of the Cauldron Design TAs, Ron Weasley. He is freaking out because he has no idea what he's doing. He begs for your help in sizing non-isothermal, adiabatic cauldrons (similar to the reactors that muggles use). He says that the liquid-phase, reversible reaction has the chemical equation



and follows an elementary rate law. The class instructor, Prof. Snape, said the reactor should have an inlet flow rate of 100 m³/hr and equimolar concentrations of A and B equal to 8 mol/L, or else there will be "consequences," whatever that means.

You also know the following information:

$$C_{P,A} = 140 \text{ cal}/(\text{mol K})$$

$$k_f(30^\circ\text{C}) = 1.8 \text{ L}/(\text{mol hr})$$

$$E_a = 25.3 \text{ kcal/mol}$$

$$C_{P,B} = 100 \text{ cal}/(\text{mol K})$$

$$K_C(30^\circ\text{C}) = 25.0$$

$$T_{inlet} = 20^\circ\text{C}$$

$$C_{P,C} = 120 \text{ cal}/(\text{mol K})$$

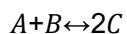
$$H_{rxn}^\circ(30^\circ\text{C}) = -9.6 \text{ kcal/mol}$$

X	0.1	0.2	0.3	0.4	0.5	0.6
F _{A0/-r_A} [m ³]						

- a.** Calculate and tabulate F_{A0/-r_A} values for the conversions in the table above and generate a Levenspiel plot. Be sure to label axes appropriately. (Note: deriving each relationship and then using Python to calculate all values at once probably makes life easier)
- b.** Assuming the data generated in part (a) sufficiently approximates the Levenspiel plot and that a continuously stirred tank cauldron will be used first, followed by a plug-flow cauldron, what are the volumes of each cauldron such that the total volume is minimized?
- c.** Ron was originally going to assume a single plug-flow cauldron would give the smallest volume. How much bigger would a single plug-flow cauldron be compared to the volume of cauldrons in series from your answer in part (b)?

#3.

You were lucky enough to be selected for a Summer REU position at Hogwarts School of Witchcraft and Wizardry in the Potion Engineering Department. Upon arrival, you immediately are pulled aside by one of the CauldronDesign TAs, Ron Weasley. He is freaking out because he has no idea what he's doing. He begs for your help in sizing non-isothermal, adiabatic cauldrons(similar to the reactors that muggles use). He says that the liquid-phase, reversible reaction has the chemical equation



and follows an elementary rate law. The class instructor, Prof. Snape, said the reactor should have an inlet flow rate of $100\text{m}^3/\text{hr}$

and equimolar concentrations of A and B equal to 8mol/L

or else there will be "consequences," whatever that means. You also know the following information:

$$\text{CPA} = 140 \text{ cal}/(\text{mol K})$$

$$k_f(30 \text{ }^\circ\text{C}) = 1.8 \text{ L}/(\text{mol hr})$$

$$E_a = 25.3 \text{ kcal/mol CP}$$

$$B = 100 \text{ cal}/(\text{mol K})$$

$$K_C(30 \text{ }^\circ\text{C}) = 25.0$$

$$T_{inlet} = 20 \text{ }^\circ\text{C}$$

$$\text{CPC} = 120 \text{ cal}/(\text{mol K})$$

$$H_{rxn}^\circ(30 \text{ }^\circ\text{C}) = -9.6 \text{ kcal/mol}$$

$$X_0 = 0.1 \ 0.2 \ 0.3 \ 0.4 \ 0.5 \ 0.6$$

$$F_A0/-r_A \text{ m}^3 = ? ? ? ? ?$$

A.Calculate and tabulate FA0/-rA values for the conversions in the table above and generate a Levenspielplot.

