

# Donovan Feist

## CH EN 3553

### Homework 9

#### Problem 1

##### *Problem 1: Non-ideal reactors*

Experiments are being performed using a reactor with non-ideal flow. The exit concentration in response to a pulse input with an inlet volumetric flow rate of 0.1 L/s is given below.

$$\begin{aligned} C &= 0 && \text{for } t < 3 \text{ s} \\ C &= 0.5t - 1.5 && \text{for } 3\text{s} < t < 5\text{s} \\ C &= -t + 6 && \text{for } 5\text{s} < t < 6\text{s} \\ C &= 0 && \text{for } t > 6\text{s} \end{aligned}$$

C has units of mol/L.

- What is the total amount of tracer fed at  $t = 0$ ? [0.15 mol]
- Find an algebraic expression for the residence time distribution function  $E(t)$  and graph this as a function of time.
- Plot  $F(t)$  of this reactor to a step change in inlet concentration from 0 to 1 mol/L at  $t = 0$ .
- What is the mean residence time in this reactor? [4.5 s] What is the volume of this reactor? [0.45 L]
- Using the segregation model of mixing, what is the mean conversion for the second order reaction  $A \rightarrow B$  with  $k = 0.5 \text{ L}/(\text{mol}\cdot\text{s})$ , and  $C_{A0} = 1 \text{ mol/L}$ ? [0.7] How does this compare to the conversions achieved in a CSTR and a PFR operating at the same residence time?

#### part a solution

$$N_0 = \int_0^\infty \dot{V} C(t) dt \Rightarrow$$

$$N_0 = \dot{V} \left[ \int_0^3 0 dt + \int_3^5 (0.5t - 1.5) dt + \int_5^6 (-t + 6) dt + \int_6^\infty 0 dt \right] \Rightarrow$$

$$N_0 = \dot{V} \left[ 0 + \left( \frac{0.5t^2}{2} - 1.5t \right) \Big|_3^5 + \left( \frac{-t^2}{2} + 6t \right) \Big|_5^6 + 0 \right]$$

```
In [1]: import numpy as np
        Vdot=0.1 #L/s
        t=np.array([3,5,6])
        N_0=Vdot*(.5/2*(t[1]**2-t[0]**2)-1.5*(t[1]-t[0])-1/2*(t[2]**2-t[1]**2)+6*(t[2]-t[1])) #mol
        print('N_0=',N_0,'mol')
```

N\_0= 0.15000000000000002 mol

Total amount of tracer fed at  $t = 0$  is  $N_0 = 0.150 \text{ mol}$ .

## part b solution

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt}$$

$$\int_0^\infty C(t)dt = \left[ 0 + \left( \frac{0.5t^2}{2} - 1.5t \right) \Big|_3^5 + \left( \frac{-t^2}{2} + 6t \right) \Big|_5^6 + 0 \right] = 1.5 \frac{\text{mol}}{L}$$

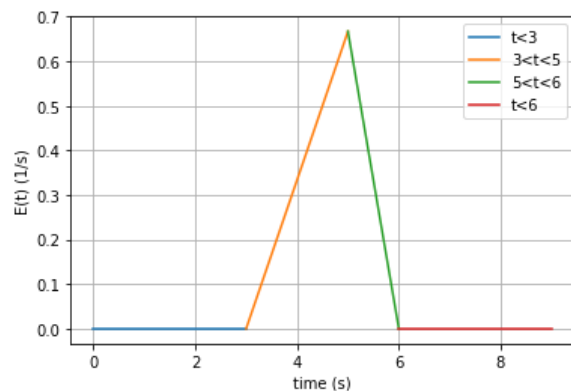
Because this is a piecewise function

$$E(t) = \begin{cases} 0 & t < 3s \\ \frac{0.5t-1.5}{1.5} & 3s \leq t \leq 5s \\ \frac{-t+6}{1.5} & 5s \leq t \leq 6s \\ 0 & t > 6s \end{cases}$$

```
In [3]: t1=np.linspace(0,3)
t2=np.linspace(3,5)
t3=np.linspace(5,6)
t4=np.linspace(6,9)
E1=0*t1
E2=(0.5*t2-1.5)/1.5
E3=(-t3+6)/1.5
E4=0*t4

import matplotlib.pyplot as plt

plt.plot(t1,E1,label='t<3')
plt.plot(t2,E2,label='3<t<5')
plt.plot(t3,E3,label='5<t<6')
plt.plot(t4,E4,label='t<6')
plt.legend(loc='best')
plt.grid()
plt.xlabel('time (s)')
plt.ylabel('E(t) (1/s)')
plt.show()
```



