1. Problem 1

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

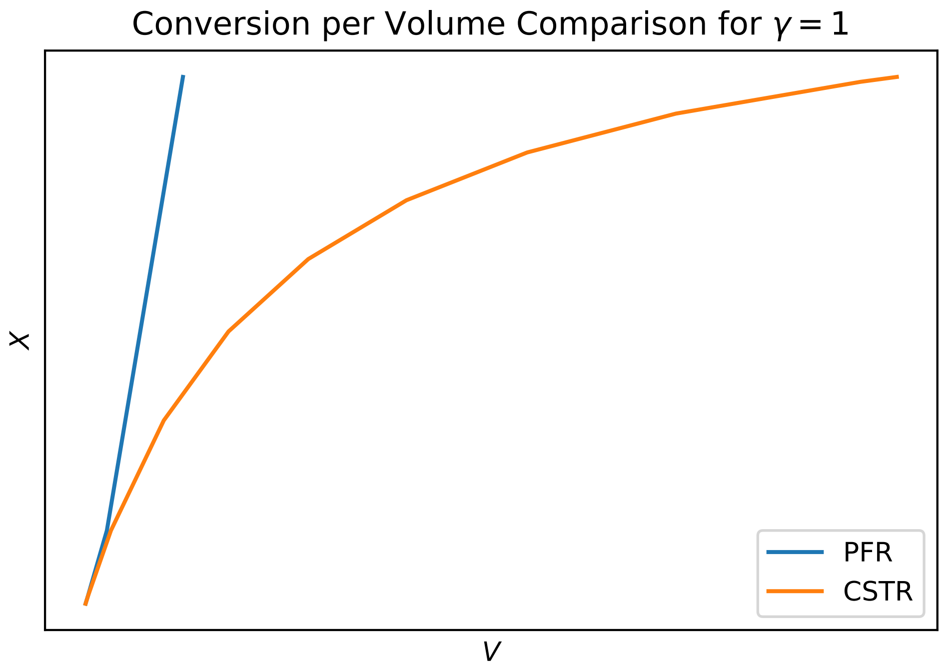
CSTR:

$$V = \frac{XF_{A0}}{-r_A}$$
$$V = \frac{XF_{A0}}{kC_{A0}(1 - X)}$$
$$\gamma = \frac{F_{A0}}{kC_{A0}}$$
$$V = \frac{\gamma X}{(1 - X)}$$
$$\frac{d}{dX}(V) = \frac{d}{dX}\left(\frac{\gamma X}{(1 - X)}\right)$$
$$\frac{dV}{dX} = \frac{\gamma}{(1 - X)^2}$$

PFR:

$$F_{A0}\frac{dV}{dX} = -r_A$$
$$F_{A0}\frac{dV}{dX} = kC_{A0}(1 - X)$$
$$\frac{dV}{dX} = \frac{1 - X}{\gamma}$$

Compare conversion per volume between the CSTR and PFR:



For any given volume change, the PFR will have a much larger conversion change because it has a higher conversion per volume than the CSTR. Add more volume to the PFR because it will give more conversion.

2. Problem 2

(a)

$$A + B \rightarrow C$$

$$\begin{aligned}
F_{A0}\frac{dX}{dW} &= -r'_A \\
-r'_A &= k'C_AC_B \\
\epsilon &= (1-1-1)\cdot\frac{1}{2} = -\frac{1}{2} \\
C_A = C_B &= C_{A0}\left(\frac{1-X}{1-\frac{1}{2}X}\right)p \\
C_C &= C_{A0}\left(\frac{X}{1-\frac{1}{2}X}\right)p \\
\frac{dX}{dW} &= \frac{k'C_{A0}^2p^2}{F_{A0}}\left(\frac{1-X}{1-\frac{1}{2}X}\right)^2 \\
C_{A0} &= \frac{F_{A0}}{v_0} \\
\frac{dX}{dW} &= \frac{k'F_{A0}p^2}{v_0^2}\left(\frac{1-X}{1-\frac{1}{2}X}\right)^2 \\
\frac{dp}{dW} &= -\frac{\alpha\left(1-\frac{1}{2}X\right)}{2p}
\end{aligned}$$

