1. Problem 1

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

Reactor 1 mole balances

$$\begin{aligned}
\frac{dN_{A,1}}{dt} &= -r_{A,1}V_1 - \frac{FN_{A,1}}{V_1} \\
\frac{dN_{C,1}}{dt} &= r_{A,1}V_1 - \frac{FN_{C,1}}{V_1} \\
V_1 &= V_{1,0} - Ft \\
N_A &= N_B \text{ equimolar initial composition}
\end{aligned}$$

Reactor 2 mole balances

$$\begin{aligned}
\frac{dN_{A,2}}{dt} &= -r_{A,2}V_2 + \frac{FN_{A,1}}{V_1} \\
\frac{dN_{C,2}}{dt} &= r_{A,2}V_2 + \frac{FN_{C,1}}{V_1} \\
V_2 &= Ft
\end{aligned}$$

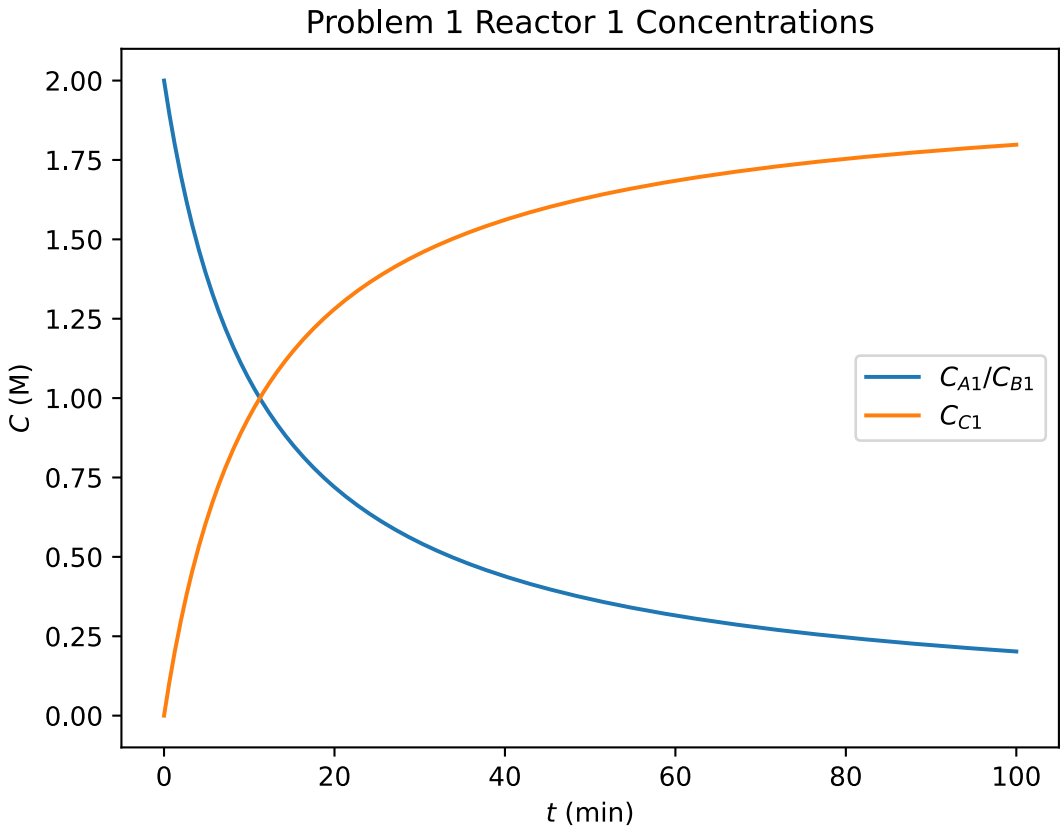
Reactions

$$\begin{aligned}
r_{A,1} = kC_AC_B &= k\frac{N_{A,1}^2}{V_1^2} \\
r_{A,2} &= k\frac{N_{A,2}^2}{V_2^2}
\end{aligned}$$