## part c solution

$$F(t) = \int_0^t E(t)dt \Rightarrow$$

$$F(t) = \begin{cases} \int_0^t E(t) & t < 3s \\ \int_0^3 E(t) + \int_3^t E(t) & 3s \leq t \leq 5s \\ \int_0^3 E(t) + \int_3^5 E(t) + \int_5^t E(t) & 5s \leq t \leq 6s \\ \int_0^3 E(t) + \int_3^5 E(t) + \int_5^6 E(t) + \int_6^t E(t) & t > 6s \end{cases} \Rightarrow$$

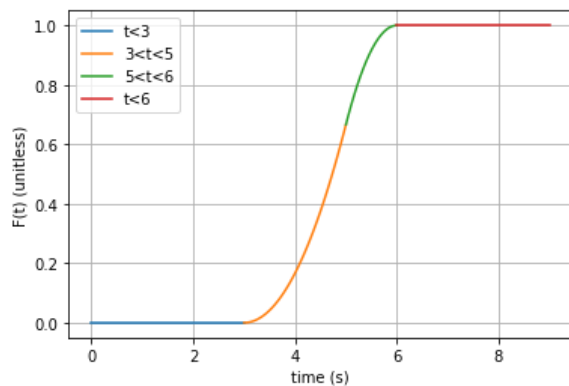
$$F(t) = \begin{cases} \int_0^3 0 & t < 3s \\ \int_0^3 0 + \int_3^t \frac{0.5t-1.5}{1.5} & 3s \leq t \leq 5s \\ \int_0^3 0 + \int_3^5 \frac{0.5t-1.5}{1.5} + \int_5^t \frac{-t+6}{1.5} & 5s \leq t \leq 6s \\ \int_0^3 0 + \int_3^5 \frac{0.5t-1.5}{1.5} + \int_5^6 \frac{-t+6}{1.5} + \int_6^t 0 & t > 6s \end{cases} \Rightarrow$$

$$F(t) = \begin{cases} 0 & t < 3s \\ 0 + \frac{1}{1.5} \cdot \left( \frac{0.5t^2}{2} - 1.5t \right) \Big|_3^t & 3s \leq t \leq 5s \\ 0 + \frac{1}{1.5} \cdot \left( \frac{0.5t^2}{2} - 1.5t \right) \Big|_3^5 + \frac{1}{1.5} \cdot \left( \frac{-t^2}{2} + 6t \right) \Big|_5^t & 5s \leq t \leq 6s \\ 0 + \frac{1}{1.5} \cdot \left( \frac{0.5t^2}{2} - 1.5t \right) \Big|_3^5 + \frac{1}{1.5} \cdot \left( \frac{-t^2}{2} + 6t \right) \Big|_5^6 + 0 & t > 6s \end{cases} \Rightarrow$$

$$F(t) = \begin{cases} 0 & t < 3s \\ 0 + \frac{1}{1.5} \cdot \left( \frac{0.5t^2}{2} - 1.5t + 2.25 \right) & 3s \leq t \leq 5s \\ 0 + \frac{1}{1.5} \cdot (1) + \frac{1}{1.5} \cdot \left( \frac{-t^2}{2} + 6t - 17.5 \right) & 5s \leq t \leq 6s \\ 0 + \frac{1}{1.5} \cdot (1) + \frac{1}{1.5} \cdot (0.5) + 0 & t > 6s \end{cases}$$

```
In [4]: F1=0*t1
F2=1/1.5*(0.5/2*t2**2-1.5*t2+2.25)
F3=1/1.5+1/1.5*(-1/2*t3**2+6*t3-17.5)
F4=1/1.5+.5/1.5+0*t4

plt.plot(t1,F1,label='t<3')
plt.plot(t2,F2,label='3<t<5')
plt.plot(t3,F3,label='5<t<6')
plt.plot(t4,F4,label='t<6')
plt.legend(loc='best')
plt.grid()
plt.xlabel('time (s)')
plt.ylabel('F(t) (unitless)')
plt.show()
```



