Solutions to workshop 04: Isothermal reactor design

Lecture notes for chemical reaction engineering

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Try following problems from Fogler 5e(Fogler 2016).

P 5-7, P 5-8, P 5-9, P 5-11, P 5-24, P 6-4, P 6-6, P 6-7

We will go through some of these problems in the workshop.

P 5-7

The gas-phase reaction

 $A \longrightarrow B + C$

follows an elementary rate law and is to be carried out first in a PFR and then in a separate experiment in a CSTR. When pure A is fed to a 10 dm³ PFR at 300 K and a volumetric flow rate of 5 dm³/s, the conversion is 80%. When a mixture of 50% A and 50% inert (I) is fed to a 10 dm³ CSTR at 320 K and a volumetric flow rate of 5 dm³/s, the conversion is also 80%. What is the activation energy in cal/mol?

Solution

Gas phase elementary reaction

$$A \longrightarrow B + C$$

Data:

PFR: $V = 10dm^3$; $V_0 = 5dm^3/s$; T = 300K; X = 0.8CSTR: $V = 10dm^3$; $V_0 = 5dm^3/s$; T = 320K; X = 0.8; $y_{A0} = 0.5$; $y_{I0} = 0.5$ Rate: $-r_A = kC_A = k_0 e^{-E/RT} C_{A0}(1 - X)$ For PFR:

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

$$\frac{dX}{dV} = \frac{kC_{A0}(1-X)}{C_{A0}v_0(1+\epsilon X)}$$
$$\therefore k\tau = \int_0^{0.8} \frac{(1+\epsilon X)}{(1-X)} dX$$
$$\epsilon = y_{A0}\delta = 1 + (1+1-1) = 1$$

import numpy as np
from scipy.integrate import quad
def RHS(X, epsilon):
return (1 + epsilon * X) / (1 - X)
epsilon = 1
volume = 10
v_0 = 5
tau = volume/ v_0
X = 0.8
result, _ = quad(RHS, 0, X, args=(epsilon,))
k_pfr = result / tau
k from PFR experiment = 1.209 at 300 K
For CSTR:

$$\begin{split} V &= \frac{F_{A0}X}{-r_A|_{exit}} \\ V &= \frac{v_0 C_{A0}X}{k C_{A0} \frac{(1-X)}{(1+\epsilon X)}} = \frac{v_0 X(1+\epsilon X)}{k(1-X)} \\ \epsilon &= \frac{1}{2}(1+1-1) = 0.5 \\ \tau &= \frac{10}{2} = 2s \\ k &= \frac{X(1+\epsilon X)}{\tau(1-X)} \end{split}$$

epsilon = 0.5
tau = 2
X = 0.8

k_cstr = (X * (1 + epsilon * X))/ (tau * (1 - X))

k from CSTR experiment = 2.800 at 320 K

$$\ln \frac{k_2}{k_1} = \frac{E}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right]$$

```
R = 1.987
activation_energy = np.log(k_cstr/k_pfr) * R /((1/300) - (1/320))
```

```
Activation energy = 8006.47 cal/mol
```

P 5-8

The elementary gas-phase reaction

 $A \longrightarrow B$

takes place isobarically and isothermally in a PFR where 63.2% conversion is achieved. The feed is pure A.

It is proposed to put a CSTR of equal volume upstream of the PFR. Based on the entering molar flow rate to A to the first reactor, what will be the intermediate from the CSTR, X_1 , and exit conversion from the PFR, X_2 , based on the feed to first reactor?

The entering flow rates and all other variables remain the same as that for the single PFR.



CSTR added upstream of PFR. \rightarrow equal volume. Therefore τk = 1.00.

$$\begin{split} V &= \frac{F_{A0}X}{kC_{A0}(1-X)} \Rightarrow \tau k = \frac{X}{1-X} \\ 1 &= \frac{X}{1-X} \Rightarrow X_1 = 0.5 \end{split}$$

For X_2

$$\tau k = \int_{X_1}^{X_2} \frac{dX}{1-X}$$

This integral can be easily solved by analytical method

$$\begin{split} 1 &= \ln \frac{1}{1-X_2} - \ln \frac{1}{1-X_1} \\ 1 &- \ln 2 = \ln \frac{1}{1-X_2} \Rightarrow X_2 = 0.82 \end{split}$$

Here's alternative numerical way to solve it.

