ChE445_HW4_Winter2020_Solution_and_Code

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T.A. Maryam Azhin, Department of Chemical and Materials Engineering, University of Alberta

Multiple reactions in isothermal PBR with pressure drop, reactor descriptors

D is a target product of conversion of A via the multiple reactions:

$A \rightarrow 2B$

$3B \rightarrow D$

The rate laws are:

$-r_{A1} = k_{A1} C_A^{0.5}$

$-r_{B2} = k_{B2} C_B^2$

The rate constants (at the reaction temperature) are $k_{A1} = 75 kg_{cat}^{-1} mol^{0.5} m_{fluid}^{-0.5} s^{-1}$, $k_{B2} = 4 m_{fluid}^2 kg_{cat}^{-1} mol^{-1} s^{-1}$.

A tubular reactor of 0.25 m i.d., packed with 0.2 kg of catalyst with a particle diameter of 125 μm, catalyst density 2500 $kg/m3$ and bed porosity of 0.35 is used for the reaction. The entering pressure is 800 kPa. The feed is pure A with entering molar flow rate 30 mol/s. The entering feed dynamic viscosity is $3 * 10^{-5}$ $kg/(ms)$. The molar mass of A is 50 g/mol, of D is 40 g/mol. The reactor is maintained isothermal at 550 K. The gas phase can be assumed to be in ideal gas state. Assume that an ideal plug flow profile is developed in the reactor and no catalyst deactivation occurs. However, pressure drop must be accounted for.

Q1.

1a). Build a model and write code to find molar flow rates of A, B, and D and pressure drop "y" at the reactor exit. Include the calculation of particle Reynolds number in the program.

In your submission, include your code and a plot of all molar flow rates vs catalyst weight (W). Also include a plot of the pressure drop vs. W and report the overall pressure drop in the reactor. **Each student has to set up their own program.**

Mole Balance:

$$\frac{dF_A}{dW} = r_A \frac{dF_B}{dW} = r_B \frac{dF_D}{dW} = r_D \tag{1}$$

Reactions:

$$k_{A1} = 75 \frac{mol^{0.5}}{kg_{cat} m_{fluid}^{0.5} s} k_{B2} = 4 \frac{m_{fluid}^2}{kg_{cat} mol.s} \tag{2}$$

Stoich.:

$$A \rightarrow 2B; \;\; r_{B1} = -2r_{A1}3B \rightarrow D; \;\; r_{D2} = -\frac{1}{3}r_{B2} \tag{3}$$

$$r_A = r_{A1}r_B = r_{B1} + r_{B2}r_D = r_{D2} \tag{4}$$

$$C_A = C_{T0}\frac{F_A}{F_T}yC_B = C_{T0}\frac{F_B}{F_T}y \tag{5}$$

$$C_{T0} = C_{A0} = \frac{P_0}{R*T}F_{T0} = F_{A0}F_T = F_A + F_B + F_D \tag{6}$$

$$Ergun\ equation: \;\; \frac{dy}{dW} = \frac{-\alpha}{2y}\frac{F_T}{F_{T0}}At\ \ W = 1:\ y = 1\alpha = \frac{2\beta_0}{A_c(1-\Phi)\rho_c P_0}\beta_0 = \frac{G(1-\Phi)}{\rho_0 g_c D_p \Phi^3}[\frac{150(1-\Phi)\mu}{D_p} + 1.75G] \tag{7}$$

$$A_c = \pi * r^2 \;\; [for\ reactor]Q_0 = \frac{F_{T0}}{C_{T0}} = \frac{F_{T0}*R*T}{P_0} = \frac{30[mol/s]*8.314[J/(mol.K)]*550[K]}{800000[Pa]} = 0.1715[m^3/s]\dot{m} = F \tag{8}$$

Particle Re:

$$\rho_0[feed] = \frac{\dot{m}}{Q_0} = \frac{F_{A0}MW_A}{Q_0} = \frac{30[mol/s]*50[g/mol]}{0.1715[m^3/s]} = 8.7475Re_p = \frac{D_p\rho_0 u_s}{\mu} = \frac{125.e-6*8.746*(\frac{0.1715*4}{3.14*(0.25)^2})}{3.e-5} = \tag{9}$$