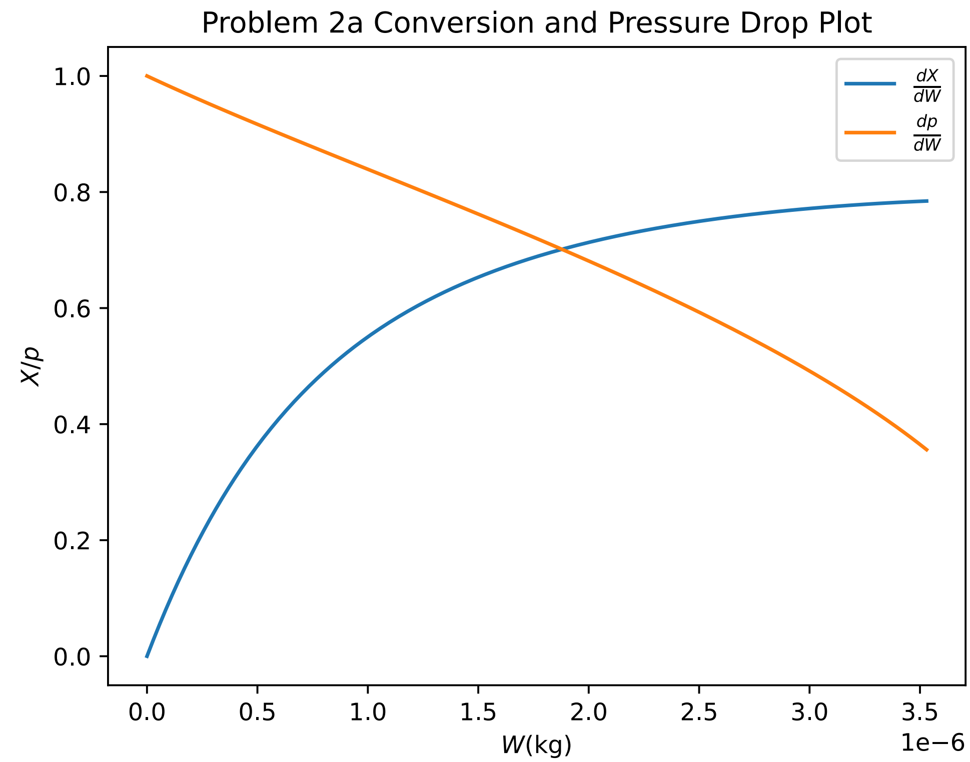
Solve this system of ODEs:

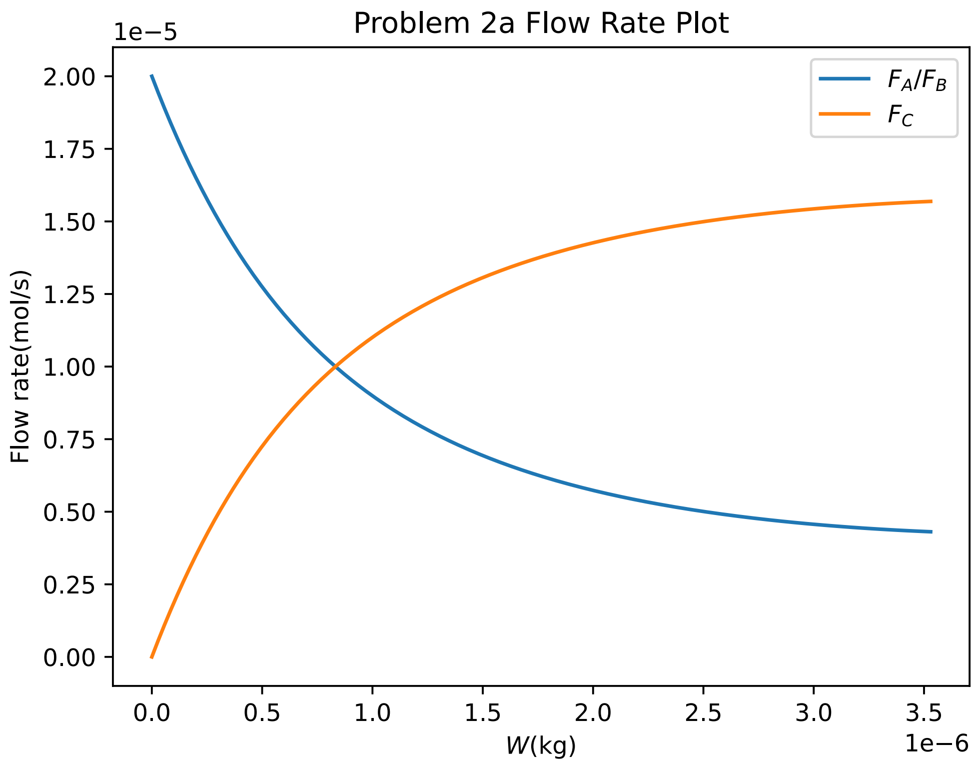
$$\begin{aligned}
\frac{dX}{dW} &= \frac{k'F_{A0}p^2}{v_0^2}\left(\frac{1-X}{1-\frac{1}{2}X}\right)^2 \\
\frac{dp}{dW} &= -\frac{\alpha\left(1-\frac{1}{2}X\right)}{2p} \\
k' &= 0.004 \\
F_{A0} &= 2\cdot 10^{-5} \\
v_0 &= 2.83\cdot 10^{-7} \\
\alpha &= 3.55\cdot 10^{5}
\end{aligned}$$