To calculate X_2 from a given X_1 and τk , where τk is the result of the definite integral from X_1 to X_2 of $\frac{dX}{1-X}$, you'll need to perform the inverse operation. Essentially, you need to solve for X_2 in the equation $\tau k = \int_{X_1}^{X_2} \frac{dX}{1-X}$.

This operation is not straightforward because it requires finding the roots of a function, which is an iterative numerical process. Python's scipy library has methods such as fsolve for root finding.

```
import numpy as np
from scipy.integrate import quad
from scipy.optimize import fsolve

def func(x2, x1, tau_k):
    result, _ = quad(lambda x: 1 / (1 - x), x1, x2)
    return result - tau_k

x1 = 0.5
tau_k = 1

# provide a good initial guess for x2
x2_guess = x1 + 0.1

# Solve for x2
x2 = fsolve(func, x2_guess, args=(x1, tau_k))

X<sub>2</sub> = 0.816.
```

P 5-9

The liquid-phase reaction

 $A+B \longrightarrow C$

follows an elementary rate law and is carried out isothermally in a flow system. The concentrations of the A and B feed streams are 2 M before mixing. The volumetric flow rate of each stream is 5 dm³/min, and the entering temperature is 300 K. The streams are mixed immediately before entering. Two reactors are available. One is a gray, 200.0 dm³ CSTR that can be heated to 77 °C or cooled to 0 °C, and the other is a white, 800.0 dm³ PFR operated at 300 K that cannot be heated or cooled but can be painted red or black. Note that $k = 0.07 dm^3/mol \cdot min$ at 300 K and E = 20 kcal/mol.

- Which reactor and what conditions do you recommend? Explain the reason for your choice (e.g., color, cost, space available, weather conditions). Back up your reasoning with the appropriate calculations.
- How long would it take to achieve 90% conversion in a 200 dm³ batch reactor with $C_{A0} = C_{B0} = 1$ M after mixing at a temperature of 77°C?
- What would your answer to part (b) be if the reactor were cooled to 0° C?
- What conversion would be obtained if the CSTR and PFR were operated at 300 K and connected in series? In parallel with 5 mol/min to each?
- Keeping Table 1 in mind, what batch reactor volume would be necessary to process the same amount of species A per day as the flow reactors, while achieving 90% conversion?

Table 1: Concentrations in a variable-volume gas flow system

$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v}$	$= \frac{F_{A0}(1-X)}{v_0(1+eX)} \left(\frac{T_0}{T}\right) \frac{P}{P_0}$	$= C_{A0} \tfrac{(1-X)}{(1+eX)} \left(\tfrac{T_0}{T} \right) \tfrac{P}{P_0}$
$C_B = \frac{F_B}{v} = \frac{F_{A0}(\Theta_B - (b/a)X)}{v}$	$= \frac{F_{A0}(\Theta_B-(b/a)X)}{v_0(1+eX)} \left(\frac{T_0}{T}\right) \frac{P}{P_0}$	$= C_{A0} \tfrac{(\Theta_B - (b/a)X)}{(1 + eX)} \left(\tfrac{T_0}{T} \right) \tfrac{P}{P_0}$
$C_C = \frac{F_C}{v} = \frac{F_{A0}(\Theta_C + (c/a)X)}{v}$	$= \frac{F_{A0}(\Theta_C + (c/a)X)}{v_0(1 + eX)} \left(\frac{T_0}{T}\right) \frac{P}{P_0}$	$= C_{A0} \tfrac{\left(\Theta_C + (c/a)X\right)}{(1+eX)} \left(\tfrac{T_0}{T}\right) \tfrac{P}{P_0}$
$C_D = \frac{F_D}{v} = \frac{F_{A0}(\Theta_D + (d/a)X)}{v}$	$= \frac{F_{A0}(\Theta_D + (d/a)X)}{v_0(1 + eX)} \left(\frac{T_0}{T}\right) \frac{P}{P_0}$	$= C_{A0} \tfrac{(\Theta_D + (d/a)X)}{(1+eX)} \left(\tfrac{T_0}{T} \right) \tfrac{P}{P_0}$
$C_1 = \frac{F_1}{v} = \frac{F_{A0}\Theta_1}{v}$	$= \frac{F_{A0}\Theta_1}{v_0(1+eX)} \left(\frac{T_0}{T}\right) \frac{P}{P_0}$	$= C_{A0} \Theta_1 \tfrac{1}{(1+eX)} \left(\tfrac{T_0}{T} \right) \tfrac{P}{P_0}$

