1. Problem 1

   (a)

   Rate law:

   $$\boxed{-r_A = kC_AC_B}$$

   (b)

   Rate law:

   Catalyst k and r_A

   $$\boxed{-r'_A = k'P_AP_B}$$

   (c)

   Rate law:

   $$\boxed{-r_A = kC_A}$$

   (d)

   Rate law:

   $$\boxed{-r_A = k}$$

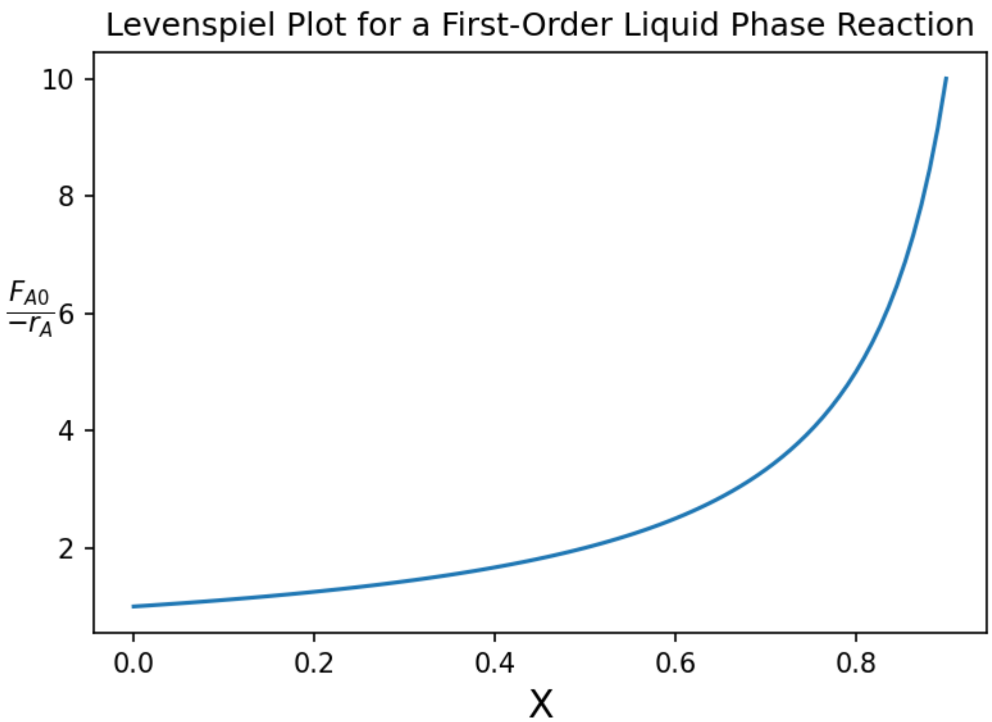
   The fourth rate law is strange because it is zeroth order. It does not make sense for a reaction to be independent of the concentration of any reactants. Why would a reaction be occurring if the concentration of the reactants is zero?

2. Problem 2

$$A \rightarrow B + C$$

$$\begin{aligned}
-r_A &= kC_A \\
C_A &= C_{A0}(1-X) \\
\frac{F_{A0}}{-r_A} &= \frac{v_0 C_{A0}}{kC_{A0}(1-X)} \\
\frac{F_{A0}}{-r_A} &= \frac{v_0}{k(1-X)}
\end{aligned}$$

Plot:



3. Problem 3

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C}$$

CSTR design equation:

$$\begin{aligned}
V_{CSTR} &= \frac{XF}{-r_A} \\
V_{CSTR} &= \frac{Xv_0C_{A0}}{-r_A} \\
\frac{V_{CSTR}}{v_0} &= \frac{XC_{A0}}{-r_A} \\
\tau &= \frac{XC_{A0}}{-r_A}
\end{aligned}$$

Elementary rate law:

$$\begin{aligned}
-r_A &= kC_AC_B \\
C_A &= C_{A0}(1-X) \\
C_B &= C_{A0}\left(\frac{C_{B0}}{C_{A0}} - \frac{1}{1}X\right) \\
-r_A &= kC_{A0}^2(1-X)\left(\frac{C_{B0}}{C_{A0}} - X\right) \\
\tau &= \frac{XC_{A0}}{kC_{A0}^2(1-X)\left(\frac{C_{B0}}{C_{A0}} - X\right)} \\
\tau &= \frac{X}{kC_{A0}(1-X)\left(\frac{C_{B0}}{C_{A0}} - X\right)} \\
X &= 0.9 \\
C_{A0} &= 16.3 \\
C_{B0} &= 55.5 \\
k &= 0.01
\end{aligned}$$