For plotting flow rates over time:

$$\begin{aligned}
F_A = F_B &= F_{A0}(1-X) \\
F_C &= F_{A0}X
\end{aligned}$$

Output plots:


Problem 2a Conversion and Pressure Drop Plot
$\frac{dX}{dW}$
$\frac{dp}{dW}$
X/p
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
1e−6
W(kg)


Problem 2a Flow Rate Plot
1e−5
$F_A/F_B$
$F_C$
Flow rate(mol/s)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
1e−6
W(kg)

Code that creates the plots:

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

# ode system to solve dp/dW and dX/dW
def ode(t, y):
    X = y[0]
    p = y[1]
    # constants
    F_A0 = 2e-5
    v_0 = 2.83e-7
    alpha = 3.55e5
    k = 0.004

    f = np.zeros(len(y))

    f[0] = k * F_A0 * p**2 / v_0**2 * ((1 - X) / (1 - X/2)) **2
    f[1] = -alpha / 2 / p * (1 - X/2)

    return f

# arguments to pass to the ode solver
ode_kwargs = {
    'method': 'Radau',
    'atol': 1e-8,
    'rtol': 1e-8,
}

# solving the ode system
solution = solve_ivp(ode, [0, 3.53e-6], [0, 1], **ode_kwargs)

# plottting
plt.plot(solution.t, solution.y[0])
plt.plot(solution.t, solution.y[1])
plt.legend([r'$\frac{dX}{dW}$', r'$\frac{dp}{dW}$'])
plt.xlabel(r"$W$(kg)")
plt.ylabel(r"$X/p$")
plt.title("Problem 2a Conversion and Pressure Drop Plot")
plt.show()