### part d solution

$$t_m = \int_0^\infty t E(t) dt \Rightarrow$$

$$t_m = \int_0^3 t E(t) dt + \int_3^5 t E(t) dt + \int_5^6 t E(t) dt + \int_6^\infty t E(t) dt \Rightarrow$$

$$t_m = \int_0^3 t(0)dt + \int_3^5 t \left( \frac{0.5t-1.5}{1.5} \right) dt + \int_5^6 t \left( \frac{-t+6}{1.5} \right) dt + \int_6^\infty t(0)dt$$

```
In [5]: from scipy.integrate import quad
t=np.linspace(0,9)
def tE2(t):
    return t/1.5*(0.5*t-1.5)
def tE3(t):
    return t/1.5*(-t+6)
tm=quad(tE2,3,5)[0]+quad(tE3,5,6)[0]
print( 'tm=',tm, 's')
```

tm= 4.666666666666667 s

$$V = \dot{V} t_m$$

```
In [6]: V=Vdot*tm
print( 'V=',V, 'L')
```

V= 0.46666666666666673 L

The mean residence time in this reactor is  $t_m = 4.67 \text{ s}$ . The volume of this reactor is  $V = 0.467 \text{ L}$ .

## part e solution

First the equation for  $\bar{X}$  must be derived, starting with the moles balance for a batch reactor (since we're using the segregation model).

$$r_A V = \frac{dN_A}{dt} \Rightarrow$$

$$r_A V = -N_{A0} \frac{dX}{dt} \Rightarrow$$

$$-kc_A^2 V = -N_{A0} \frac{dX}{dt} \Rightarrow$$

$$kN_A c_A = N_{A0} \frac{dX}{dt} \Rightarrow$$

$$kc_{A0}(1-X)^2 = \frac{dX}{dt} \Rightarrow$$

$$\int_0^X \frac{dX}{(1-X)^2} = kc_{A0}t \Rightarrow$$

$$\frac{1}{1-X} - 1 = kc_{A0}t \Rightarrow$$

$$X = 1 - \frac{1}{1+kc_{A0}t}$$

Proceeding to the calculation of the mean conversion,

$$\bar{X} = \int_0^\infty X(t)E(t)dt \Rightarrow$$

$$\bar{X} = \int_0^\infty \left(1 - \frac{1}{1+kc_{A0}t}\right)E(t)dt \Rightarrow$$

$$\bar{X} = \int_0^\infty E(t)dt - \int_0^\infty \frac{E(t)}{1+kc_{A0}t}dt \Rightarrow$$

$$\bar{X} = 1 - \int_0^\infty \frac{E(t)}{1+kc_{A0}t}dt \Rightarrow$$

$$\bar{X} = 1 - \left[ \int_0^3 \frac{0}{1+kc_{A0}t}dt + \int_3^5 \frac{0.5t-1.5}{1.5(1+kc_{A0}t)}dt + \int_5^6 \frac{-t+6}{1.5(1+kc_{A0}t)}dt + \int_6^\infty \frac{0}{1+kc_{A0}t}dt \right]$$

$$\bar{X} = 1 - \left[ \int_3^5 \frac{0.5t-1.5}{1.5(1+kc_{A0}t)}dt + \int_5^6 \frac{-t+6}{1.5(1+kc_{A0}t)}dt \right]$$

```
In [7]: k=0.5 #L/(mol*s)
c_A0=1 #mol/L

def integrand1(t):
    return (0.5*t-1.5)/(1.5*(1+k*c_A0*t))
def integrand2(t):
    return (-t+6)/(1.5*(1+k*c_A0*t))

X_bar=1-(quad(integrand1,3,5)[0]+quad(integrand2,5,6)[0])
print('X=',X)
```

X= 0.6972392674091351

Using the segregation model of mixing, the mean conversion with second order kinetics is  $\bar{X} = 0.697$ .