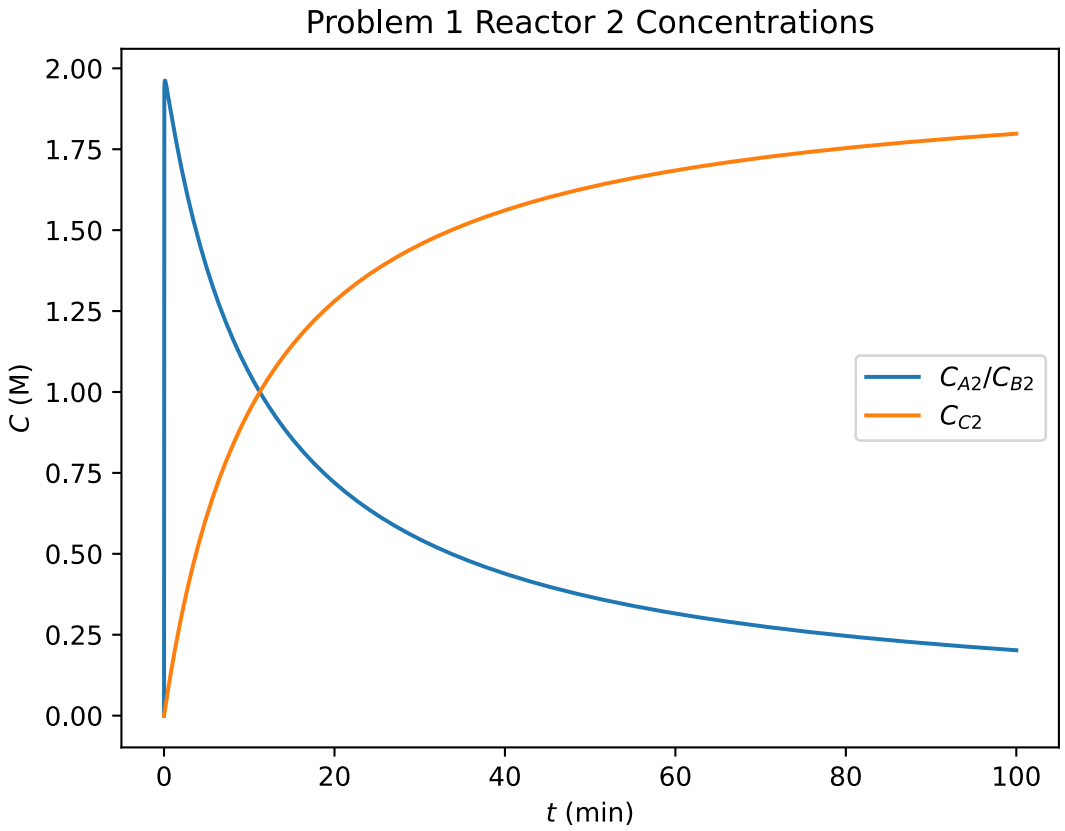
Solve the system of ODEs with the following paramters

$$\begin{aligned}
k &= 0.0445 \text{ L/mol/min} \\
F &= 10 \text{ L/min} \\
V_{1,0} &= 1000 \text{ L} \\
C_{A0} &= 2 \text{ M} \\
C_A &= \frac{N_A}{V}
\end{aligned}$$

Reactor 1 plot:



Reactor 2 plot:



Code:

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

def ode(t, y):
    f = y*0

    N_A1 = y[0]
    N_C1 = y[1]
    N_A2 = y[2]
    N_C2 = y[3]

    k = 0.0445
    F = 10
    V_1_0 = 1000

    V_1 = V_1_0 - F * t
    V_2 = F * t

    r_A1 = k * N_A1**2 / V_1**2
```

```
    if V_2 == 0:
        r_A2 = 0
    else:
        r_A2 = k * N_A2**2 / V_2**2

    f[0] = -r_A1 * V_1 - F * N_A1 / V_1
    f[1] = r_A1 * V_1 - F * N_C1 / V_1
    f[2] = -r_A2 * V_2 + F * N_A1 / V_1
    f[3] = r_A2 * V_2 + F * N_C1 / V_1

    return f

V_1_0 = 1000.
C_A1_0 = 2.
N_A1_0 = V_1_0 *  C_A1_0


init_cond = [N_A1_0, 0., 0., 0.]

ode_kwargs = {
    'method': 'Radau',
    'atol': 1e-8,
    'rtol': 1e-8,
}

sol = solve_ivp(ode, [0.001, 99.999], init_cond, **ode_kwargs)

