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

$$-r_A = kC_A^2$$

3. Stoichiometry

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

4. Combine

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

5. Evaluate

   For constant batch volume $V = V_0$ solve

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

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

   Integrate:

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

```python
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 $80^{\circ}C$, there is a significant by-product formation, while at temperatures below $40^{\circ}C$, the reaction does not proceed at a significant rate; consequently, a temperature of $55^{\circ}C$ 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.

$$\mathrm{C_2H_4O + H_2O \xrightarrow{H_2SO_4} (CH_2{-}OH)_2}$$

$$\mathrm{A + B \xrightarrow{catalyst} C}$$

   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 $55^{\circ}C$. The concentration of ethylene glycol (C) was recorded as a function of time (Table 1).

   a) Derive an equation for the concentration of ethylene glycol as a function of time.

   b) Rearrange the equation derived in (a) to obtain a linear plot of a function concentration versus time.

   c) Using the data in (Table 1), determine the specific reaction rate at $55^{\circ}C$.

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)

$$C_C = C_A 0 - C_A = C_{A0}(1 - e^{-kt}) \tag{1}$$

3. Rearranging Equation 1 we get

$$\ln \frac{C_A 0 - C_C}{C_A 0} = t$$

The plot of $\ln[(C_A 0 - C_C)/C_A 0]$ vs. t will be a straight line with slope $-k$.

```python
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/m^3

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()
```

```
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  plt.ylabel('$\ln[(C_{A0}-C_C)/C_{A0}]$')
C:\Users\Ranjeet\AppData\Local\Temp\ipykernel_30880\3618357485.py:24: SyntaxWarning: i
  plt.title('Linear Fit of $\ln[(C_{A0}-C_C)/C_{A0}]$ vs t')
```

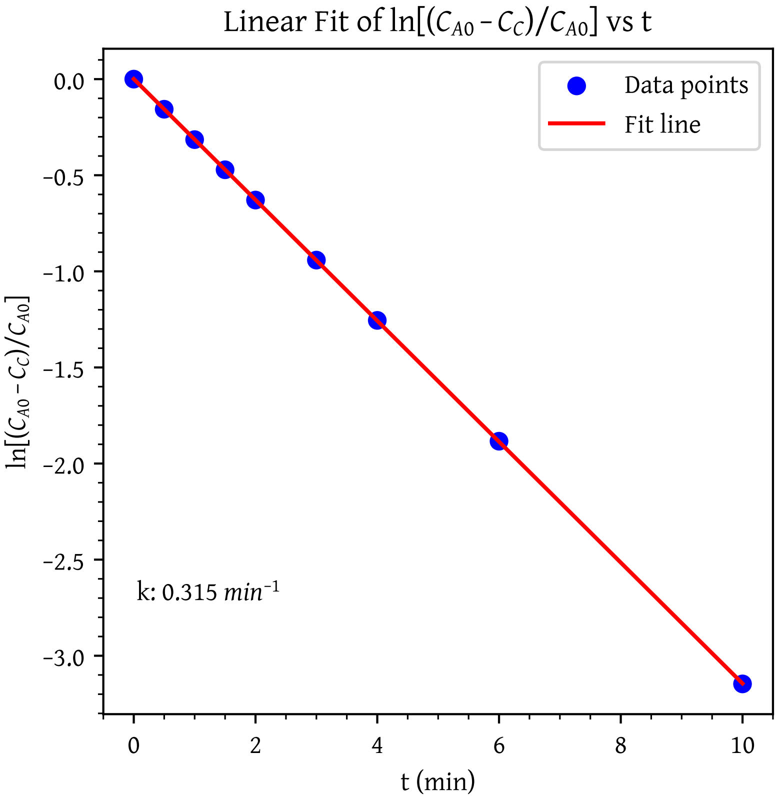

3. Exit concentration for CSTR in series using the algorithm:

   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 2 A $\longrightarrow$ 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

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

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

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

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