Solution

Hand written solution

1. recommended reactor and conditions

```
import numpy as np
from scipy.integrate import quad
from scipy.optimize import fsolve
# Data
k 300 = 0.07 \# dm^3/mol min
E = 20*1000 \ \# \ cal/mol
R = 1.987 # cal/mol K
V CSTR = 200 # dm^3
V PFR = 800 # dm<sup>3</sup>
v OA = 5 # dm<sup>3</sup>/min
v OB = 5 # dm^3/min
v_0 = v_0A + v_0B
C_{Ain} = 2  # mol/dm<sup>3</sup>
C Bin = 2  # mol/dm<sup>3</sup>
F_AO = C_Ain * v_OA
F_BO = C_Bin * v_OB
C AO = F AO / v O
C BO = F BO/v O
# Calculate k at 77 degC (350 K)
k_{350} = k_{300} * np.exp((E/R) * ((1/300) - (1/350)))
k_273 = k_300 * np.exp((E/R) * ((1/300) - (1/273)))
# CSTR conversion
# Calculate concentrations and rate
CA = lambda x: C_A0 * (1 - x)
CB = lambda x: C_B0 * (1 - x)
rA = lambda x,k: k * CA(x) * CB(x)
# Function to find the root of
def func(x, *args):
   v, fa0, k = args
   rate = rA(x,k)
    return x - v * rate/ fa0
x_guess = 0
x_cstr = fsolve(func, x2_guess, args=(V_CSTR, F_A0, k_350))
```

 X_{CSTR} at 350 K = 0.926. To calculate the PFR conversion we solve

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

using similar approach from problem P 5-8.

```
# PFR conversion

def find_x(x1, *args):
    v, k, fa0 = args
    result, _ = quad(lambda x: 1 / rA(x,k), 0, x1)
    return fa0 * result - v

x_guess = 0
x_pfr = fsolve(find_x, x_guess, args=(V_PFR, k_300, F_A0))
```

```
X_{PFR} at 300 K = 0.848.
```

As the PFR conversion is lower than CSTR conversion, use of CSTR operating at 350 K is recommended.

2. Batch time

```
# Batch time
v = 200 # dm<sup>3</sup>
N_A0 = 200 # moles
N_B0 = 200 # moles
X = 0.9
batch_time, _ = quad(lambda x: N_A0 / (rA(x, k_350) * v), 0, X)
```

Batch time at 350 K = 1.065 min.

3. Batch time at 273 K

batch_time, _ = quad(lambda x: N_A0 / (rA(x, k_273) * v), 0, X)

Batch time at 273 K = 3550.191 min (2.5 days).