F = 10
V_1 = V_1_0 - F * sol.t
V_2 = F * sol.t

C_A1 = sol.y[0] / V_1
C_C1 = sol.y[1] / V_1
C_A2 = sol.y[2] / V_2
C_C2 = sol.y[3] / V_2

plt.plot(sol.t, C_A1, label=r"$C_{A1}/C_{B1}$")
plt.plot(sol.t, C_C1, label=r"$C_{C1}$")
plt.xlabel(r"$t$ (min)")
plt.ylabel(r"$C$ (M)")
plt.title("Problem 1 Reactor 1 Concentrations")
plt.legend()
plt.show()


plt.plot(sol.t, C_A2, label=r"$C_{A2}/C_{B2}$")
plt.plot(sol.t, C_C1, label=r"$C_{C2}$")
```

```
plt.xlabel(r"$t$ (min)")
plt.ylabel(r"$C$ (M)")
plt.title("Problem 1 Reactor 2 Concentrations")
plt.legend()
plt.show()
```

2. Problem 2

Assume Constant volume

(a)

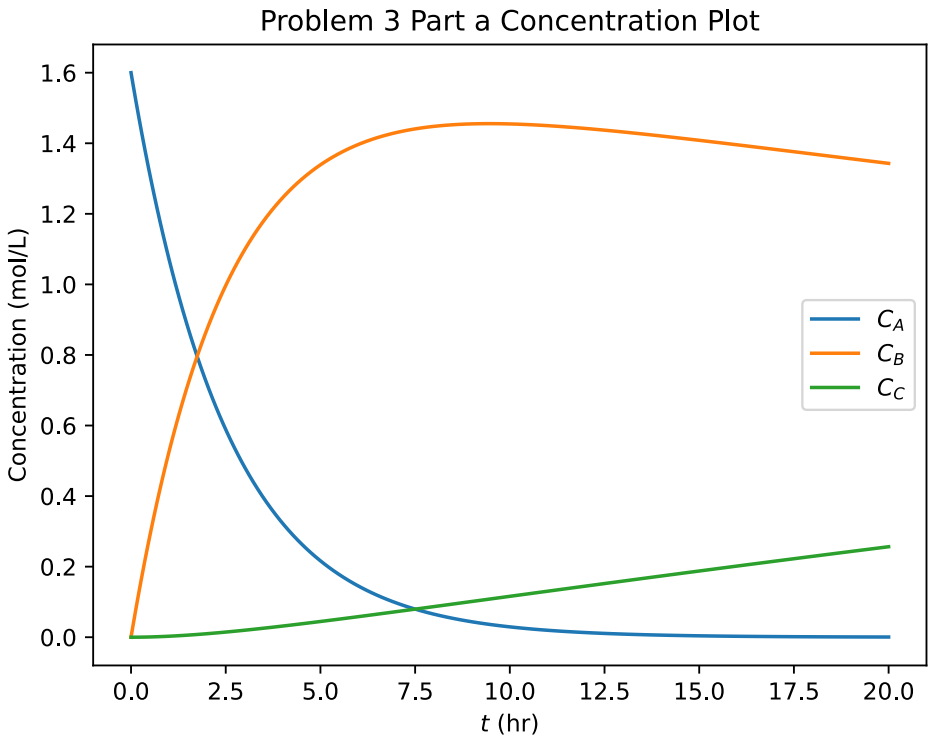
Mole balances

$$\frac{dC_A}{dt} = -r_1$$
$$\frac{dC_B}{dt} = r_1 - r_2$$
$$\frac{dC_C}{dt} = r_2$$
$$r_1 = k_1 C_A$$
$$r_2 = k_2 C_B$$

Solve the system of ODEs with the following paramters

$$k_1 = 0.4 \text{ h}^{-1}$$
$$k_2 = 0.01 \text{ h}^{-1}$$

Concentration plot:



(b)