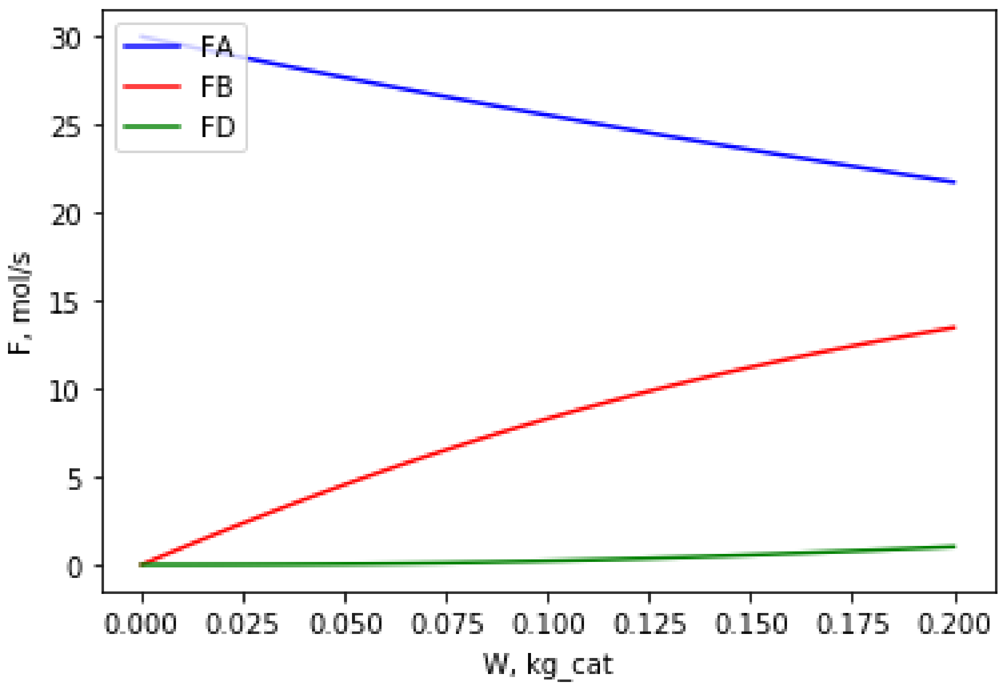
[1]:
```python
#Q1.a
from scipy.integrate import odeint
import matplotlib.pyplot as plt
import numpy as np

W0=np.linspace(0.,0.2,100)
W=W0
FA=np.zeros(len(W))
FB=np.zeros(len(W))
FD=np.zeros(len(W))
Y=np.zeros(len(W))

def fun(F,W):
    Dr=0.25
    Ac=(np.pi)*(pow(Dr,2))/4
    Wcat=0.2
    Dp=125.e-6
    Rhoc=2500.
    Phi=0.35
    P0=800000.
```

```
    FA0=30.
    FT0=FA0
    Mu=0.00003
    MWA=50. #0.050
    MWD=40. #0.040
    T=550.
    R=8.314
    CT0=P0/(R*T)
    Q0=FT0/CT0
    m=FA0*MWA/1000.
    Rho0=m/Q0
    Us=Q0/Ac
    G=m/Ac#Rho0*Us#
    Q0=FT0/CT0
    Rhofeed=m/Q0
    Reb=Dp*Rhofeed*Us/Mu
    FT=F[0]+F[1]+F[2]
    CA0=P0/(R*T)
    CT0=CA0
    CA=CT0*(F[0]*F[3]/FT)
    CB=CT0*(F[1]*F[3]/FT)
    CD=CT0*(F[2]*F[3]/FT)
    Ac=(np.pi/4.)*(pow(Dr,2.))
    beta=(G*(1.-Phi))/(Rho0*Dp*(pow(Phi,3)))*(((150.*(1-Phi)*Mu)/Dp)+(1.75*G))
    alpha=2.*beta/(Ac*(1.-Phi)*Rhoc*P0)

    kA1=75.*Ac
    kB2=4.*pow(Ac,2)

    dFAdW=-kA1*pow(CA,0.5)
    dFBdW=2.*kA1*pow(CA,0.5)-kB2*pow(CB,2)
    dFDdW=1./3*kB2*pow(CB,2)
    dYdW=(-alpha*FT)/(2.*F[3]*FT0)
    y=np.array([dFAdW,dFBdW,dFDdW,dYdW])
    return y

init_F= [30.,0.,0.,1.]
FS=odeint(fun,init_F,W)

print ("FA={0:.3f}".format(FS[len(FS)-1,0]),'mol/s')
print ("FB={0:.3f}".format(FS[len(FS)-1,1]),'mol/s')
print ("FD={0:.3f}".format(FS[len(FS)-1,2]),'mol/s')

plt.plot(W,FS[:,0],"-b", label="FA")
plt.plot(W,FS[:,1],"-r", label="FB")
plt.plot(W,FS[:,2],"-g", label="FD")
plt.legend(loc="upper left")
```

```
plt.ylabel('F, mol/s')
plt.xlabel('W, kg_cat')
```