Be sure to label axes appropriately. (Note: deriving each relationship and then using Python to calculate all values at once probably makes life easier)

```
In [334]: CPA = 140
CPB = 100
CPC = 120
k_F = 1.8
K_C = 25.0
Hrxn = -9.6
E_a = 25.3
T0 = 293
T_ref = 303
R = 1.9859 * 10 ** -3
Fa_0 = 800000
v0 = 100
Ca_0 = 8
```

```
In [335]: def Kc(T):
    return K_C * np.exp((Hrxn/R)*((1/T_ref) - (1/T)))

def kf(T):
    return k_F * np.exp((E_a/R)*((1/T_ref) - (1/T)))

def temp(X):
    return T0 - (Hrxn* X * 1000)/(CPA + CPB)

def rate(X, T):
    return (kf(T) * Ca_0**2 * ((1 - X)**2 - (4*X*X / Kc(T)))) * 1000
```

In [336]:

```
x1 = 0.1
x2 = 0.2
x3 = 0.3
x4 = 0.4
x5 = 0.5
x6 = 0.6

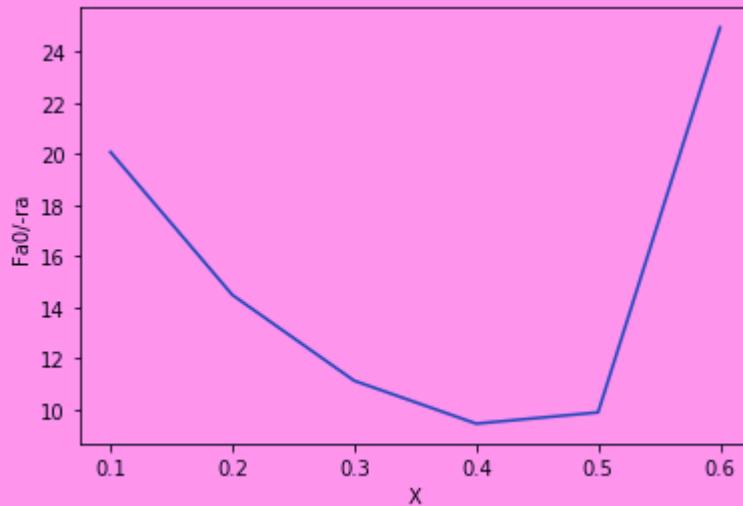
t1 = temp(x1)
t2 = temp(x2)
t3 = temp(x3)
t4 = temp(x4)
t5 = temp(x5)
t6 = temp(x6)

a = Fa_0 / (rate(x1, t1))
b = Fa_0 / (rate(x2, t2))
c = Fa_0 / (rate(x3, t3))
d = Fa_0 / (rate(x4, t4))
e = Fa_0 / (rate(x5, t5))
f = Fa_0 / (rate(x6, t6))
print(a, b, c, d, e, f)

conv = np.array([0.1,0.2,0.3,0.4,0.5,0.6])
fa_by_ra = np.array([a,b,c,d,e,f])
plt.plot(conv, fa_by_ra)
plt.xlabel("X")
plt.ylabel("Fa0/-ra")
```

```
20.075518549714694 14.478093158840718 11.120119253127436 9.441676964356544 9.
881632195740092 24.944198060443508
```

Out[336]: Text(0, 0.5, 'Fa0/-ra')



X0 =**[0.1 , 0.2 , 0.3 , 0.4 , 0.5 , 0.6]****FA0/-rA m^3 =****[20.0755185 , 14.47809316 , 11.120119253 , 9.44167696 , 9.881632 , 24.944198]**

B.Assuming the data generated in part (a) sufficiently approximates the Levenspiel plot and that a continuously stirred tank cauldron will be used first, followed by a plug-flow cauldron,

what are the volumes of each cauldron such that the total volume is minimized?

```
In [317]: #PFR = Integral (FA0/-rA) from .4 to .6
V = 1/3 * ((.6-.4) / 2) * (9.44 + (4*(9.88)) + 24.94)
print("Volume of the PFR Reactor",V,"m^3")
```

Volume of the PFR Reactor 2.4633333333333333 m³

```
In [318]: #CSTR = X * FA0 / -rA ; when x = .4
V_CSTR = .4 * 9.44
print("Volume of the CSTR Reactor",V_CSTR,"m^3")
```

Volume of the CSTR Reactor 3.776 m³

```
In [319]: V_total = V_CSTR + V

print("Total Volume of the CSTR and PFR Reactor",V_total,"m^3")
```

Total Volume of the CSTR and PFR Reactor 6.2393333333333333 m³

C.Ron was originally going to assume a single plug-flow cauldron would give the smallest volume.