# functions to calculate flow rates
F_A0 = 2e-5
F_A = lambda X: F_A0 * (1 - X)
F_C = lambda X: F_A0 * X
```

```python
# plotting
plt.plot(solution.t, F_A(solution.y[0]))
plt.plot(solution.t, F_C(solution.y[0]))
plt.legend([r'$F_A/F_B$', r'$F_C$'])
plt.xlabel(r"$W$(kg)")
plt.ylabel(r"Flow rate(mol/s)")
plt.title("Problem 2a Flow Rate Plot")
plt.show()
```

(b) The total conversion is 0.784.

Convert to kg/yr:

$$\dot{m}_C = 0.784 \cdot 2 \cdot 10^{-5} \text{ mol/s} \cdot 99 \text{ g/mol} = 0.00155 \text{ g/s}$$
$$N = \frac{10000 \text{ kg/yr} \cdot 1000 \text{ g/kg}}{0.00155 \text{ g/s} \cdot 3600 \text{ s/hr} \cdot 24 \text{ hr/day} \cdot 365 \text{ day/yr}}$$
$$\boxed{N = 204}$$

204 reactors are needed to achieve a production of 10,000 kg/yr.

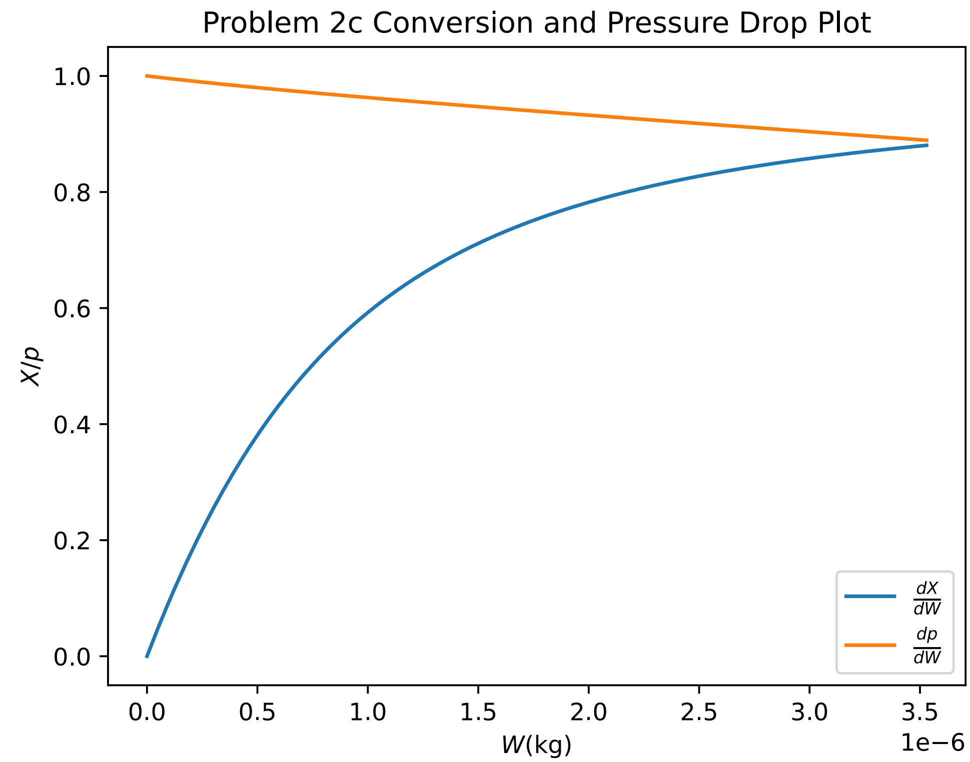
(c)

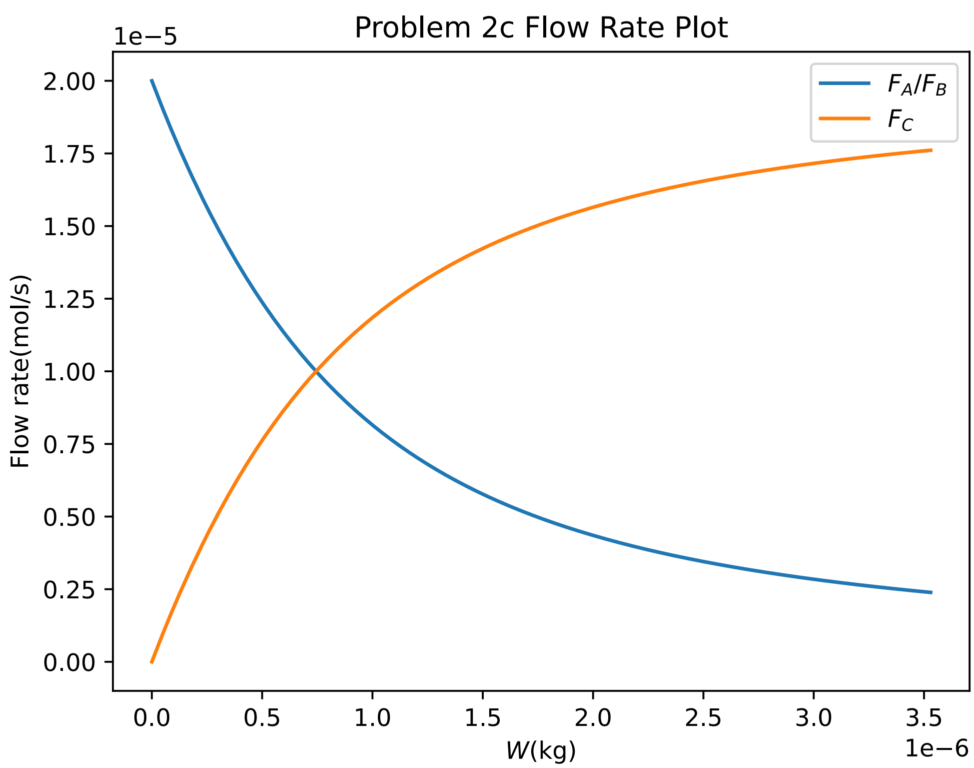
$$\alpha = \alpha_0 \frac{D_0^2}{D^2}$$
$$D = 2D_0$$
$$\alpha = \alpha_0 \frac{D_0^2}{(2D_0)^2}$$
$$\alpha = \frac{\alpha_0}{4}$$

Solve the ODE system with the new alpha value.

$$\frac{dX}{dW} = \frac{k' F_{A0} p^2}{v_0^2} \left( \frac{1 - X}{1 - \frac{1}{2}X} \right)^2$$
$$\frac{dp}{dW} = -\frac{\frac{\alpha_0}{4} \left(1 - \frac{1}{2}X\right)}{2p}$$

Output plots:




The conversion compared to part a is slightly higher, and the pressure drop is lower. Nothing unusual.

Code that creates the plots:

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

def ode(t, y):
    X = y[0]
    p = y[1]

    F_A0 = 2e-5
    v_0 = 2.83e-7
    alpha = 3.55e5 / 4
    k = 0.004

    f = np.zeros(len(y))

    f[0] = k * F_A0 * p**2 / v_0**2 * ((1 - X) / (1 - X/2)) **2
    f[1] = -alpha / 2 / p * (1 - X/2)

    return f


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

solution = solve_ivp(ode, [0, 3.53e-6], [0, 1], **ode_kwargs)

plt.plot(solution.t, solution.y[0])
plt.plot(solution.t, solution.y[1])
plt.legend([r'$\frac{dX}{dW}$', r'$\frac{dp}{dW}$'])
plt.xlabel(r"$W$(kg)")
plt.ylabel(r"$X/p$")
plt.title("Problem 2c Conversion and Pressure Drop Plot")
plt.show()

# functions to calculate flow rates
F_A0 = 2e-5
F_A = lambda X: F_A0 * (1 - X)
F_C = lambda X: F_A0 * X

# plotting
plt.plot(solution.t, F_A(solution.y[0]))
plt.plot(solution.t, F_C(solution.y[0]))
plt.legend([r'$F_A/F_B$', r'$F_C$'])
plt.xlabel(r"$W$(kg)")
```

```
plt.ylabel(r"Flow rate(mol/s)")
plt.title("Problem 2c Flow Rate Plot")
plt.show()
```