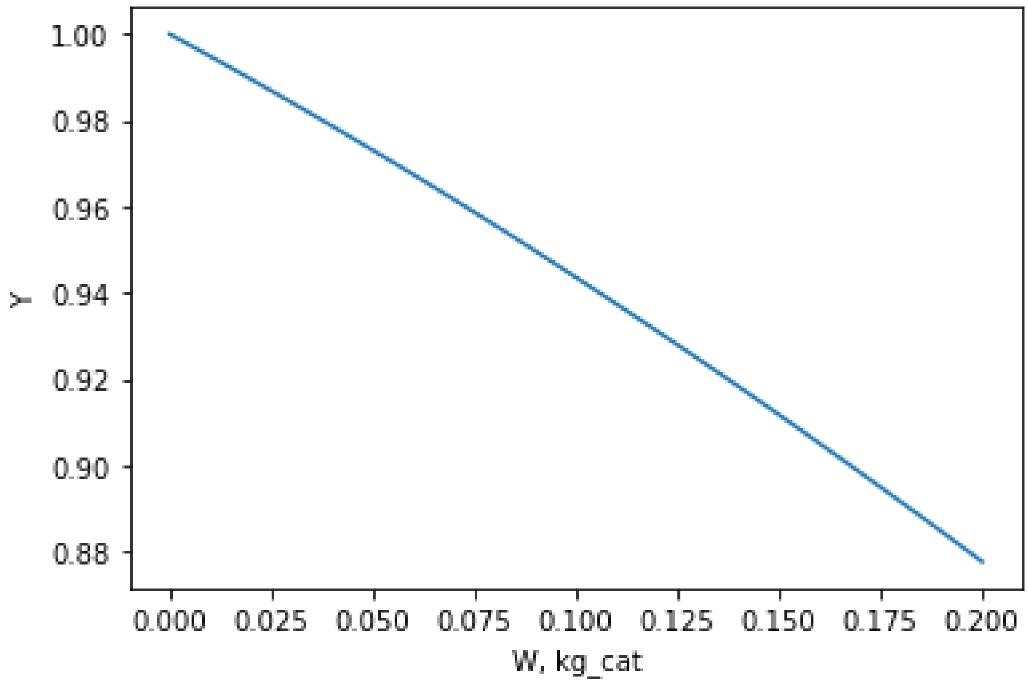
```
FA=21.736 mol/s
FB=13.470 mol/s
FD=1.020 mol/s
```

[1]: Text(0.5, 0, 'W, kg_cat')



[2]:
```
import matplotlib.pyplot as plt
plt.plot(W,FS[:,3])
plt.ylabel('Y')
plt.xlabel('W, kg_cat')
```

[2]: Text(0.5, 0, 'W, kg_cat')



[11]:
```
Dr=0.25
Ac=(np.pi)*(pow(Dr,2))/4
Dp=125.e-6
P0=800000.
FA0=30.
FT0=FA0
Mu=0.00003
MWA=50. #0.050
MWD=40. #0.040
T=550.
R=8.314
CT0=P0/(R*T)
Q0=FT0/CT0
m=FA0*MWA/1000.
Rho0=m/Q0
Us=Q0/Ac
Rhofeed=m/Q0
Rhoc=2500.
Phi=0.35
Wcat=0.2
MWD=40. #0.040
Reb=Dp*Rhofeed*Us/Mu
print ("Re={0:.3f}".format(Reb))
    # Overall_P_Drop
```

```
Overall_P_Drop=P0-FS[len(FS)-1,3]*P0
print ("Overall_P_Drop={0:.3f}".format(Overall_P_Drop),'Pa')
Rhofeed
```

```
Re=127.324
Overall_P_Drop=97775.384 Pa
```

[11]: 8.747567082905068

1b). Calculate WHSV $[1/h]$, GHSV $[1/h]$, WTYD in $[kg_D/kg_{cat}h]$, X_A and integral selectivity to D.

$$\dot{m}_T = \dot{m}_{A0} = F_{A0} * MW_A = 30[mol/s] * 0.050[kg/mol] = 1.5[kg/s] WHSV = \frac{\dot{m}_T}{W_{cat}} = \frac{1.5[kg/s]}{0.2[kg]} * \frac{3600[s]}{1[hr]} WHSV = \tag{10}$$

[4]:
```
#Q1.b
WHSV=(m/0.2)*3600
print ("WHSV={0:.1f}".format(WHSV),'1/h')
Q0STP=R*273.15*30/100000
Rhob= Rhoc*(1.-Phi)
Vbed=Wcat/Rhob
GHSV=(Q0STP/Vbed)*3600
print ("GHSV={0:.3f}".format(GHSV))
Wprod=FS[len(FS)-1,2]*MWD/1000.
WTY=(Wprod/Wcat)*3600
print ("WTY={0:.3f}".format(WTY),'kg_D/kg_cat.hr')
X_A=(MWA-FS[len(FS)-1,0])/MWA
print ("X_A={0:.3f}".format(X_A))
S_D=FS[len(FS)-1,2]/(FS[len(FS)-1,1]+FS[len(FS)-1,2])
print ("S_D={0:.3f}".format(S_D))
```

```
WHSV=27000.0 1/h
GHSV=19927753.852
WTY=734.105 kg_D/kg_cat.hr
X_A=0.565
S_D=0.070
```

1c). Based on the particle Reynolds number, is our assumption of ideal plug flow profile reasonable? (assuming no channeling or bypassing).