How much bigger would a single plug-flow cauldron be compared to the volume of cauldrons in series from your answer in part (b)?

```
In [320]: #PFR_series= Integral (FA0/-rA) from .1 to .4 and then .4 to .6
V_PFR1 = 3/8*((.4-.1)/3)*(20.0755 + 3*14.478 + 3*11.12 + 9.44)

V_PFR2 = 1/3 * ((.6-.4) / 2) * (9.44 + (4*(9.88)) + 24.94)

V_series = V_PFR1 + V_PFR2

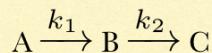
print("Total Volume of two PFR Reactors in Series",V_series,"m^3")
```

Total Volume of two PFR Reactors in Series 6.44993958333334 m³

```
In [321]: V_diff = V_series - V_total  
print("A single plug-flow cauldron will be",V_diff,"m^3 Larger than a our answer in part B")
```

A single plug-flow cauldron will be 0.21060625000000144 m³ Larger than a our answer in part B

4. The elementary liquid-phase reactions



take place in a non-isothermal 100-L CSTR with heat effects. The volumetric feed rate is 1000 L/min at a concentration of A of 0.3 mol/L with an inlet temperature of 20 °C.

Additional Information

$$C_{P,A} = C_{P,B} = C_{P,C} = 200 \text{ J/mol}\cdot\text{K}$$

$$k_1 = 1.3 \text{ min}^{-1} \text{ at } 300 \text{ K, with } E_1 = 11.9 \text{ kcal/mol}$$

$$k_2 = 3.5 \text{ min}^{-1} \text{ at } 500 \text{ K, with } E_2 = 23.0 \text{ kcal/mol}$$

$$\Delta H_{RxnA} = -38.0 \text{ kJ/mol A}$$

$$\Delta H_{RxnB} = -65.0 \text{ kJ/mol B}$$

$$UA = 30.0 \text{ kJ/mol}\cdot\text{K} \text{ with } T_a = 57 \text{ °C}$$

- a.** At what temperatures are the different steady states and what are the effluent concentrations for each species at each steady state? Be sure to include your plot of $G(T)$, $R(T)$ vs T with properly labeled axes and a legend. (Note: you do not need Polymath to plot $G(T)$ and $R(T)$ vs T , Python can be used to plot them)
- b.** By comparing the selectivities of B/C, which steady state would you choose if you wanted to maximize formation of B?

Note: Include all code used in this homework, clearly labeled for the problem it belongs to.

#4.

The elementary liquid-phase reactions A \rightarrow B \rightarrow C take place in a non-isothermal 100-L CSTR with heat effects. The volumetric feed rate is 1000 L/min at a concentration of A of 0.3 mol/L with an inlet temperature of 20 °C.

Additional Information

$$CP_A = 200 \text{ J/mol}\cdot\text{K}$$

$$CP_B = 200 \text{ J/mol}\cdot\text{K}$$

$$CP_C = 200 \text{ J/mol}\cdot\text{K}$$

$$k_1 = 1.3 \text{ min}^{-1} \text{ at } 300 \text{ K with } E_1 = 11.9 \text{ kcal/mol}$$

$$k_2 = 3.5 \text{ min}^{-1} \text{ at } 500 \text{ K, with } E_2 = 23.0 \text{ kcal/mol}$$

$$\Delta H_{rxn1A} = -38.0 \text{ kJ/mol A}$$

$$\Delta H_{rxn1B} = -65.0 \text{ kJ/mol B}$$

$$U_A = 30.0 \text{ kJ/mol}\cdot\text{K}$$

$$\text{with } T_a = 57 \text{ }^\circ\text{C}$$

A. At what temperatures are the different steady states and what are the effluent concentrations for each species at each steady state?