3. Problem 3

   (a) Suppose first order reaction:

$$-r_A = kC_A$$

Isothermal and isobaric

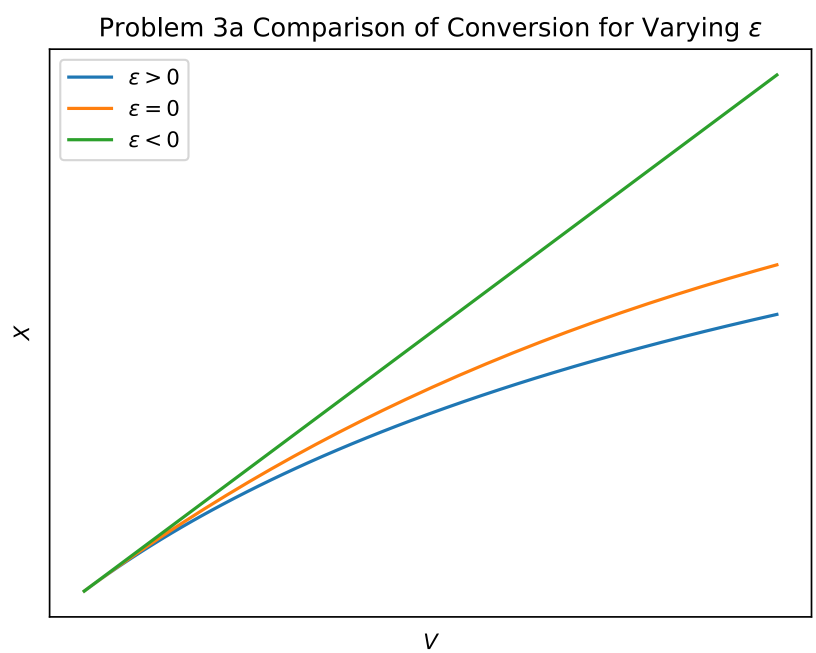
$$C_A = C_{A0}\left(\frac{1-X}{1+\epsilon X}\right)$$
$$\frac{dX}{dV} = -r_A$$
$$\frac{dX}{dV} = kC_{A0}\left(\frac{1-X}{1+\epsilon X}\right)$$
$$\gamma = kC_{A0}$$