4. CSTR / PFR connected in series

```
# Function to find the root of
def func(x, *args):
   v, fa0, k = args
   rate = rA(x,k)
    return x - v * rate/ fa0
x_guess = 0
x_cstr_1 = fsolve(func, x2_guess, args=(V_CSTR, F_A0, k_300))
def find x(x2, *args):
   x1, v, k, fa0 = args
    result, _ = quad(lambda x: 1 / rA(x,k), x1, x2)
    return fa0 * result - v
x_guess = x_cstr_1
x_pfr_2 = fsolve(find_x, x_guess, args=(x_cstr_1, V_PFR, k_300, F_A0))
X_{1,CSTR} at 300 K = 0.440.
X_{2,PFR} at 300 K = 0.865.
  5. CSTR and PFR connected in parallel
# Function to find the root of
def func(x, *args):
   v, fa0, k = args
   rate = rA(x,k)
    return x - v * rate/ fa0
x_guess = 0
x cstr 1 = fsolve(func, x2 guess, args=(V CSTR, F A0/2, k 300))
def find x(x2, *args):
    x1, v, k, fa0 = args
    result, _ = quad(lambda x: 1 / rA(x,k), x1, x2)
    return fa0 * result - v
x guess = 0
x_pfr_2 = fsolve(find_x, x_guess, args=(0, V_PFR, k_300, F_A0/2))
X_{1,CSTR} at 300 K = 0.555.
X_{2.PFR} at 300 K = 0.918.
X_{Final} = 0.736.
```

P 5-11

The irreversible elementary gas-phase reaction

 $A+B \longrightarrow C+D$

is carried out isothermally at 305 K in a packed-bed reactor with 100 kg of catalyst.

The entering pressure was 20 atm and the exit pressure is 2 atm. The feed is equal molar in A and B and the flow is in the turbulent flow regime, with $F_{A0} = 10 \text{ mol/min}$ and $C_{A0} = 0.4 \text{ mol/dm}^3$. Currently 80% conversion is achieved. What would be the conversion if the catalyst particle size were doubled and everything else remained the same?



Figure 1: Packed bed reactor

Solution

Hand written solution Elementary reaction

$$A + B \longrightarrow C + D$$

From the initial conversion data given, we will determine rate constant. And use this rate constant to calculate coversion when catalyst particle size is dubbled. Isothermal reaction

$$C_A = C_{A0}(1-X)\frac{P}{P_0}$$

let $P/P_0=y.$ For single isothermal reactions with $\epsilon=0, y^2=1-\alpha w$ Equimolar flow of A and B. Therefore, $C_A=C_B$

$$-r'_A = kC_A C_B = kC_A^2 = kC_{A0}^2 (1-X)^2 y^2$$
(1)

$$\frac{dX}{dW} = \frac{-r'_A}{F_{A0}} \tag{2}$$

$$\frac{dy}{dW} = -\frac{\alpha}{2p} \tag{3}$$

$$\frac{dX}{dW} = \frac{kC_{A0}^2(1-X)^2y^2}{F_{A0}}$$

$$\frac{dX}{(1-X)^2} = \frac{kC_{A0}^2}{F_{A0}}(1-\alpha w)^2 dW$$

$$\int_{0}^{X} \frac{dX}{(1-X)^{2}} = \frac{kC_{A0}^{2}}{F_{A0}} \int_{0}^{W} (1-\alpha w)^{2} dW$$
$$\frac{X}{(1-X)} = \frac{kC_{A0}^{2}}{F_{A0}} \left[W - \frac{\alpha W^{2}}{2} \right]$$
(4)

y = 2/20 = 0.1, $y^2 = 1 - \alpha W$. Therefore, $\alpha = (1 - (0.1)^2)/(100) = 9.9 \times 10^{-3} 1/kg$ Substituting in Equation 4 we get $k = 4.95 dm^6/(kg - cat \ mol \ min)$.

For Turbulent flow, $\alpha \approx 1/Dp$. Therefore, as the particle size doubles, α will be halved. $\alpha = 4.95 \times 10^{-3}$

Substituting in Equation 4: X = 0.86

Alternate approach

We can solve Equation 1, Equation 2, and Equation 3 simultaneously to obtain conversion and pressure as a function of weight.