Be sure to include your plot of G(T), R(T) vs T with properly labeled axes and a legend. (Note: you do not need Polymath to plot G(T) and R(T) vs T, Python can be used to plot them)

Combined mole balance and rate law for A

$$V = v_0 (C_{A0} - C_A) / (k_1 C_A)$$

Solving CA gives us

$$C_A = C_{A0} / (1 + (\tau * k_1))$$

Combined mole balance and rate law for B

$$V = 0 - (C_B * v_0) / -r_B$$

$$= C_B v_0 / ((k_1 C_A) - (k_2 C_B))$$

Solving CB gives us

$$C_B = (\tau k_1 C_A) / (1 + (\tau * k_2))$$

$$= (\tau k_1 C_{A0}) / ((1 + (\tau k_1)) (1 + (\tau * k_2)))$$

Rate laws

$$r_{1A} = -(k_1 C_A) = (k_1 C_{A0}) / (1 + (\tau * k_1))$$

$$r_{2B} = -(k_2 C_B) = -((k_2 \tau k_1 C_{A0}) / ((1 + (\tau k_1)) (1 + (\tau * k_2))))$$

$$F = UA(T_a - T) - F A_0 C_P A (T - T_0) + V((r_{1A} H R_x 1A) + (r_{2B} H R_x 2B)) = 0$$

```
In [322]: v0 = 1000
C_A0 = 0.3
T0 = 293.15 #K
V = 100
Cp = 200
k1 = 1.3 # at 300 K
E1 = 11.9
k2 = 3.5 #at #500 K
E2 = 23.0
DH1 = -38000.0
DH2 = -65000.0
UA = 30000
Ta = 330.15 #K

rA = -k1*C_A
rB = -k2*C_B

F_A0 = v0*C_A0 #mol/min
F_B0 = 0 #mol/min
F_C0 = 0 #mol/min

T = np.arange(0,1000)

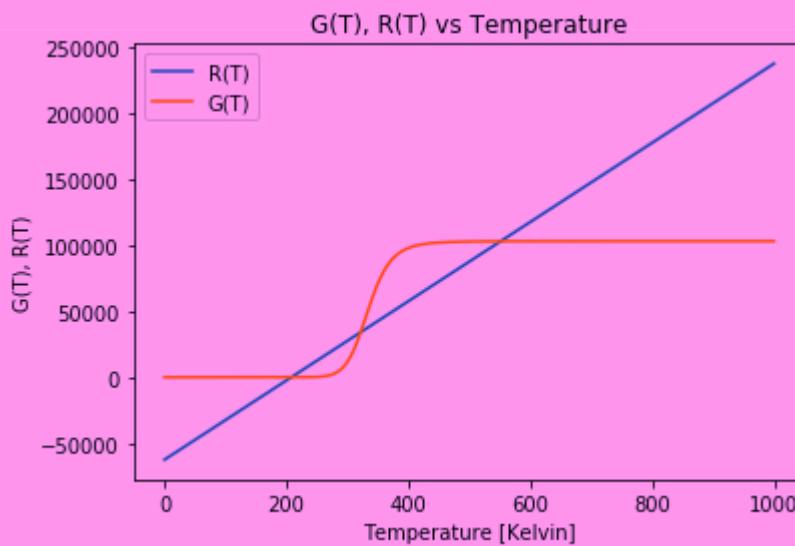
C_p = 200 # =Cp*(1 + F_B0/F_A0 + F_C0/F_A0)

K = UA/(C_p*F_A0)
Tc = K*(Ta+T0)/(1+K)
R = C_p*(1+K)*(T-Tc)
H = DH1 + DH2
tau = V/v0
R_const = 1.987*10**(-3)
A1 = k1/np.exp(-E1/(R_const*300))
k = A1*np.exp(-E1/(R_const*T))
X = tau*k/(1+tau*k)
G = -H*X
```