Deriving an equation for a CSTR with 2nd order kinetics operating at the same residence time:

$$V = \frac{F_{A0}X}{-r_A} \Rightarrow$$

$$V = \frac{c_{A0}\dot{V}X}{kc_{A0}^2(1-X)^2} \Rightarrow$$

$$t_m = \frac{X}{kc_{A0}(1-X)^2} \Rightarrow$$

```
In [8]: def functionCSTR(X):
        r=tm-X/(k*c_A0*(1-X)**2)
        return r

from scipy.optimize import fsolve

sol=fsolve(functionCSTR,0.5)
print('X_CSTR=',sol)
```

X\_CSTR= [ 0.52545352]

The conversion in a CSTR with the same residence time is  $\bar{X}_{CSTR} = 0.525$ .

Deriving an equation for a PFR with 2nd order kinetics operating at the same residence time:

$$V = F_{A0} \int_0^X \frac{dX}{-r_A} \Rightarrow$$

$$t_m \dot{V} = c_{A0} \dot{V} \int_0^X \frac{dX}{kc_A^2} \Rightarrow$$

$$t_m = \frac{1}{kc_{A0}} \int_0^X \frac{dX}{(1-X)^2} \Rightarrow$$

$$t_m = \frac{1}{kc_{A0}} \left( \frac{1}{1-X} \right) \Big|_0^X \Rightarrow$$

$$t_m = \frac{1}{kc_{A0}} \left( \frac{1}{1-X} - 1 \right) \Rightarrow$$

```
In [9]: def functionPFR(X):
        r=tm-1/(k*c_A0)*(1/(1-X)-1)
        return r

solPFR=fsolve(functionPFR,0.5)
print('X_PFR=',solPFR)
```

X\_PFR= [ 0.7]

The conversion in a PFR with the same residence time is  $\bar{X}_{PFR} = 0.700$ .

Comparing the conversions obtained from the three reactor types, we see that

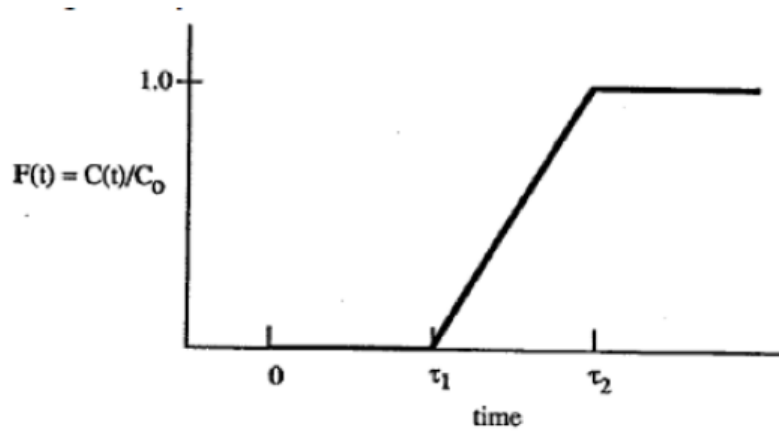
$$\bar{X}_{PFR} > \bar{X} > \bar{X}_{CSTR} \Rightarrow 0.700 > 0.697 > 0.525$$

This is in agreement with our intuition about reactors and back-mixing. In a PFR there is no back-mixing, so the conversion will be highest. In a CSTR everything is back-mixed. It seems reasonable that a reactor which has some dead zones, where not every particle has the same residence time, would have a conversion greater than a CSTR but less than a PFR.

## Problem 2

### Problem 2: Writing $E(t)$ from $F(t)$

The response of an isothermal tubular reactor to a step change in concentration at  $t = 0$  is given by the following graph.



- Write an expression for  $E(t)$  and sketch the predicted response of this reactor to a pulse input.
- Calculate the conversion of A in this reactor using a segregated model for this non-ideal tubular reactor for the liquid phase reaction. The experimental conversion is 35%. [0.35]