General form:

$$\frac{dX}{dV} = \gamma\left(\frac{1-X}{1+\epsilon X}\right)$$

When $\epsilon$ is less than zero, the numerator of the differential above becomes less than zero which increases $\frac{dX}{dV}$. The rate of change of conversion increases which increases conversion overall. When $\epsilon$ is greater than zero, the numerator is greater than one which decreases $\frac{dX}{dV}$. The decrease causes the rate of change of conversion to slow which decreases conversion. The way $\epsilon$ changes $\frac{dX}{dV}$ changes the overall conversion. Negative $\epsilon$ increases the rate which increases conversion.

The increase in conversion can be seen in the plot below which shows conversion with different $\epsilon$ values.

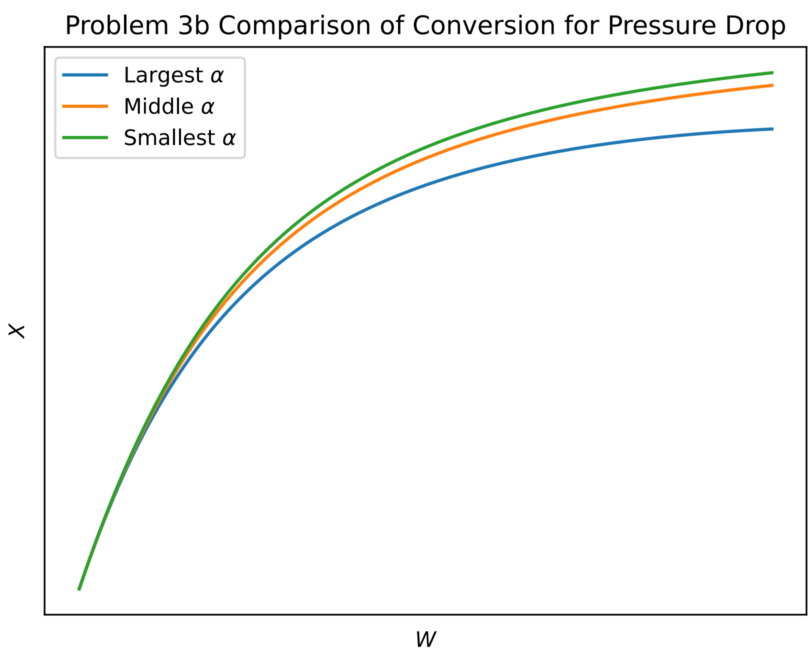


(b) Reorder the above differential for catalyst weight and pressure drop:

$$\frac{dX}{dW} = \gamma \left( \frac{1-X}{1+\epsilon X} \right) p$$
$$\frac{dp}{dW} = -\frac{\alpha(1+\epsilon X)}{p}$$

Smaller values of $\alpha$ in $\frac{dp}{dW}$ decrease the rate at which pressure drops in the reactor. From the differential for $\frac{dX}{dW}$, the pressure ratio, $p$, is proportional to the rate at which conversion increases. If the pressure ratio is decreasing at a slower rate, then the rate at which $\frac{dX}{dW}$ decreases will be lower. If lower values for $\alpha$ lower $\frac{dp}{dW}$, then lower values of $\alpha$ should result in higher conversions. Essentially, a lower $p$ results in the conversion increasing at a slower rate. The lower $p$ is a result of a larger pressure drop.

The plot below demonstrates this relationship. Notice that the reactor with the lowest $\alpha$ has the highest conversion. A lower $\alpha$ corresponds to a lower pressure drop.