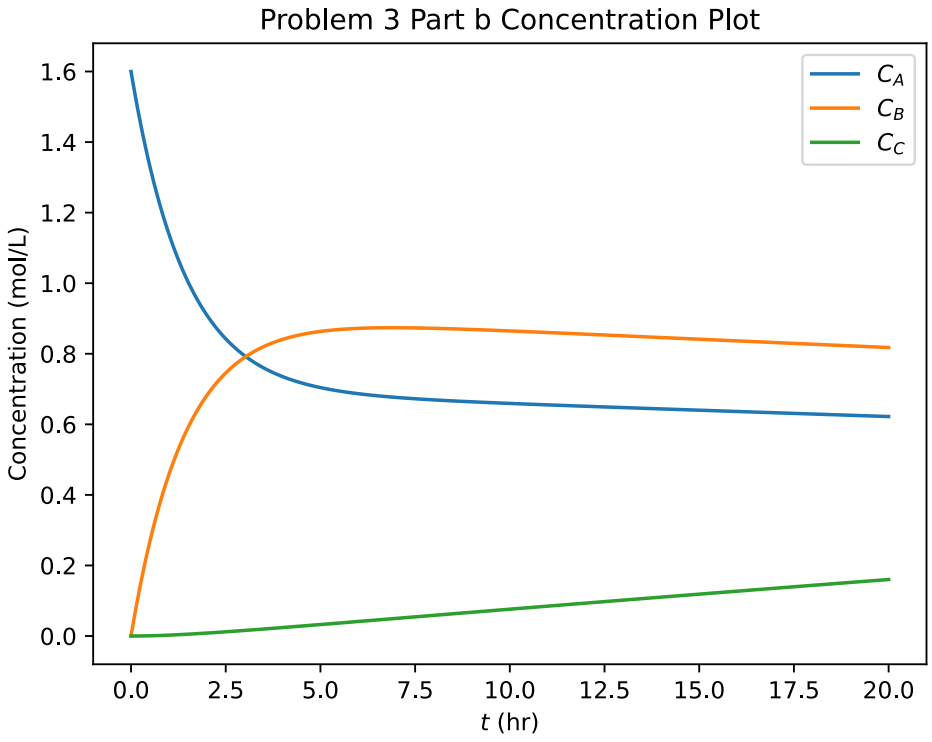
Mole balances

$$\frac{dC_A}{dt} = -r_1 + r_{-1}$$
$$\frac{dC_B}{dt} = r_1 - r_2 - r_{-1}$$
$$\frac{dC_C}{dt} = r_2$$
$$r_1 = k_1 C_A$$
$$r_2 = k_2 C_B$$
$$r_{-1} = k_{-1} C_B$$

Solve the system of ODEs with the following paramters

$$k_1 = 0.4 \text{ h}^{-1}$$
$$k_2 = 0.01 \text{ h}^{-1}$$
$$k_{-1} = 0.3 \text{ h}^{-1}$$

Concentration plot:



(c)

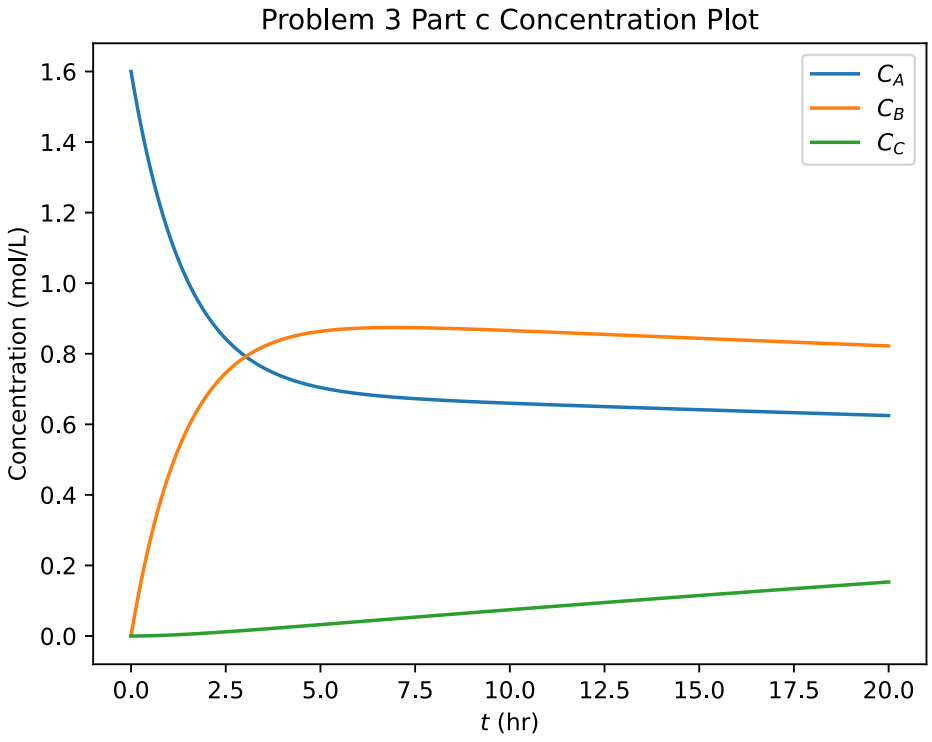
Mole balances

$$\begin{aligned}
\frac{dC_A}{dt} &= -r_1 + r_{-1} \\
\frac{dC_B}{dt} &= r_1 - r_2 - r_{-1} + r_{-2} \\
\frac{dC_C}{dt} &= r_2 - r_{-2} \\
r_1 &= k_1 C_A \\
r_2 &= k_2 C_B \\
r_{-1} &= k_{-1} C_B \\
r_{-2} &= k_{-2} C_C
\end{aligned}$$

Solve the system of ODEs with the following paramters

$$\begin{aligned}
k_1 &= 0.4 \text{ h}^{-1} \\
k_2 &= 0.01 \text{ h}^{-1} \\
k_{-1} &= 0.3 \text{ h}^{-1} \\
k_{-2} &= 0.005 \text{ h}^{-1}
\end{aligned}$$

Concentration plot:



Code for all three parts:

```python
import numpy as np
import matplotlib.pyplot as plt

from scipy.integrate import solve_ivp

ode_kwargs = {
    'method': 'Radau',
    'atol': 1e-8,
    'rtol': 1e-8,
}

'''
####################
#      Part A      #
####################
'''

def ode_a(t, y):
    f = y*0

    C_A = y[0]
    C_B = y[1]
    C_C = y[2]

    k_1 = 0.4
    k_2 = 0.01
    k_b1 = 0.3
    k_b2 = 0.005

    r_1 = k_1 * C_A
    r_2 = k_2 * C_B

    f[0] = -r_1
    f[1] = r_1 - r_2
    f[2] = r_2

    return f

C_A0 = 1.6

init_cond = [C_A0, 0, 0]

sol_a = solve_ivp(ode_a, [0, 20], init_cond, **ode_kwargs)

plt.plot(sol_a.t, sol_a.y[0], label=r"$C_{A}$")
plt.plot(sol_a.t, sol_a.y[1], label=r"$C_{B}$")
plt.plot(sol_a.t, sol_a.y[2], label=r"$C_{C}$")
```

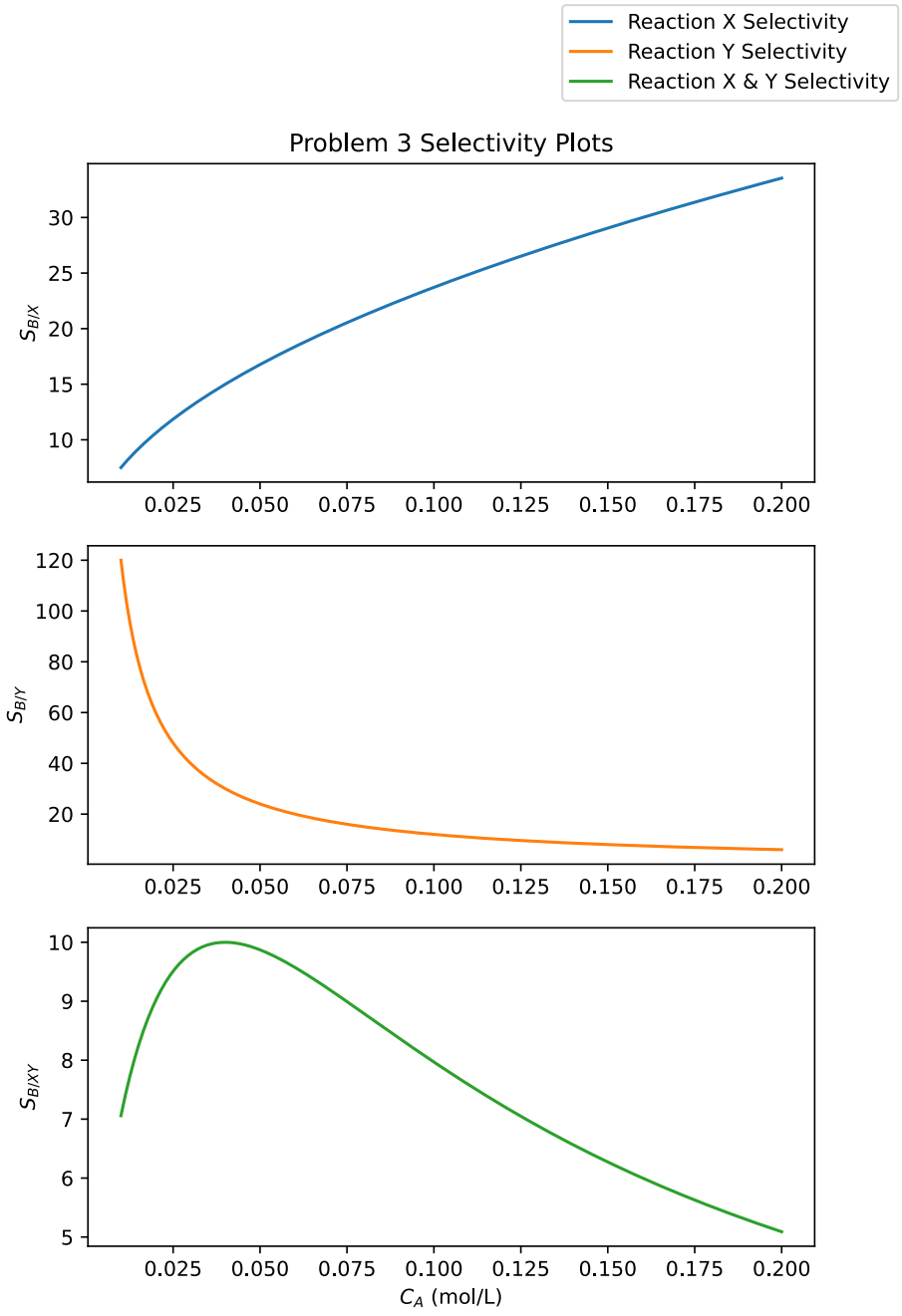
```
plt.title("Problem 3 Part a Concentration Plot")
plt.xlabel(r"$t$ (hr)")
plt.ylabel("Concentration (mol/L)")
plt.legend()
plt.show()