$$C_{A0} = 2C_{B0}$$

$$\tau_1 = 30\text{ s}$$

$$kC_{A0} = 0.05\text{ s}^{-1}$$

$$\tau_2 = 50\text{ s}$$

### part a solution

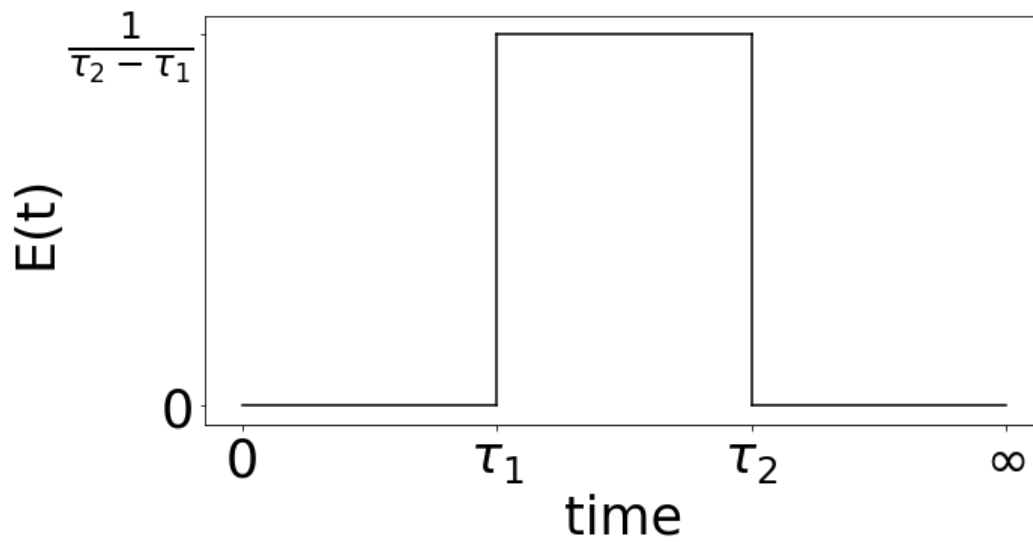
$$F(t) = \frac{C(t)}{C_0}$$

$$E(t) = \frac{d}{dt} \left( \frac{C(t)}{C_0} \right)_{\text{step}} \Rightarrow$$

$$E(t) = \begin{cases} 0 & 0 \leq t < \tau_1 \\ \frac{1}{\tau_2 - \tau_1} & \tau_1 \leq t \leq \tau_2 \\ 0 & t > \tau_2 \end{cases}$$

```
In [11]: t1=np.linspace(0,1)
t2=np.linspace(1,2)
t3=np.linspace(2,3)
E1=0*t1
E2=1*np.ones(len(t2))
E3=0*t3
v1=np.linspace(0,1)
u1=np.ones(len(v1))
v2=np.linspace(0,1)
u2=2*np.ones(len(v2))
x=np.arange(4)
y=np.arange(2)

plt.figure(figsize=(10,5))
plt.plot(t1,E1,'k')
plt.plot(t2,E2,'k')
plt.plot(t3,E3,'k')
plt.plot(u1,v1,'k')
plt.plot(u2,v2,'k')
plt.rcParams.update({'font.size': 35})
plt.xlabel('time')
plt.ylabel('E(t)')
plt.xticks(x, (0, r'$\tau_1$', r'$\tau_2$', r'$\infty$'))
plt.yticks(y, (0, r'$\frac{1}{\tau_2-\tau_1}$'))
plt.show()
```



## part b solution

First, an equation for the conversion must be derived using the segregated model.

$$r_A V = \frac{dN_A}{dt} \Rightarrow$$

$$-k C_A C_B V = \frac{d(N_{A0}(1-X))}{dt} \Rightarrow$$

$$k C_{A0} (1-X) C_{A0} \left(\frac{1}{2} - X\right) V = N_{A0} \frac{dX}{dt} \Rightarrow$$

$$k C_{A0}^2 (1-X) \left(\frac{1}{2} - X\right) V = C_{A0} V \frac{dX}{dt} \Rightarrow$$

$$kC_{A0}(1-X)(\frac{1}{2}-X) = \frac{dX}{dt} \Rightarrow$$

$$\int \frac{dX}{(1-X)(\frac{1}{2}-X)} = \int kC_{A0} dt \Rightarrow$$

$$-2 \int \frac{dX}{1-X} + 2 \int \frac{dX}{\frac{1}{2}-X} = kC_{A0}t \Rightarrow$$

$$2\ln(1-X)\Big|_0^X - 2\ln(\frac{1}{2}-X)\Big|_0^X = kC_{A0}t \Rightarrow$$

$$\ln(1-X) - \ln(1) - (\ln(\frac{1}{2}-X) - \ln(\frac{1}{2})) = \frac{kC_{A0}t}{2} \Rightarrow$$

