CASE
Determining Reactor Length

Case Description

A catalytic reaction is carried out in an isothermal circulating fluidized bed reactor. For reactions with surface-reaction limited mechanisms, where A and B are adsorbed on the surface of the catalyst, the reaction rate $(-r_A)$ equation is:

$$-r_A = \frac{k_1 C_A}{1 + k_2 C_A + k_3 C_B}$$

Where reaction rates r_A in kmol/m^3.s, C_A and C_B are the concentrations of A and B in kmol/m^3, and k_1, k_2, and k_3 are reaction rate constants. It is assumed that the catalyst moves at the same speed as the gas, ie U m/s.

From mass balance in reactor, the equation is obtained as below:

$$z = C_{A0} U \int_0^x \frac{1}{(-r_A)} dx$$

$$C_A = C_{A0}(1 - x), C_B = C_{B0}(1 + x)$$

Where:

z	= Reactor length (m)
C_{A0}	= Concentration of A at inlet reactor (z = 0)
C_{B0}	= Concentration of B at inlet reactor (z = 0)
x	= Reaction conversion

Known data: C_{A0} = 0,2 kmol/m^3, C_{B0} = 0, U = 7,5 m/s, k_1 = 8 s^{-1}, k_2 = 3 m^3/kmol, k_3 = 0,01 m^3/kmol.

Objective

Determine the required length of reactor to reach reaction conversion of 90% and show the relationship between reactor length and reaction conversion in graph and table.

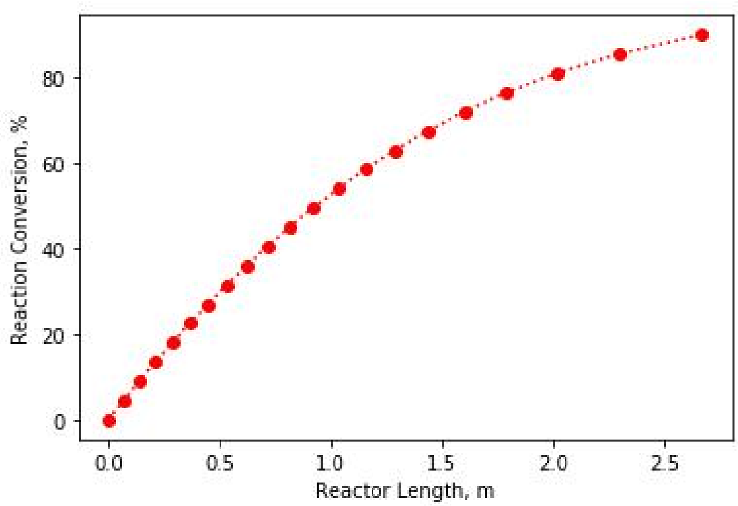
Solution

To determine the required length of reactor, we need to solve the equations of reactor length (z) and reaction rate $(-r_A)$ as functions of reaction conversion (x) simultaneously using numerical calculation method in python. Integration in reactor length (z) equation will be carried out using Simpson method. Python coding script is attached to this file or it can also be seen in the folder with filename ‘Code.py’.

Result

Calculation Results:

Reactor Length, m	Reaction Conversion, %
0.00	0.00
0.07	4.50
0.14	9.00
0.21	13.50
0.29	18.00
0.37	22.50
0.45	27.00
0.53	31.50
0.62	36.00
0.71	40.50
0.81	45.00
0.92	49.50
1.03	54.00
1.15	58.50
1.29	63.00
1.43	67.50
1.60	72.00
1.79	76.50
2.01	81.00
2.29	85.50
2.67	90.00



Conclusion

From the calculation result, it is found that the required length of reactor to reach 90% conversion reaction is 2.67 meters.

```python
# Case: Determining Reactor Length

# Import library
import numpy as np
import matplotlib.pyplot as plt


# Data
CA0 = 0.2  # Concentration of A at inlet reactor (kmol/m3)
CB0 = 0    # Concentration of B at inlet reactor (kmol/m3)
U = 7.5    # Gas velocity (m/s)
k1 = 8     # constants
k2 = 3     # constants
k3 = 0.01  # constants
x0 = 0     # initial conversion at z=0
xf = 0.90  # target conversion


# Function for reaction rate
def reactionRate(xi):
    CA = CA0*(1-xi)
    CB = CB0*(1-xi)
    _RA = k1*CA/(1+k2*CA+k3*CB)
    fi = 1/_RA
    return fi


# Function for reactor length
def reactorLength(xfj):
    #Integration is carried out using Simpson method
    n = 20 # number of integration segment
    dx = (xfj-x0)/n
    xj = np.linspace(x0,xfj,n+1)
    f = np.zeros(n+1)
    fsim = np.zeros(n+1)
    for j in range(n+1):
        f[j] = reactionRate(xj[j])
        if j == 0:
            fsim[j] = f[j]
        elif j == n:
            fsim[j] = f[j]
        elif (-1)**j < 0:
            fsim[j] = 4*f[j]
        else:
            fsim[j] = 2*f[j]
    z = U*CA0*dx/3*sum(fsim)
    return z


# Calling out the results
nx = 21
x = np.linspace(x0,xf,nx)
z = np.zeros(nx)
for i in range(0,nx):
    z[i] = reactorLength(x[i])


# Showing the Table
print('Calculation Results:')
garis = '-'*53
tabel = np.zeros([nx,2])
```

```python
tabel[:,0] = z
tabel[:,1] = x*100
header = ['Reactor Length, m','Reaction Conversion, %']
print(garis)
print('{:^25s} {:^25s}'.format(*header))
print(garis)
for baris in tabel:
    print('{:^25.2f} {:^25.2f}'.format(*baris))
print(garis)


# Showing the Graph
plt.plot(z,x*100,'o:r')
plt.xlabel('Reactor Length, m')
plt.ylabel('Reaction Conversion, %')
```