As we do not know k value, we will use root finding to find the value of k that satisfies the condition where X reaches X_{final} at W_{final} .

```
import numpy as np
from scipy.integrate import solve_ivp
from scipy.optimize import root_scalar
T = 305 \# K
W = 100 \# kg
F AO = 10 \# mol/min
C AO = 0.4 \# mol/dm^{3}
X final = 0.8
P_0 = 20 \# \text{ atm}
P = 2 # atm
# Calculate alpha using pressure drop data
y = P/P 0
alpha_1 = (1 - y * * 2) / W
# System of differential equations
def system(W, y, *args):
    X, p = y
    k, ca0, fa0, alpha = args
    rate = k * ca0**2 * (1-X)**2 * p**2
    dX_dW = rate / fa0
    dp dW = -alpha / (2*p)
    return [dX dW, dp dW]
# initial conditions
# at start of reactor, conversion is 0 and p is 1
y0 = [0, 1]
# Function to integrate over W
def solve k(k):
    system args = (k, C AO, F AO, alpha 1)
    sol = solve_ivp(system, [0, W], y0, args=system_args, dense_output=True)
    X = sol.sol(W)[0]
    return X - X final
# Use root finding to solve for k
# since we don't know the value of k we provide a very large search space
result = root_scalar(solve_k, bracket=[1e-4, 1e4], method='bisect')
k = result.root
# Now alpha is alpha/2
alpha_2 = alpha_1/2
# Calculate the final conversion with this new alpha value
system_args = (k, C_A0, F_A0, alpha_2)
sol = solve_ivp(system, [0, W], y0, args=system_args, dense_output=True)
X = sol.sol(W)[0]
```

k = 4.963. X (for α = 0.005) = 0.856.

P 5-24

The gas-phase reaction

 $A + B \longrightarrow C + D$

takes place isothermally at 300 K in a packed-bed reactor in which the feed is equal molar in A and B with $C_{A0} = 0.1 \text{ mol/dm}^3$. The reaction is second order in A and zero order in B. Currently, 50% conversion is achieved in a reactor with 100 kg of catalysts for a volumetric flow rate 100 dm³/min. The pressure-drop parameter, α , is $\alpha = 0.0099 \text{ kg}^{-1}$. If the activation energy is 10,000 cal/mol, what is the specific reaction rate constant at 400 K?

💡 Solution

```
import numpy as np
from scipy.integrate import solve_ivp
from scipy.optimize import root_scalar
T = 300 \# K
W = 100 \# kg
v 0 = 100 \# dm^{3}/min
C AO = 0.1 \# mol/dm^3
F_AO = C_AO * v_O \# mol/min
X_final = 0.5
alpha 1 = 0.0099 \# 1/kg
# System of differential equations
def system(W, y, *args):
    X, p = y
    k, ca0, fa0, alpha = args
    rate = k * ca0**2 * (1-X)**2 * p**2
    dX dW = rate / fa0
    dp dW = -alpha / (2*p)
    return [dX_dW, dp_dW]
# initial conditions
# at start of reactor, conversion is 0 and p is 1
y0 = [0, 1]
# Function to integrate over W
def solve_k(k):
    system_args = (k, C_A0, F_A0, alpha_1)
    sol = solve_ivp(system, [0, W], y0, args=system_args, dense_output=True)
    X = sol.sol(W)[0]
    return X - X final
# Use root finding to solve for k
# since we don't know the value of k we provide a very large search space
result = root_scalar(solve_k, bracket=[1e-4, 1e4], method='bisect')
k = result.root
EA = 10000 # cal/mol
T2 = 400
R = 1.987
\ln_k 2k1 = (EA/R) * ((1/T) - (1/T2))
k2 = k*np.exp(ln k2k1)
k at 300 K = 19.832 dm^6/(kg - cat \ mol \ min).
k at 400 K = 1314.531 dm^6/(kg - cat \ mol \ min).
```

P 6-4

The elementary gas-phase reaction

$$(CH_3)_3COOC(CH_3)_3 \longrightarrow C_2H_6 + 2 CH_3COCH_3$$

 $A \longrightarrow B + 2 C$

is carried out isothermally at 400 K in a flow reactor with no pressure drop. The specific reaction rate at 50°C is 10^{-4} min⁻¹ (from pericosity data) and the activation energy is 85 kJ/mol. Pure *di-tert*-butyl peroxide enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min, i.e., $F_A = 2.5$ mol/min.