C:\Users\jerem\Anaconda3\lib\site-packages\ipykernel_launcher.py:33: RuntimeWarning: divide by zero encountered in true_divide

```
In [323]: plt.plot(T,R, label = 'R(T)')
plt.plot(T,G, label = 'G(T)')
plt.title('G(T), R(T) vs Temperature')
plt.xlabel('Temperature [Kelvin]')
plt.ylabel('G(T), R(T)')
plt.legend()
```

Out[323]: <matplotlib.legend.Legend at 0x280614dcf88>



```
In [324]: for i in range(0,1000):
    if R[i]>G[i]:
        T1 = T[i]
        i1 = i
        break

for i in range(T1,1000):
    if R[i]<G[i]:
        T2 = T[i]
        i2 = i
        break

for i in range(T2,1000):
    if R[i]>G[i]:
        T3 = T[i]
        i3 = i
        break

print('Steady State #1 Temperature:', T1, 'Kelvin')
print('Steady State #2 Temperature:', T2, 'Kelvin')
print('Steady State #3 Temperature:', T3, 'Kelvin')
```

Steady State #1 Temperature: 208 Kelvin
 Steady State #2 Temperature: 322 Kelvin
 Steady State #3 Temperature: 551 Kelvin

```
In [325]: A2 = k2/np.exp(-E2/(R_const*500))
k_2 = A2*np.exp(-E2/(R_const*T))

C_A = C_A0*(1-X)
C_B = (tau*k*C_A0)/((1+tau*k)+(1+tau*k_2))
C_C = (((tau)**2)*k*k_2*C_A0)/((1+tau*k)+(1+tau*k_2))

print(T1,"Kelvin", "CA =",C_A[i1], "CB =", C_B[i1], "CC =",C_C[i1])
print(T2,"Kelvin", "CA =",C_A[i2], "CB =", C_B[i2], "CC =",C_C[i2])
print(T3,"Kelvin", "CA =",C_A[i3], "CB =", C_B[i3], "CC =",C_C[i3])
```

```
208 Kelvin CA = 0.29999429428608015 CB = 2.85288408948301e-06 CC = 7.67198254
9684922e-21
322 Kelvin CA = 0.19887256358203503 CB = 0.06081356527551282 CC = 5.891124835
130713e-08
551 Kelvin CA = 0.000259044320318913 CB = 0.29871358099785666 CC = 0.89109210
23224894
```

```
C:\Users\jerem\Anaconda3\lib\site-packages\ipykernel_launcher.py:2: RuntimeWarning: divide by zero encountered in true_divide
```

Effluent Concentrations

280K:

$$C_A = 0.30 \text{ mol/L}$$

$$C_B = 2.85 \times 10^{-6} \text{ mol/L}$$

$$C_C = 7.67 \times 10^{-21} \text{ mol/L}$$

322K:

$$C_A = 0.20 \text{ mol/L}$$

$$C_B = 0.06 \text{ mol/L}$$

$$C_C = 5.89 \times 10^{-8} \text{ mol/L}$$

551K:

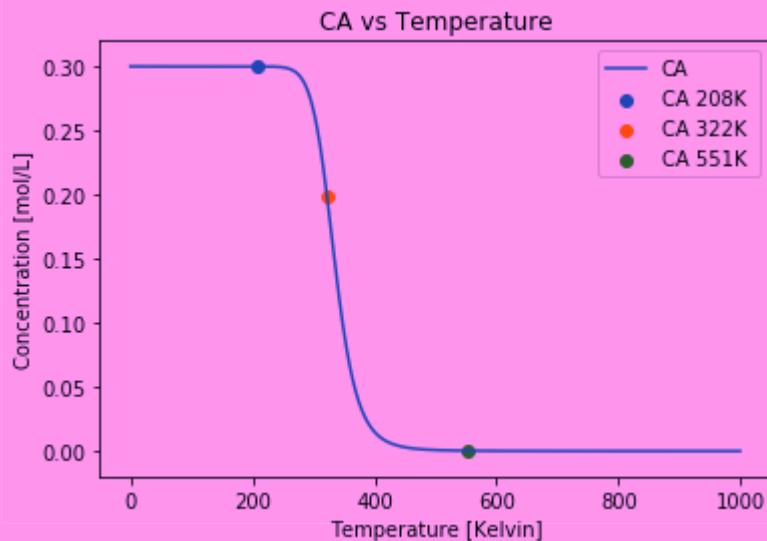
$$C_A = 2.59 \times 10^{-4} \text{ mol/L}$$