$$\ln\left(\frac{1-X}{\frac{1}{2}-X}\right) = \frac{kC_{A0}t}{2} - \ln(\frac{1}{2}) \Rightarrow$$

$$\frac{1-X}{\frac{1}{2}-X} = \exp(\frac{kC_{A0}t}{2} \ln(\frac{1}{2})) = \alpha \Rightarrow$$

$$X = \frac{1 - \frac{1}{2}\alpha}{1 - \alpha}$$

```
In [13]: τ1=30 #s
τ2=50 #s
kC_A0=0.05 #1/s
X0=0.35

def crazy(t):
    α=np.exp(kC_A0*t/2-np.log(.5))
    integrand=(1-.5*α)/((1-α)*(τ2-τ1))
    return integrand

sol=quad(crazy,τ1,τ2)
print(sol)

(0.38518450855159614, 4.2764071012290754e-15)
```

The conversion is  $\boxed{X = 0.385}$ .

Alternatively, a method of numerically integrating two coupled ODEs could be used. Following the same derivation given above, the two ODEs would be

$$\frac{dX}{dt} = kC_{A0}(1-X)(\frac{1}{2}-X)$$

$$\frac{d\bar{X}}{dt} = X(t)E(t)$$

```
In [16]: def coupled(z,t):
    x=z[0]
    dxdt=kC_A0*(1-x)*(0.5-x)
    dxbardt=x/(τ2-τ1)
    return (dxdt,dxbardt)

z0=[X0,0]

t=np.linspace(τ1,τ2,100)

from scipy.integrate import odeint

sol=odeint(coupled,z0,t)
print(sol[-1][1])

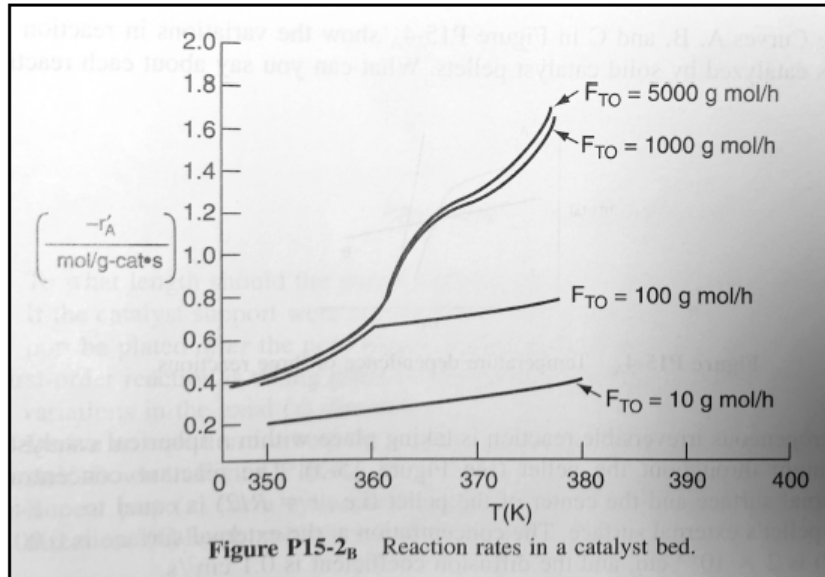
0.38842213999732506
```

Using this method, the conversion is  $\boxed{X = 0.388}$ .

## Problem 3



### Problem 3: Mass transfer limited or kinetically limited systems



Answer the following questions using the figure above from Fogler.

- Is the reaction limited by external diffusion?
- If your answer from part a was Yes, under what conditions (flow rate and temperature) is the reaction limited by external diffusion?
- Is the reaction "kinetically limited?"
- If your answer from part c was Yes, under what conditions (flow rate and temperature) is the reaction limited by the rate of chemical reaction?
- Is the reaction limited by internal diffusion?
- If your answer from part e was Yes, under what conditions (flow rate and temperature) is the reaction limited by internal diffusion?

#### part a solution

The reaction IS limited by external diffusion.

#### part b solution

The reaction is limited by external diffusion when the temperature is between 350 K and 380 K, and when the flow rate is 10 gmol/hr.

#### part c solution

When the reaction is kinetically limited  $k_r \gg k_c$ .

