

In class activity: Isothermal reactor design

Lecture notes for chemical reaction engineering

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Apply reaction engineering algorithm

1. Derive the **equation for batch time** as a function of conversion for a second order reaction
$$-r_A = k_2 C_A^2$$

Solution

1. Mole balance

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

2. Rate law

$$-r_A = k C_A^2$$

3. Stoichiometry

$$C_A = C_{A0}(1 - X_A)$$

4. Combine

$$N_{A0} \frac{dX_A}{dt} = k C_{A0}^2 (1 - X_A)^2 V$$

5. Evaluate

For constant batch volume $V = V_0$ solve

$$N_{A0} \frac{dX_A}{dt} = k C_{A0}^2 (1 - X_A)^2 V_0$$

$$\frac{dX_A}{dt} = k C_{A0} (1 - X_A)^2$$

Integrate:

$$\frac{1}{k C_{A0}} \int_0^X \frac{dX_A}{(1 - X_A)^2} = \int_0^t dt$$

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from sympy import symbols, integrate, simplify, pprint

k, CA0, X, XA = symbols('k CA0 X XA')

expression = 1 / (1 - XA)**2
integral_result = integrate(expression, (XA, 0, X))
simplified_integral = simplify(integral_result)

t = (1 / (k * CA0)) * simplified_integral

pprint(t)

```

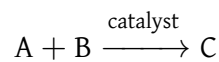
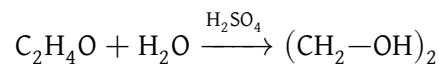
-X

CA k (X - 1)

$$t = \frac{1}{kC_{A0}} \frac{X}{1 - X}$$

2. Determining k from Batch Data

It is desired to design a CSTR to produce 200 million pounds of ethylene glycol per year by hydrolyzing ethylene oxide. However, before the design can be carried out, it is necessary to perform and analyze a batch-reactor experiment to determine the specific reaction-rate constant, k . Because the reaction will be carried out isothermally, the specific reaction rate will need to be determined only at the reaction temperature of the CSTR. At temperatures above 80°C , there is a significant by-product formation, while at temperatures below 40°C , the reaction does not proceed at a significant rate; consequently, a temperature of 55°C has been chosen. Because water is present in excess, its concentration (55.5 mol/dm^3) may be considered constant during the course of the reaction. The reaction is first-order in ethylene oxide.



In the laboratory experiment, 500 mL of a 2 M solution (2 kmol/m^3) of ethylene oxide (A) in water was mixed with 500 mL of water (B) containing 0.9 wt% sulfuric acid, which is a catalyst. The temperature was maintained at 55°C . The concentration of ethylene glycol (C) was recorded as a function of time (Table 1).

- Derive an equation for the concentration of ethylene glycol as a function of time.
- Rearrange the equation derived in (a) to obtain a linear plot of a function concentration versus time.
- Using the data in (Table 1), determine the specific reaction rate at 55°C .

Table 1: Concentration-Time Data

Time (min)	0.00	0.50	1.00	1.50	2.00	3.00	4.00	6.00	10.00
Concentration of Ethylene Glycol (C) ($kmol/m^3$)	0.00	0.14	0.27	0.38	0.47	0.61	0.71	0.85	0.96

💡 Solution

1. See [slides 9 and 10](#).

2.

$$\ln \frac{C_{A0}}{C_A} = kt$$

Concentration of ethylene oxide (A)

$$C_A = C_{A0}e^{-kt}$$

Concentration of ethylene oxide (C)

$$C_C = C_{A0} - C_A = C_{A0}(1 - e^{-kt}) \quad (1)$$

3. Rearranging Equation 1 we get

$$\ln \frac{C_{A0} - C_C}{C_{A0}} = t$$

The plot of $\ln[(C_{A0} - C_C)/C_{A0}]$ vs. t will be a straight line with slope $-k$.

