Portfolio 06: Nonisothermal reactor design

CHEN3010/ CHEN5040: chemical reaction engineering

Student ID:

General Instructions for in class Portfolios

1. The portfolio is an open-book task.
2. You can use textbooks, the resources provided during class/ workshop etc. to answer the questions.
3. The portfolio task is made available in both pdf format and as a print.
4. You are free to choose a solution technique. It is **not** required that you use the provided python code to answer the questions. You can use any tool (pen and paper, excel, ...) and any technique (graphical, numerical, analytical) that you are comfortable with.
5. Irrespective of your solution method, you are expected to write your answers on to the printed question paper provided. **This is what gets marked.**
6. The portfolio will take place during designated time slot communicated earlier by the unit coordinator. Please refer to the portfolio schedule on blackboard for the portfolio dates and topics.
7. The tasks will be a mix of theory questions, short calculation type and long numerical examples.
8. You have **50 minutes** to complete the tasks in the portfolio.
9. The portfolios will be marked immediately after completion by your peers using a provided marking rubric.
10. The portfolios will be collected by the instructors to verify peer marking and record the marks. You will receive your portfolio back within a week.
11. When you are required to upload the portfolio answers on to blackboard:

   - Save your report as a pdf file.
   - Rename the file as STUDENTID_Portfolio_x.pdf (Where STUDENTID is your student ID, and x is the portfolio number) and
   - Upload it using assessment submission link on blackboard.

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Introduction

The ethylene (E) epoxydation is to be carried out using a cesium-doped silver catalyst in a packed-bed reactor.

$$C_2H_4 + \frac{1}{2}O_2 \longrightarrow C_2H_4O \qquad \Delta H_{rxn,1} = -0.17\,kJ/mol \tag{1}$$
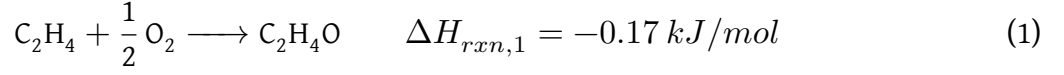
Along with the desired reaction, the complete combustion of ethylene also occurs

$$C_2H_4 + 3\,O_2 \longrightarrow 2\,CO_2 + 2\,H_2O \qquad \Delta H_{rxn,2} = -1306\,kJ/mol \tag{2}$$
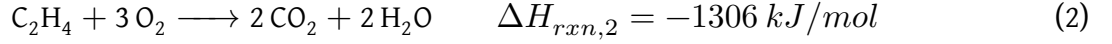
Lafarga et al. (2000) have proposed following reaction kinetics for the reaction system.

$$-r_{1E} = \frac{k_{1E}P_E P_O^{0.58}}{(1 + K_{1E}P_E)^2} \tag{3}$$

$$-r_{2E} = \frac{k_{2E}P_E P_O^{0.3}}{(1 + K_{2E}P_E)^2} \tag{4}$$

The reaction rate constants are:

$$k_{1E} = 0.15 \frac{mol}{kg \cdot s\,atm^{1.58}} \text{ at 523 K with } E_1 = 60.7\,kJ/mol \tag{5}$$

$$k_{2E} = 0.0888 \frac{mol}{kg \cdot s\,atm^{1.3}} \text{ at 523 K with } E_2 = 73.2\,kJ/mol \tag{6}$$

The adsorption constants are: $K_{1E} = 6.50\,atm^{-1}$; and $K_{2E} = 4.33\,atm^{-1}$

The feed enters the reactor at 250 °C and a pressure of 2 atm. The molar flow rate is 0.0093 mol/s. The reactor contains 100g of catalyst. Pressure drop in the reactor can be neglected. Inlet gas composition along with thermochemical data for the species involved is given in Table 1.

Table 1: Inlet gas composition

Gas	volume fraction at inlet (%)	ΔH_f^0 at 298 K (kJ/mol)	$C_P\,(J/mol\,K)$
C_2H_4	6	-52.47	65
O_2	12	0	30
C_2H_4O	0	-52.64	80
CO_2	0	-393.5	45
H_2O	0	-285.83	35
N_2	82	0	30

Questions

1. Assuming isothermal conditions, what conversion and selectivity of ethylene oxide to CO_2 are expected at the exit of the PBR? (10 marks)

2. The reactor is cooled by boiling kerosene with a boiling point of 250 °C (The ambient temperature can be assumed to be constant at 250 °C). The heat transfer coefficient for the system is $Ua = 300 J/kg - cat\ s\ K$.

   Write energy balance for the system. (10 marks)

3. What would happen if the reactor is operated adiabatically? (10 marks)

   Modify the code given in appendix to include energy balance. Simulate adiabatic operations and report the temperature, conversion, and selectivity for adiabatic operations. Briefly comment on the results.