$$C_B = 0.299 \text{ mol/L}$$

$$C_C = 0.891 \text{ mol/L}$$

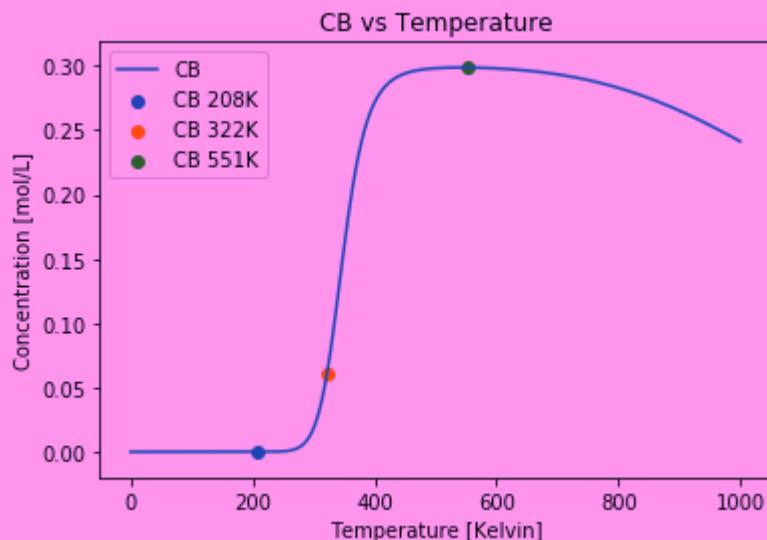
```
In [326]: plt.plot(T,C_A, label = 'CA')
plt.scatter(T[i1],C_A[i1], label = 'CA 208K')
plt.scatter(T[i2],C_A[i2], label = 'CA 322K')
plt.scatter(T[i3],C_A[i3], label = 'CA 551K ')
plt.title('CA vs Temperature')
plt.xlabel('Temperature [Kelvin]')
plt.ylabel('Concentration [mol/L]')
plt.legend()
```

Out[326]: <matplotlib.legend.Legend at 0x28061578b48>



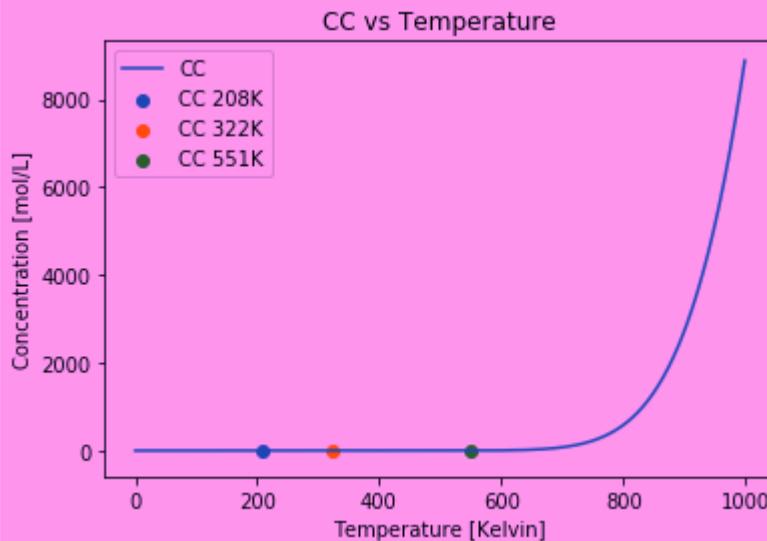
```
In [327]: plt.plot(T,C_B, label = 'CB')
plt.scatter(T[i1],C_B[i1], label = 'CB 208K')
plt.scatter(T[i2],C_B[i2], label = 'CB 322K')
plt.scatter(T[i3],C_B[i3], label = 'CB 551K')
plt.title('CB vs Temperature')
plt.xlabel('Temperature [Kelvin]')
plt.ylabel('Concentration [mol/L]')
plt.legend()
```