At 300K:

$$\begin{aligned}
\tau &= \frac{0.9}{0.01 \cdot 16.3 \cdot (1-0.9)\left(\frac{55.5}{16.3} - 0.9\right)} \\
&\boxed{\tau = 21.96\mathrm{s}}
\end{aligned}$$

At 350K:

$$
\begin{aligned}
k' &= k \exp \frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \\
E &= 12500 \cdot 4.184 \\
T_1 &= 300 \\
T_2 &= 350 \\
R &= 8.314 \\
\tau &= \frac{0.9 \cdot (1 - 0.9)}{0.01 \cdot \exp \frac{12500 \cdot 4.184}{8.314}\left(\frac{1}{300} - \frac{1}{350}\right) \cdot 16.3 \cdot (1 - 0.9)\left(\frac{55.5}{16.3} - 0.9\right)} \\
&\boxed{\tau = 1.098\text{s}}
\end{aligned}
$$

Reactor volume:

$$
\begin{aligned}
V &= v_0 \tau \\
v_0 &= 200
\end{aligned}
$$

At 300K:

$$
\begin{aligned}
V &= 200 \cdot 21.96 \\
&\boxed{V = 4392\text{L}}
\end{aligned}
$$

At 350K:

$$
\begin{aligned}
V &= 200 \cdot 1.098 \\
&\boxed{V = 219.6\text{L}}
\end{aligned}
$$

4. Problem 4

$$\frac{3}{2}\text{A} + \frac{1}{2}\text{B} \rightarrow \text{C}$$

$$\text{A} + \frac{1}{3}\text{B} \rightarrow \frac{2}{3}\text{C}$$

(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)

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

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

$$y_{A0} = 0.5$$

$$y_{B0} = 0.5$$

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

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

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

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

$$T = 227°\text{C} = 500.15\text{K}$$

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

$$\boxed{C_{A0} = 0.2}$$

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

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

$$\boxed{C_A = 0.1}$$

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

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

$$\boxed{C_C = 0.1}$$

(c)

Constant volumetric flow rate flow reactor:

$$-r_A = kC_A^{\frac{3}{2}}C_B^{\frac{1}{2}}$$

$$C_A = C_{A0}\left[\frac{1-X}{1+\epsilon X}\right]\frac{P}{P_0}\frac{T_0}{T}$$

$$C_B = C_{A0}\left[\frac{\Theta_B - \frac{1}{3}X}{1+\epsilon X}\right]\frac{P}{P_0}\frac{T_0}{T}$$

$$\frac{P}{P_0} = \frac{T_0}{T}$$

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

$$C_B = C_{A0}\left[\frac{\Theta_B - \frac{1}{3}X}{1+\epsilon X}\right]$$

$$C_{A0} = C_{B0}$$

$$\Theta_B = 1$$

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

$$-r_A = k\left(C_{A0}\left[\frac{1-\frac{1}{3}X}{1-\frac{1}{3}X}\right]\right)^{\frac{1}{2}}\left(C_{A0}\left[\frac{1-X}{1-\frac{1}{3}X}\right]\right)^{\frac{3}{2}}$$

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

$$-r_A = 40\cdot 0.2^2\left(\frac{1-X}{1-\frac{1}{3}X}\right)^{\frac{3}{2}}$$

$$\boxed{-r_A = 1.6\cdot\left(\frac{1-X}{1-\frac{1}{3}X}\right)^{\frac{3}{2}}}$$

(d)

PFR design equation:

$$
\begin{aligned}
F_{A0}\frac{dX}{dV} &= -r_A \\
-r_A &= kC_{A0}^2\left(\frac{1-X}{1-\frac{1}{3}X}\right)^{\frac{3}{2}} \\
F_{A0}\frac{dX}{dV} &= kC_{A0}^2\left(\frac{1-X}{1-\frac{1}{3}X}\right)^{\frac{3}{2}} \\
\int_0^V dV &= \frac{F_{A0}}{kC_{A0}^2}\int_0^X\left(\frac{1-X'}{1-\frac{1}{3}X'}\right)^{-\frac{3}{2}} dX' \\
F_{A0} &= 100 \\
k &= 40 \\
C_{A0} &= 0.2 \\
X &= 0.6
\end{aligned}
$$

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:

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