```

import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import linregress

time = np.array([0.0, 0.5, 1.0, 1.5, 2.0, 3.0, 4.0, 6.0, 10.0])
conc_C = np.array([0.000, 0.145, 0.270, 0.376, 0.467, 0.610, 0.715, 0.848, 0.957])

conc_A0 = 1.0 # kmol/m3

lhs = np.log((conc_A0 - conc_C)/conc_A0)

slope, intercept, r_value, p_value, std_err = linregress(time, lhs)
line = slope * time + intercept

k = -slope

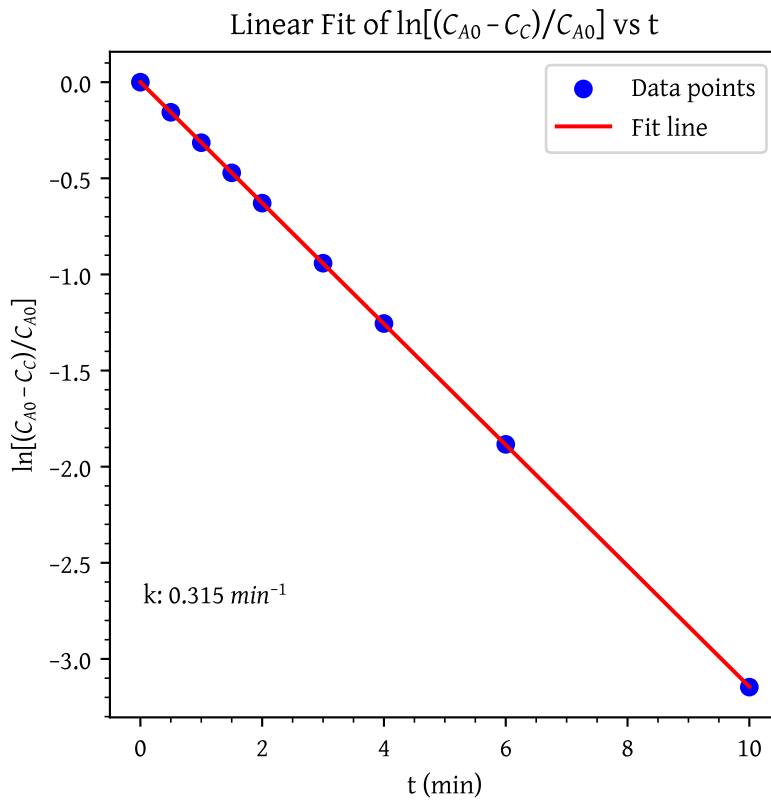
# Plot
plt.scatter(time, lhs, color='blue', label='Data points')
plt.plot(time, line, color='red', label='Fit line')

# Labels and title
plt.xlabel('t (min)')
plt.ylabel('$\ln[(C_{A0}-C_C)/C_{A0}]$')
plt.title('Linear Fit of $\ln[(C_{A0}-C_C)/C_{A0}]$ vs t')
plt.legend()

k_text = f'k: {k:.3f} $min^{{-1}}$'
plt.annotate(f'{k_text}', xy=(0.05, 0.20), xycoords='axes fraction', verticalalignment=

# Show plot
plt.show()

```



3. Exit concentration for CSTR in series using the algorithm:

Obtain C_{A2} in terms of C_{A0} and Da for two CSTRs operating in series. The reaction is first order isothermal liquid phase reaction.

Solution

Relate C_{A2} to k & t

$$C_{A2} = \frac{C_{A1}}{1 + \tau k}; C_{A1} = \frac{C_{A0}}{1 + \tau k}$$

Substitute:

$$C_{A2} = \frac{C_{A0}}{1 + \tau k} \frac{1}{1 + \tau k}$$

$$C_{A2} = \frac{C_{A0}}{(1 + \tau k)^2}$$

4. Derive **equation for conversion in a liquid phase PFR** for second order reaction $2A \longrightarrow$ products; $-r_A = kC_A^2$ in terms of Damköhler number $Da_2 = \tau k C_{A0}$

Solution

1. Mole balance

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

2. Rate law

$$-r_A = kC_A^2$$

3. Stoichiometry

$$C_A = C_{A0}(1 - X_A)$$

4. Combine

$$F_{A0} \frac{dX_A}{dV} = kC_{A0}^2(1 - X_A)^2$$

5. Evaluate

$$V = \frac{v_0}{kC_{A0}} \int_0^X \frac{dX_A}{(1 - X_A)^2}$$

$$V = \frac{v_0}{kC_{A0}} \frac{X}{1 - X}$$

$$Da_2 = \tau kC_{A0} = \frac{X}{1 - X}$$

$$X = \frac{Da_2}{1 + Da_2}$$