- Use the algorithm for molar flow rates to formulate and solve the problem. Plot F_A , F_B , F_C , and then X as a function of plug-flow reactor volume and space time to achieve 90% conversion.
- Calculate the plug-flow volume and space time for a CSTR for 90% conversion.

Solution

```
import numpy as np
from scipy.integrate import quad
import matplotlib.pyplot as plt
T ref = 273.15
R = 0.0821
TO = 127 + T ref \# K
EA = 85000 # J/mol
PO = 10 \# atm
yA0 = 1
F_AO = 2.5 \# mol/min
C AO = yAO * PO/(R * TO)
delta = 1 + 2 - 1
epsilon = yA0 * delta
k 50 = 1e-4 # 1/min
k_{127} = k_{50*} \text{ np.exp}((EA/8.314) * (1/(50 + T_ref) - (1/T0)))
CA = lambda x: C_A0 * (1 - x) / (1 + epsilon * x)
rA = lambda k, x: k * CA(x)
# Molar flow rates
FA = lambda x: F AO * (1 - x)
FB = lambda x: F_AO * (x)
FC = lambda x: F_A0 * (2 * x)
def integral(x, *args):
    fa0, k = args
    return fa0/ rA(k, x)
system_args = (F_A0, k_127)
X_range = np.linspace(0, 0.9, 100)
V = []
# Calculate volume for each X
for X in X_range:
    v, _ = quad(integral, 0, X, args=system_args)
    V.append(v)
plt.plot(V, X_range, label='X vs. Volume')
plt.xlabel('Volume ($dm^3$)')
plt.ylabel('Conversion (X)')
plt.title('Conversion X as a Function of Reactor Volume')
plt.legend()
plt.grid(True)
plt.ylim(0,1)
plt.xlim(0,1000)
```





P 6-6

(Membrane reactor) The first-order, gas-phase, reversible reaction

$$A \rightleftharpoons B + 2C$$

is taking place in a membrane reactor. Pure A enters the reactor, and B diffuses out through the membrane. Unfortunately, a small amount of the reactant A also diffuses through the membrane.

• Plot and analyze the flow rates of A, B, and C and the conversion X down the reactor, as well as the flow rates of A and B through the membrane.

- Next, compare the conversion profiles in a conventional PFR with those of a membrane reactor from part (a). What generalizations can you make?
- Would the conversion of A be greater or smaller if C were diffusing out instead of B?
- Discuss qualitatively how your curves would change if the temperature were increased significantly or decreased significantly for an exothermic reaction. Repeat the discussion for an endothermic reaction.

Additional information:

F _{A0} = 100 mol/min
v_0 = 100 dm ³ /min
$V_{reactor}$ = 20 dm ³

Solution

```
import numpy as np
from scipy.integrate import solve_ivp
import matplotlib.pyplot as plt
# Data
k = 10
            # 1/min
K eq = 0.01 \# mol/dm^3^{-1}
k CA = 1
          # min^-1^
k_CB = 40
          # min^-1^
F AO = 100 \# mol/min
v_0 = 100
           # dm^3^/min
V reactor = 20 \# dm^3
C_TO = F_AO/v_O
r_A = lambda ca, cb, cc: - k * (ca - cb * cc**2/ K_eq)
r_B = lambda ca, cb, cc: - r_A(ca, cb, cc)
r C = lambda ca, cb, cc: - r A(ca, cb, cc)/2
r_diff_A = lambda ca: k_CA * ca
r diff B = lambda cb: k CB * cb
C = lambda f, ft: C_TO * f/ft
# System of differential equations for membrane reactor
def membrane_reactor(V, y, *args):
    FA, FB, FC = y
    FT = FA + FB + FC
    CA = C(FA, FT)
    CB = C(FB, FT)
    CC = C(FC, FT)
    dFA_dV = r_A(CA, CB, CC) - r_diff_A(CA)
    dFB_dV = r_B(CA, CB, CC) - r_diff_B(CB)
    dFC dV = r C(CA, CB, CC)
    return [dFA_dV, dFB_dV, dFC_dV]
# System of differential equations for pfr
def pfr(V, y, *args):
   FA, FB, FC = y
    FT = FA + FB + FC
    CA = C(FA, FT)
    CB = C(FB, FT)
    CC = C(FC, FT)
    dFA_dV = r_A(CA, CB, CC)
    dFB_dV = r_B(CA, CB, CC)
    dFC_dV = r_C(CA, CB, CC)
```