4. Using the conditions for heat transfer fluid in question 2, calculate the maximum temperature in the reactor, the temperature, conversion, and selectivity at the exit of the reactor considering heat transfer. Briefly comment on the results. (10 marks)

Appendix

The code is also available as `ipython` notebook. Download the file `portfolio_6.ipynb` from blackboard. Open Google colab. From menu, click on File > Upload notebook. Upload the downloaded file and modify as per needed.

```python
import numpy as np
from scipy.integrate import solve_ivp
import matplotlib.pyplot as plt

# constants

R = 8.314      # J/ (mol K)
RATM = 0.082     # atm dm^3/ (mol K)
TRR = 523      # K

# Components
# 0: ethylene
# 1: oxygen
# 2: ethylene oxide
# 3: CO2
# 4: water
# 5: nitrogen

# Heats of formation at 298 K in J/mol
HF = np.array([-52470, 0, -52640, -393500, -285830, 0])

# Specific Heat Capacities J/mol K
CP = np.array([65, 30, 80, 45, 35, 30])

# reactions
# 0. C2H4 + 1/2 O2 -> C2H4O
# 1. C2H4 + 3O2 -> 2CO2 + 2H2O

# Stoichiometry
NU = np.array([
    [-1, -0.5, 1, 0, 0, 0],  # Reaction 0: C2H4 + 0.5 O2 -> C2H4O
    [-1, -3, 0, 2, 2, 0]     # Reaction 1: C2H4 + 3 O2 -> 2 CO2 + 2 H2O
])

# Adsorption constants (1/atm)
KE0, KE1 = 6.5, 4.33

# Heat of reaction at reference temperature J/mol
DELTA_HR_TR = np.dot(NU, HF)

# Functions

k0e = lambda t: 0.15 * np.exp((60700/R) * ((1/TRR) - (1/t)))
k1e = lambda t: 0.0888 * np.exp((73200/R) * ((1/TRR) - (1/t)))
```

```python
# rates
r0e = lambda t, pe, po: k0e(t) * pe * po**0.58 / (1 + KE0*pe)**2
r1e = lambda t, pe, po: k1e(t) * pe * po**0.3 / (1 + KE1*pe)**2

def pbr(w,y,*args):

  # convert dependent variables
  f = y[:-1]
  t = y[-1]

  # convert args
  (pt, ua, ta) = args

  # total molar flow rate
  ft = np.sum(f)

  # mol fr.
  phi = f/ft

  # partial pressures
  p = pt * phi

  # extract partial pressure for ethylene and oxygen
  pe = p[0]
  po = p[1]

  # calculate reaction rates
  r0 = r0e(t,pe,po)
  r1 = r1e(t,pe,po)

  # Could also be written as an array
  # r = np.array([r1e(t,pe,po), r2e(t,pe,po)])

  # calculate rates of individual species
  r_e = -r0 -r1
  r_o = -0.5 * r0 - 3 * r1
  r_eo = r0
  r_co2 = 2 * r1
  r_h2o = 2 * r1
  r_n2 = 0

  # could also be written as
  # ri = np.dot(NU.T, r)

  # write mole balances
  # dfdw = ri

  df_e = r_e
  df_o = r_o
```

```
    df_eo = r_eo
    df_co2 = r_co2
    df_h2o = r_h2o
    df_n2 = r_n2

    # energy balance

    delta_cp = np.dot(NU,CP)
    delta_hr = DELTA_HR_TR + delta_cp * (t - 298)

    # isothermal case
    dtdw = 0

    # non-isothermal case
    # replace dtdw with appropriate expression

    # dydw = np.append(dfdw,dtdw)
    dydw = [df_e, df_o, df_eo, df_co2, df_h2o, df_n2, dtdw]

    return dydw


# Problem data

# Heat transfer properties
ua = 300  # J/kg-cat s K

ta = 250 + 273.15 # k

# Inlet pressure and temperature
t0 = 250 + 273.15 # K
p0 = 2 # atm

# inlet flow rate mol/s
ft0 = 0.0093

# Inlet volume (mol) fraction
phi = np.array([0.06,0.12,0,0,0,0.82])

# Inlet molar flow rates for components mol/s
f0  = phi*ft0

# total catalyst weight kg
wcat = 0.1

# Differential equations
# 0: dF_e/dW
# 1: dF_o/dW
# 2: dF_eo/dW
# 3: dF_co2/dW
```

```python
# 4: dF_h2o/dW
# 5: dF_n2/dW
# 6: dT/dW

initial_conditions = np.append(f0,t0)
args = (p0, ua, ta)


w_final = wcat


sol = solve_ivp(pbr,
                [0, w_final],
                initial_conditions,
                args=args,
                method='LSODA',
                dense_output=True)


# Extract solution

w = np.linspace(0,w_final, 1000)

# molar flow rate
f = sol.sol(w)[:-1]


f_e = f[0]
f_o = f[1]
f_eo = f[2]
f_co2 = f[3]
f_h2o = f[4]
f_n2 = f[5]


# temperature
t = sol.sol(w)[-1]

# Calculate conversion, selectivity, max temperature etc. as required # after
# this point
```

References

Lafarga, David, Mohammed A. Al-Juaied, Christina M. Bondy, and Arvind Varma. 2000. "Ethylene Epoxidation on Ag-Cs/α-Al2O3 Catalyst: Experimental Results and Strategy for Kinetic Parameter Determination." *Industrial & Engineering Chemistry Research* 39 (7): 2148–56. https://doi.org/10.1021/ie990939x.