When the reaction is kinetically limited, there are temperature effects on  $k_c$  such that  $r'_A \propto T^{3/2} C_A$ . Therefore, we expect the graph of  $r'_A$  vs temperature to be approximately parabolically upward in direction. Examining the graph above, we see that this upward parabolic shape is present.

The reaction IS kinetically limited.

#### part d solution

The conditions under which the reaction is kinetically limited is in the temperature range of 345 K to 360 K, for flow rates between 100 gmol/hr and 5000 gmol/hr.

## part e solution

The reaction IS limited by internal diffusion.

## part f solution

For a flow rate of 10 gmol/hr, the reaction is limited by internal diffusion up until T=361 K.

For flow rates of 1000 gmol/hr and 5000 gmol/hr, the reaction is limited by internal diffusion up until T=363 K.

## Problem 4

### *Problem 4: Concentration gradients and internal effectiveness factor*

Consider an irreversible first-order heterogeneous reaction inside a porous spherical pellet that is coated on the inside with platinum. Let the reactant concentration halfway between the external surface and the center of the pellet ( $r = R/2$ ) be equal to one-tenth of the concentration of the pellet's external surface. At the external surface, the concentration is 0.001 mol/L, the effective diffusion coefficient is 0.1 cm<sup>2</sup>/s, and the diameter is 0.002 cm. Assume that the pellet is isothermal.

- At a radial distance of 0.0003 cm inside from the external pellet surface, what is the concentration of the reactant? [ $2 \times 10^{-4}$  M]
- What diameter of particle must be used to have an effectiveness factor of 0.8? [ $7 \times 10^{-4}$  cm]

## part a solution

$$\frac{C_A}{C_{AS}} = \frac{1}{\lambda} \frac{\sinh(\phi_1 \lambda)}{\sinh(\phi_1)}$$

$$\lambda = \frac{r}{R} \Rightarrow$$

$$\frac{C_A}{C_{AS}} = \frac{R}{r} \frac{\sinh(\phi_1 r/R)}{\sinh(\phi_1)}$$

$$\text{At } r = \frac{R}{2}, C_A = \frac{C_{AS}}{10} \Rightarrow$$

$$\frac{1}{10} = 2 \frac{\sinh(\phi_1/2)}{\sinh(\phi_1)}$$

```
In [17]: from math import sinh

def func(phi):
    r=0.1-2*sinh(phi/2)/sinh(phi)
    return r

phi=fsolve(func,0.5)
print('phi=',phi)

phi= [5.98644569]
```

$$C_A = \frac{C_{AS}R}{r} \frac{\sinh(\phi_1 r/R)}{\sinh(\phi)}$$

```
In [18]: C_AS=0.001 #mol/L
R=0.001 #cm
r=R-0.0003 #cm

C_A=C_AS*R/r*sinh(phi*r/R)/sinh(phi)
print('C_A=',C_A,'mol/L')
```

C\_A= 0.00023705060152623905 mol/L

The concentration of the reactant is  $2.37 \times 10^{-4} \frac{\text{mol}}{\text{L}}$ .

## part b solution

For a first-order reaction in a spherical pellet

$$\phi_1 = R \sqrt{\frac{k_N}{D_e}}$$

Assuming  $k_N$  is constant from the first situation to the second, we can calculate the value of  $k_N$  from the conditions in the first situation, then use that value in the second situation.

```
In [19]: De=0.1 #cm^2/s

def func(k):
    r=phi-R*np.sqrt(k/De)
    return r

k=fsolve(func,0.5)
print('k_N=',k)
```

k\_N= [3583753.20262914]

For a first-order reaction in a spherical pellet

$$\eta = \frac{3}{\phi_1^2}(\phi_1 \coth(\phi_1) - 1)$$

Because the desired value for  $\eta$  is given to us, we can solve for  $\phi$ .

```
In [20]: from numpy import tanh
eta=0.8

def func(phi):
    r=eta-3/phi**2*(phi*(tanh(phi))**(-1)-1)
    return r

sol=fsolve(func,0.5)
print('phi=',sol)
```

phi= [2.04207798]

The equation

$$\phi_1 = R \sqrt{\frac{k_N}{D_e}}$$

can now be used to solve for R.

```
In [21]: R=sol/np.sqrt(k/De)
D=2*R
print('D=',D,'cm')
```

D= [0.00068223] cm

To have an effectiveness factor of 0.8, the diameter of the particle must be  $D = 6.82 \times 10^{-4} \text{ cm}$ .

