

1. Problem 1

(a)

Rate law:

$$-r_A = kC_A C_B$$

(b)

Rate law:

Catalyst k and r_A

$$-r'_A = k'P_A P_B$$

(c)

Rate law:

$$-r_A = kC_A$$

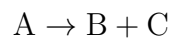
(d)

Rate law:

$$-r_A = k$$

The fourth rate law is strange because it is zeroth order. It does not make sense for a reaction to be independent of the concentration of any reactants. Why would a reaction be occurring if the concentration of the reactants is zero?

2. Problem 2



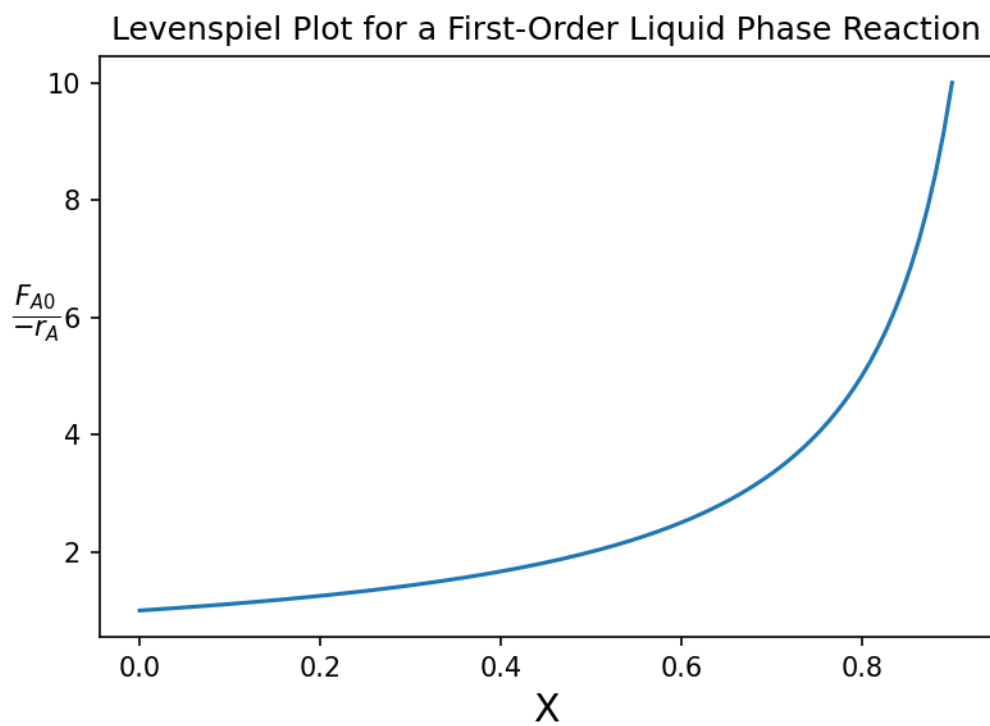
$$-r_A = kC_A$$

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

$$\frac{F_{A0}}{-r_A} = \frac{v_0 C_{A0}}{k C_{A0}(1 - X)}$$

$$\frac{F_{A0}}{-r_A} = \frac{v_0}{k(1 - X)}$$

Plot:



3. Problem 3



CSTR design equation:

$$V_{CSTR} = \frac{XF}{-r_A}$$

$$V_{CSTR} = \frac{Xv_0C_{A0}}{-r_A}$$

$$\frac{V_{CSTR}}{v_0} = \frac{XC_{A0}}{-r_A}$$

$$\tau = \frac{XC_{A0}}{-r_A}$$

Elementary rate law:

$$-r_A = kC_AC_B$$

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

$$C_B = C_{A0} \left(\frac{C_{B0}}{C_{A0}} - \frac{1}{1}X \right)$$

$$-r_A = kC_{A0}^2(1 - X) \left(\frac{C_{B0}}{C_{A0}} - X \right)$$

$$\tau = \frac{XC_{A0}}{kC_{A0}^2(1 - X) \left(\frac{C_{B0}}{C_{A0}} - X \right)}$$

$$\tau = \frac{X}{kC_{A0}(1 - X) \left(\frac{C_{B0}}{C_{A0}} - X \right)}$$

$$X = 0.9$$

$$C_{A0} = 16.3$$

$$C_{B0} = 55.5$$

$$k = 0.01$$

At 300K:

$$\tau = \frac{0.9}{0.01 \cdot 16.3 \cdot (1 - 0.9) \left(\frac{55.5}{16.3} - 0.9 \right)}$$

$\tau = 21.96s$

At 350K:

$$k' = k \exp \frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

$$E = 12500 \cdot 4.184$$

$$T_1 = 300$$

$$T_2 = 350$$

$$R = 8.314$$

$$\tau = \frac{0.9 \cdot (1 - 0.9)}{0.01 \cdot \exp \frac{12500 \cdot 4.184}{8.314} \left(\frac{1}{300} - \frac{1}{350} \right) \cdot 16.3 \cdot (1 - 0.9) \left(\frac{55.5}{16.3} - 0.9 \right)}$$

$$\tau = 1.098\text{s}$$

Reactor volume:

$$V = v_0 \tau$$

$$v_0 = 200$$

At 300K:

$$V = 200 \cdot 21.96$$

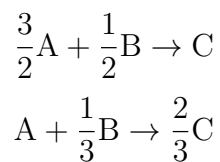
$$V = 4392\text{L}$$

At 350K:

$$V = 200 \cdot 1.098$$

$$V = 219.6\text{L}$$

4. Problem 4



(a) Stoichiometric table:

Species	Initial	Change	Final
A	F_{A0}	$-X$	$F_{A0}(1 - X)$
B	F_{B0}	$-\frac{1}{3}X$	$F_{A0}(\Theta_B - \frac{1}{3}X)$
C	$F_{C0} = 0$	$\frac{2}{3}X$	$F_{A0}(\Theta_C + \frac{2}{3}X)$

(b)

$$\delta = \frac{2}{3} - \frac{1}{3} - 1$$

$$\delta = -\frac{2}{3}$$

$$y_{A0} = 0.5$$

$$y_{B0} = 0.5$$

$$\epsilon = 0.5 \cdot -\frac{2}{3}$$

$$\epsilon = -\frac{1}{3}$$

$$P_{A0} = 8.2 \text{ atm} = 830.865 \text{ kPa}$$

$$C_{A0} = \frac{P_{A0}}{RT}$$

$$T = 227^\circ\text{C} = 500.15 \text{ K}$$

$$C_{A0} = \frac{830.865}{8.314 \cdot 500.15}$$

$$C_{A0} = 0.2$$

$$C_A = C_{A0} \left[\frac{1 - X}{1 + \epsilon X} \right]$$

$$C_A = 0.3 \cdot \left[\frac{1 - 0.6}{1 - \frac{1}{3} \cdot 0.6} \right]$$

$$C_A = 0.1$$

$$C_C = C_{A0} \left[\frac{\Theta_C - \frac{2}{3}X}{1 + \epsilon X} \right]$$

$$C_C = 0.2 \left[\frac{0 + \frac{2}{3} \cdot 0.6}{1 - \frac{1}{3} \cdot 0.6} \right]$$

$$C_C = 0.1$$

(c)

Constant volumetric flow rate flow reactor:

$$\begin{aligned} -r_A &= kC_A^{\frac{3}{2}}C_B^{\frac{1}{2}} \\ C_A &= C_{A0} \left[\frac{1-X}{1+\epsilon X} \right] \frac{P}{P_0} \frac{T_0}{T} \\ C_B &= C_{A0} \left[\frac{\Theta_B - \frac{1}{3}X}{1+\epsilon X} \right] \frac{P}{P_0} \frac{T_0}{T} \\ \frac{P}{P_0} &= \frac{T_0}{T} \\ C_A &= C_{A0} \left[\frac{1-X}{1+\epsilon X} \right] \\ C_B &= C_{A0} \left[\frac{\Theta_B - \frac{1}{3}X}{1+\epsilon X} \right] \\ C_{A0} &= C_{B0} \\ \Theta_B &= 1 \\ C_B &= C_{A0} \left[\frac{1 - \frac{1}{3}X}{1 + \epsilon X} \right] \\ -r_A &= k \left(C_{A0} \left[\frac{1 - \frac{1}{3}X}{1 - \frac{1}{3}X} \right] \right)^{\frac{1}{2}} \left(C_{A0} \left[\frac{1-X}{1 - \frac{1}{3}X} \right] \right)^{\frac{3}{2}} \\ -r_A &= kC_{A0}^2 \left(\frac{1-X}{1 - \frac{1}{3}X} \right)^{\frac{3}{2}} \\ -r_A &= 40 \cdot 0.2^2 \left(\frac{1-X}{1 - \frac{1}{3}X} \right)^{\frac{3}{2}} \\ -r_A &= 1.6 \cdot \left(\frac{1-X}{1 - \frac{1}{3}X} \right)^{\frac{3}{2}} \end{aligned}$$

(d)

PFR design equation:

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

$$-r_A = kC_{A0}^2 \left(\frac{1-X}{1-\frac{1}{3}X} \right)^{\frac{3}{2}}$$

$$F_{A0} \frac{dX}{dV} = kC_{A0}^2 \left(\frac{1-X}{1-\frac{1}{3}X} \right)^{\frac{3}{2}}$$

$$\int_0^V dV = \frac{F_{A0}}{kC_{A0}^2} \int_0^X \left(\frac{1-X'}{1-\frac{1}{3}X'} \right)^{-\frac{3}{2}} dX'$$

$$F_{A0} = 100$$

$$k = 40$$

$$C_{A0} = 0.2$$

$$X = 0.6$$

Evaluate the integral with the following code:

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

# function inside integral
def P_4_d_diff(x):
    return ( (1 - x) / (1 - x / 3) ) ** (-3 / 2)

# constants
F_A0 = 100
k = 40
C_A0 = 830.865 / 8.314 / 500.15 # = 0.2

# conversion values array
X = np.linspace(0, 0.6, 1000)

# evaluate innner function at X
dV = P_4_d_diff(X)

# analytical integral
V = trapezoid(dV, X) * F_A0 / k / C_A0 ** 2
print(V)

# Aggie Honor Code: An Aggie does not lie, cheat, or steal or tolerate
# those who do.
# I certify that this work is my own and not the work of another.
#
# Name: Mark Levchenko
# Assignment #: HW 2
# Question #: 4d
```

Output:

$$V_{\text{PFR}} = 59.91\text{L}$$