'''
####################
#      Part B      #
####################
'''

def ode_b(t, y):
    f = y*0

    C_A = y[0]
    C_B = y[1]
    C_C = y[2]

    k_1 = 0.4
    k_2 = 0.01
    k_b1 = 0.3
    k_b2 = 0.005

    r_1 = k_1 * C_A
    r_2 = k_2 * C_B
    r_b1 = k_b1 * C_B

    f[0] = -r_1 + r_b1
    f[1] = r_1 - r_2 - r_b1
    f[2] = r_2

    return f

C_A0 = 1.6

init_cond = [C_A0, 0, 0]

sol_b = solve_ivp(ode_b, [0, 20], init_cond, **ode_kwargs)

plt.plot(sol_b.t, sol_b.y[0], label=r"$C_{A}$")
plt.plot(sol_b.t, sol_b.y[1], label=r"$C_{B}$")
plt.plot(sol_b.t, sol_b.y[2], label=r"$C_{C}$")
plt.title("Problem 3 Part b Concentration Plot")
plt.xlabel(r"$t$ (hr)")
plt.ylabel("Concentration (mol/L)")
plt.legend()
```

```
plt.show()

'''
####################
#      Part C      #
####################
'''

def ode_c(t, y):
    f = y*0

    C_A = y[0]
    C_B = y[1]
    C_C = y[2]

    k_1 = 0.4
    k_2 = 0.01
    k_b1 = 0.3
    k_b2 = 0.005

    r_1 = k_1 * C_A
    r_2 = k_2 * C_B
    r_b1 = k_b1 * C_B
    r_b2 = k_b2 * C_C

    f[0] = -r_1 + r_b1
    f[1] = r_1 - r_2 - r_b1 + r_b2
    f[2] = r_2 - r_b2

    return f

C_A0 = 1.6

init_cond = [C_A0, 0, 0]

sol_c = solve_ivp(ode_c, [0, 20], init_cond, **ode_kwargs)