## Problem 5

### *Problem 5: Sizing a reactor with internal mass transfer limitations*

The second order, ideal gas phase decomposition reaction of  $A \rightarrow B$  is carried out isothermally and isobarically in a tubular reactor packed with catalyst pellets 0.4 cm in diameter. These large pellets are used to make pressure drop negligible, but as a consequence, the reaction becomes internal mass transfer limited. Pure A enters the reactor at a superficial velocity of 3 m/s, temperature of 250 degrees C and a pressure of 5 kPa. The reaction rate constant is  $k'' = 0.0005 \text{ m}^4/(\text{mol}\cdot\text{s})$ . Assume that the forced axial convection term in the mole balance is much larger than axial diffusion.

Calculate the length of the bed necessary to achieve 80% conversion with the 0.4 cm diameter pellets. [0.04 m]

#### Additional information:

Effective diffusivity:  $2.66(10^{-8}) \text{ m}^2/\text{s}$

Bed void fraction: 0.4

Pellet density  $2(10^6) \text{ g}/\text{m}^3$

Internal surface area:  $400 \text{ m}^2/\text{g}$

### **problem 5 solution**

$$\frac{d^2 C_{AB}}{dz^2} - \frac{V dC_{AB}}{dz} + r_A = 0$$

Because the axial convection is much greater than the axial diffusion,  $\frac{d^2 C_{AB}}{dz^2} \approx 0 \Rightarrow$

$$\frac{r_A}{V} = \frac{dC_{AB}}{dz}$$

$$\frac{r_A}{r_{AS}} = \eta \Rightarrow$$

$$\frac{dC_{AB}}{dz} = \frac{\eta C_{AB}}{V}$$

$$-r''_{AS} = k'' C_{AS}^2$$

Because the reaction is internally mass transfer limited

$$C_{AS} \approx C_{AB}$$

$$-r_{AS} = r''_{AS} \rho_A S_A \Rightarrow$$

$$-r_{AS} = k'' \rho_A S_A C_{AB}^2 \Rightarrow$$

$$\frac{dC_{AB}}{dz} = \frac{-\eta k'' \rho_A S_A C_{AS}^2}{V}$$

$$\phi_2 = \sqrt{\frac{k_N R^2 C_{AS}}{D_e}}$$

$$k_N = k'' \rho_A S_A \Rightarrow$$

$$\phi_2 = \sqrt{\frac{k'' \rho_A S_A R^2 C_{AS}}{D_e}}$$

$$\text{If } \phi_2 > 20 \text{ then } \eta = \frac{3}{\phi_2} \sqrt{\frac{2}{n+1}}$$

Inverting the equation of  $\frac{dC_{AB}}{dz} \Rightarrow$

$$\frac{dz}{dC_{AB}} = \frac{-V}{\eta k'' \rho_A S_A C_{AS}^2}$$

The initial concentration can be found with the equation

$$C_{A0} = \frac{P}{RT}$$

```
In [23]: kdp=0.0005 #m^4/(mol*s)
q=2*(10**6) #g/m^3
S=400 #m^2/g
R=0.4/2/100 #m
De=2.66*(10**(-8)) #m^2/s
n=2 #order of the reaction
V=3 #m/s
T=250+273.15 #K
P=5000 #Pa
Rg=8.314 #J/(mol*K)
X=0.80

def func(z,C):
    phi2=R*np.sqrt(kdp*q*S*C/De)
    eta=(3/phi2)*np.sqrt(2/(n+1))
    dzdC=-V/(eta*kdp*q*S*C**2)
    return dzdC

from scipy.integrate import odeint

C_A0=P/(Rg*T) #mol/m^3
Cend=C_A0*(1-X) #mol/m^3
C=np.linspace(C_A0,Cend,100)
z0=0

sol=odeint(func,z0,C)
print('L=',sol[-1],'m')
```

L= [0.05475363] m

The length of the bed necessary to achieve 80% conversion with 0.4 cm diameter pellets is  $L = 0.548 \text{ meters}$ .