Particle Re = corresponds to turbulent flow and ideal PBR conditions might be satisfied. 127.32>100 Assumption of ideal plug flow is not reasonable due to transition flow regime.

Q2.

2a). To minimize pressure drop, the catalyst was pelletized into spheres of 2 cm diameter. Repeat your calculations for this case (all other parameters and conditions remain the same) and report the molar flow rates and pressure drop at the outlet of the reactor.

2b). Calculate WTY of the target product D for the pelletized catalyst. Is there an improvement compared to the powered catalyst of Q1?

D_p=0.02cm Based on the attached code

$$FA = 21.5[mol/s]FB = 13.3[mol/s]F_D = 1.2[mol/s]\Delta Poverall = P_0*(1-y) = 800000*(1-0.9995) = 400[kPa]WT \tag{11}$$

WTY_D is increased compare to Q1.b. Therefore by increasing the size of the catalyst pellets the result is improved.

[10]:
```
#Q2.a
from scipy.integrate import odeint
import matplotlib.pyplot as plt
import numpy as np

W0=np.linspace(0.,0.2,100)
W=W0
FA=np.zeros(len(W))
FB=np.zeros(len(W))
FD=np.zeros(len(W))
Y=np.zeros(len(W))

def fun(F,W):
    Dr=0.25
    Ac=(np.pi)*(pow(Dr,2))/4
    Wcat=0.2
    Dp=0.02
    Rhoc=2500.
    Phi=0.35
    P0=800000.
    FA0=30.
    FT0=FA0
    Mu=0.00003
    MWA=50. #0.050
    MWD=40. #0.040
    T=550.
    R=8.314
    CT0=P0/(R*T)
    Q0=FT0/CT0
    m=FA0*MWA/1000.
    Rho0=m/Q0
    Us=Q0/Ac
    G=m/Ac#Rho0*Us#
    Q0=FT0/CT0
    Rhofeed=m/Q0
    Reb=Dp*Rhofeed*Us/Mu
    FT=F[0]+F[1]+F[2]
    CA0=P0/(R*T)
```

```
    CT0=CA0
    CA=CT0*(F[0]*F[3]/FT)
    CB=CT0*(F[1]*F[3]/FT)
    CD=CT0*(F[2]*F[3]/FT)
    Ac=(np.pi/4.)*(pow(Dr,2.))
    beta=(G*(1.-Phi))/(Rho0*Dp*(pow(Phi,3)))*(((150.*(1-Phi)*Mu)/Dp)+(1.75*G))
    alpha=2.*beta/(Ac*(1.-Phi)*Rhoc*P0)

    kA1=75.*Ac
    kB2=4.*pow(Ac,2)

    dFAdW=-kA1*pow(CA,0.5)
    dFBdW=2.*kA1*pow(CA,0.5)-kB2*pow(CB,2)
    dFDdW=1./3*kB2*pow(CB,2)
    dYdW=(-alpha*FT)/(2.*F[3]*FT0)
    y=np.array([dFAdW,dFBdW,dFDdW,dYdW])
    return y

init_F= [30.,0.,0.,1.]
FS2=odeint(fun,init_F,W)

print ("FA={0:.3f}".format(FS2[len(FS2)-1,0]),'mol/s')
print ("FB={0:.3f}".format(FS2[len(FS2)-1,1]),'mol/s')
print ("FD={0:.3f}".format(FS2[len(FS2)-1,2]),'mol/s')
print ("y={0:.3f}".format(FS2[len(FS2)-1,3]))
```

```
FA=21.508 mol/s
FB=13.337 mol/s
FD=1.215 mol/s
y=0.999
```

[6]:
```
Dp=0.02
Overall_P_Drop=P0-FS2[len(FS2)-1,3]*P0
print ("Overall_P_Drop={0:.3f}".format(Overall_P_Drop),'Pa')
```

```
Overall_P_Drop=400.101 Pa
```

[7]:
```
#Q2.b
Wprod=FS2[len(FS2)-1,2]*MWD/1000.
WTY=(Wprod/Wcat)*3600
print ("WTY={0:.3f}".format(WTY),'kg_D/kg_cat.hr')
```

```
WTY=875.145 kg_D/kg_cat.hr
```