plt.plot(sol_c.t, sol_c.y[0], label=r"$C_{A}$")
plt.plot(sol_c.t, sol_c.y[1], label=r"$C_{B}$")
plt.plot(sol_c.t, sol_c.y[2], label=r"$C_{C}$")
plt.title("Problem 3 Part c Concentration Plot")
plt.xlabel(r"$t$ (hr)")
plt.ylabel("Concentration (mol/L)")
plt.legend()
plt.show()
```

3. Problem 3

$$
\begin{aligned}
S_{B/X} &= \frac{r_B}{r_X} \\
S_{B/Y} &= \frac{r_B}{r_Y} \\
S_{B/XY} &= \frac{r_B}{r_X + r_Y} \\
r_X &= k_1 C_A^{1/2} \\
r_B &= k_2 C_A \\
r_Y &= k_3 C_A^2 \\
k_1 &= 0.004 \text{ (mol/L)}^{1/2} \cdot \text{min}^{-1} \\
k_2 &= 0.3 \text{ min}^{-1} \\
k_3 &= 0.25 \text{ L/mol} \cdot \text{min}
\end{aligned}
$$

Plot and determine the concentration at maximum selectivity.


Reaction X Selectivity
Reaction Y Selectivity
Reaction X & Y Selectivity
Problem 3 Selectivity Plots
$S_{B/X}$
$S_{B/Y}$
$S_{B/XY}$
C_A (mol/L)

$$
\begin{aligned}
C_A &= 0.04 \text{ mol/L} \\
V &= \frac{F\left(C_{A0} - C_A\right)}{-r_A} \\
V &= \frac{F\left(C_{A0} - C_A\right)}{k_1 C_A^{1/2} + k_2 C_A + k_3 C_A^2} \\
C_{A0} &= \frac{P_0}{RT_0} \\
V &= \frac{F\left(\frac{P_0}{RT_0} - C_A\right)}{k_1 C_A^{1/2} + k_2 C_A + k_3 C_A^2} \\
F &= 10 \\
T &= 300 \\
P &= 4 \\
V &= \frac{10\left(\frac{4}{0.08206 \cdot 300} - 0.04\right)}{0.004 \cdot 0.04^{1/2} + 0.3 \cdot 0.04 + 0.25 \cdot 0.04^2} \\
V &= 92.8 \text{ L}
\end{aligned}
$$

Code:

```
import numpy as np
import matplotlib.pyplot as plt

C_A_ran = np.linspace(0.01, 0.2, 10000)

k_1 = 0.004
k_2 = 0.3
k_3 = 0.25

SX = lambda C_A: k_2 * C_A / (k_1 * C_A**0.5)
SY = lambda C_A: k_2 * C_A / (k_3 * C_A**2)
SXY = lambda C_A: k_2 * C_A / (k_1 * np.sqrt(C_A) + k_3 * C_A**2)

fig, ax = plt.subplots(3, figsize=(6.4, 2*4.8))
ax[0].plot(C_A_ran, SX(C_A_ran), label="Reaction X Selectivity")
ax[0].set_ylabel(r"$S_{B/X}$")
ax[1].plot(C_A_ran, SY(C_A_ran), "tab:orange", label="Reaction Y Selectivity")
ax[1].set_ylabel(r"$S_{B/Y}$")
ax[2].plot(C_A_ran, SXY(C_A_ran), "tab:green", label="Reaction X & Y Selectivity")
ax[2].set_ylabel(r"$S_{B/XY}$")
ax[2].set_xlabel(r"$C_A$ (mol/L)")
ax[0].set_title("Problem 3 Selectivity Plots")
fig.legend()
plt.show()
```

```
C_A_opt_index = np.where(SXY(C_A_ran)==SXY(C_A_ran).max())[0][0]
C_A_opt = C_A_ran[C_A_opt_index]

print(f"Optimum C_A = {C_A_opt}")

F = 10
C_A0 = 4 / 0.08206 / (27 + 273.15)
print(f"CSTR volume = {F * (C_A0 - C_A_opt) / (k_1 * C_A_opt**0.5 + k_2 * C_A_opt + k_3 *
↪  C_A_opt**2)}")
```

4. Problem 4

$$A + B \rightarrow C + D$$

$$C + D \rightarrow U$$

A membrane that selectively removes C would cause the concentration of C in the reactor to be very low or nearly zero. Because C participates in the undersired reaction, a low concentration of C in the reactor will lead the undersired reaction to be slow, and thus very little of the undersired product would be produced.

Select a memebrane reactor that selectively allows C to leave.