P 6-7

Fuel Cells Rationale. With the focus on alternative clean-energy sources, we are moving toward an increased use of fuel cells to operate appliances ranging from computers to automobiles. For example, the hydrogen/oxygen fuel cell produces clean energy as the products are water and electricity, which may lead to a hydrogen-based economy instead of a petroleum-based economy. A large component in the processing train for fuel cells is the water-gas shift membrane reactor. (M. Gummala, N. Gupla, B. Olsomer, and Z. Dardas, *Paper 103c*, 2003, AIChE National Meeting, New Orleans, LA.)

$$CO + H_2O \Longrightarrow CO_2 + H_2$$

Here, CO and water are fed to the membrane reactor containing the catalyst. Hydrogen can diffuse out the sides of the membrane, while CO, H_2O , and CO_2 cannot. Based on the following information, plot the concentrations and molar flow rates of each of the reacting species down the length of the membrane reactor.

Assume the following: The volumetric feed is 10 dm³/min at 10 atm, and the equimolar feed of CO and water vapor with $C_{T0} = 0.4 \text{ mol/dm}^3$. The equilibrium constant is $K_e = 1.44$, with k = 1.37 dm^6 /mol kg-cat \cdot min, and the mass transfer coefficient $k_{H_2} = 0.1 dm^3/\text{kg-cat} \cdot \text{min}$

(Hint: First calculate the entering molar flow rate of CO and then relate F_A and X.)

- What is the membrane reactor volume necessary to achieve 85% conversion of CO?
- Sophia wants you to compare the MR with a conventional PFR. What will you tell her?

• For that same membrane reactor volume, Nicolas wants to know what would be the conversion of CO if the feed rate were doubled?



Figure 2: Fuel cell

Solution

```
import numpy as np
from scipy.integrate import solve_ivp
from scipy.optimize import root_scalar
import matplotlib.pyplot as plt
# Data
k = 1.37
K_{eq} = 1.44
k_H2 = 0.1
v_0 = 10
p = 10
C_{T0} = 0.4
F_AO = C_TO * v_0/2
F_{B0} = C_{T0} * v_{0}/2
F_C0 = 0
F_{D0} = 0
# A, B, C, D --> CO, H2O, CO2, H2
# System of differential equations for membrane reactor
def fuel_cell(V, y, *args):
    FA, FB, FC, FD = y
    FT = FA + FB + FC + FD
    CA = C_TO * FA / FT
    CB = C_TO * FB / FT
    CC = C TO * FC / FT
    CD = C_TO * FD / FT
    rate = -k * (CA * CB - CC * CD / K_eq)
    rA = rate
    rB = rate
    rC = -rate
    rD = -rate
    rH2 = k H2 * CD
    dFA_dV = rA
    dFB dV = rB
    dFC dV = rC
    dFD_dV = rD - rH2
    return [dFA_dV, dFB_dV, dFC_dV, dFD_dV]
# initial conditions
# at start of reactor, conversion is 0 and p is 1
yO = [F_AO, F_BO, F_CO, F_DO]
```



References

Fogler, H. Scott. 2016. Elements of Chemical Reaction Engineering. Fifth edition. Boston: Prentice Hall.