Out[327]: <matplotlib.legend.Legend at 0x280615fc4c8>



```
In [328]: plt.plot(T,C_C, label = 'CC')
plt.scatter(T[i1],C_C[i1], label = 'CC 208K')
plt.scatter(T[i2],C_C[i2], label = 'CC 322K')
plt.scatter(T[i3],C_C[i3], label = 'CC 551K')
plt.title('CC vs Temperature')
plt.xlabel('Temperature [Kelvin]')
plt.ylabel('Concentration [mol/L]')
plt.legend()
```

```
Out[328]: <matplotlib.legend.Legend at 0x280616767c8>
```



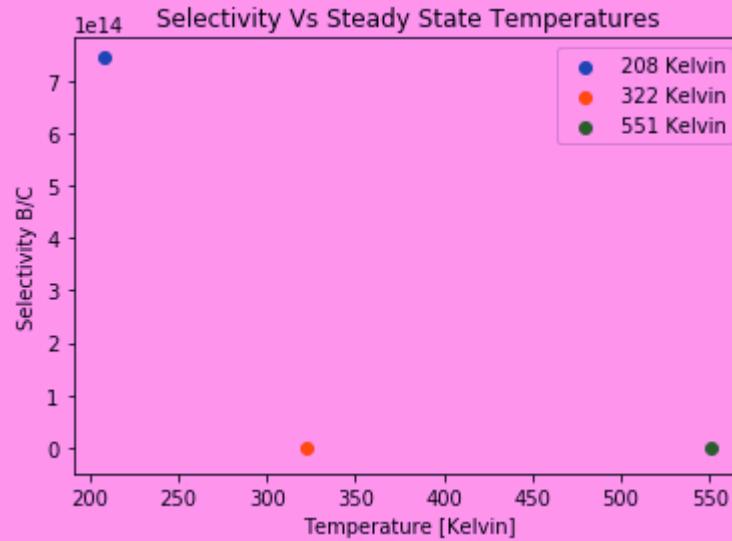
B. By comparing the selectivities of B/C, which steady state would you choose if you wanted to maximize formation of B?

```
In [329]: S_BC = (k*C_A-k_2*C_B)/(k_2*C_B)
plt.scatter(T[i1],S_BC[i1], label = '208 Kelvin')
plt.scatter(T[i2],S_BC[i2], label = '322 Kelvin')
plt.scatter(T[i3],S_BC[i3], label = '551 Kelvin')
plt.title('Selectivity Vs Steady State Temperatures')
plt.xlabel('Temperature [Kelvin]')
plt.ylabel('Selectivity B/C')
plt.legend()

print(SBC[i1])
print(SBC[i2])
print(SBC[i3])
```

```
C:\Users\jerem\Anaconda3\lib\site-packages\ipykernel_launcher.py:1: RuntimeWarning: divide by zero encountered in true_divide
    """Entry point for launching an IPython kernel.
C:\Users\jerem\Anaconda3\lib\site-packages\ipykernel_launcher.py:1: RuntimeWarning: invalid value encountered in true_divide
    """Entry point for launching an IPython kernel.
```

743707885527643.2
1716605.5776591399
-0.6636251686010487



To Maximize B select Steady State #1 where the Temperature will equals 208 degrees Kelvin