$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} + \mathrm{D} + \mathrm{E}\uparrow$$

4. Problem 4

$$r = kC_AC_B$$
$$C_A = \frac{N_A}{V}$$
$$r = k\frac{N_AN_B}{V^2}$$

Design equation:

$$\frac{dN_A}{dt} = r_A$$
$$-r_A = -r_B = r_C = r_D = r_C = r$$
$$\frac{dN_A}{dt} = -k\frac{N_AN_B}{V^2}$$
$$\frac{dN_B}{dt} = F_{B0} - k\frac{N_AN_B}{V^2}$$
$$\frac{dN_C}{dt} = k\frac{N_AN_B}{V^2}$$
$$\frac{dN_D}{dt} = k\frac{N_AN_B}{V^2}$$
$$\frac{dV}{dt} = v_0 - v_{CO_2}$$
$$v_{CO_2} = \frac{r_EVM_{CO_2}}{\rho_{CO_2}}$$
$$\frac{dV}{dt} = v_0 - \frac{k\frac{N_AN_B}{V^2}VM_{CO_2}}{\rho_{CO_2}}$$
$$\frac{dV}{dt} = v_0 - \frac{kN_AN_BM_{CO_2}}{V\rho_{CO_2}}$$
$$v_0 = \frac{F_{B0}}{C_{B0}}$$
$$\frac{dV}{dt} = \frac{F_{B0}}{C_{B0}} - \frac{kN_AN_BM_{CO_2}}{V\rho_{CO_2}}$$

Solve the system of ODEs:

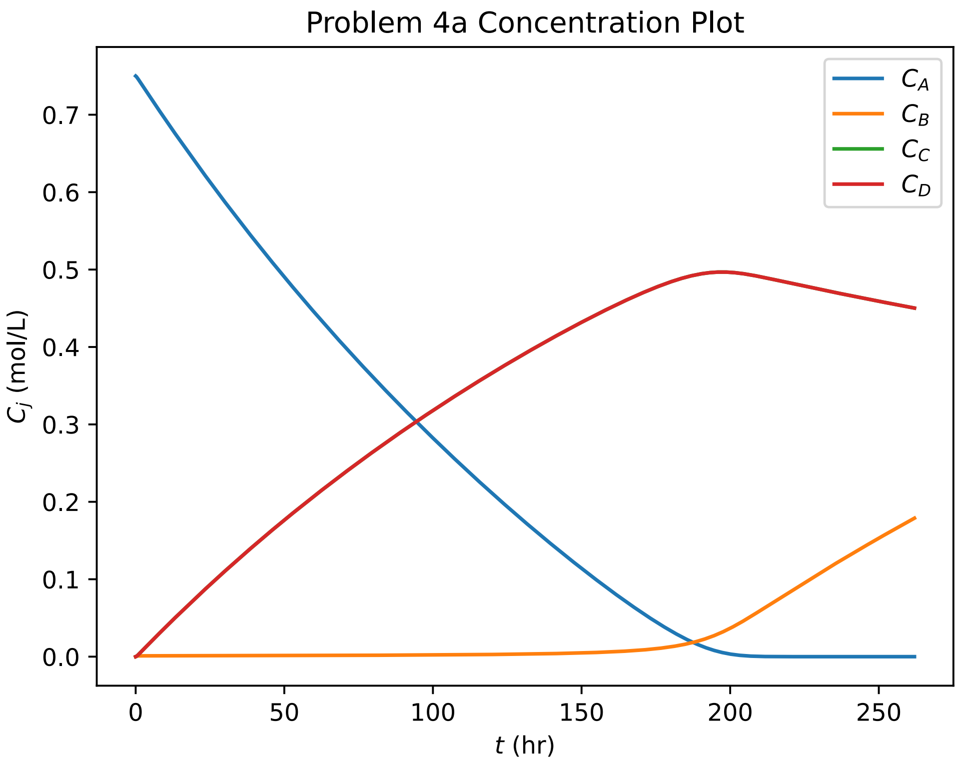
$$
\begin{aligned}
\frac{dN_A}{dt} &= -k\frac{N_A N_B}{V^2} \\
\frac{dN_B}{dt} &= F_{B0} - k\frac{N_A N_B}{V^2} \\
\frac{dN_C}{dt} &= k\frac{N_A N_B}{V^2} \\
\frac{dN_D}{dt} &= k\frac{N_A N_B}{V^2} \\
\frac{dV}{dt} &= \frac{F_{B0}}{C_{B0}} - \frac{kN_A N_B M_{CO_2}}{V\rho_{CO_2}} \\
C_{B0} &= 1.5 \\
F_{B0} &= 60 \cdot 0.1 = 6 \\
k &= 5.1 \\
M_E &= 44 \\
\rho_E &= 1000 \\
v_0 &= \frac{F_{B0}}{C_{B0}} = \frac{6}{1.5} = 4 \\
N_{A0} &= 0.75 \cdot 1500 = 1125
\end{aligned}
$$

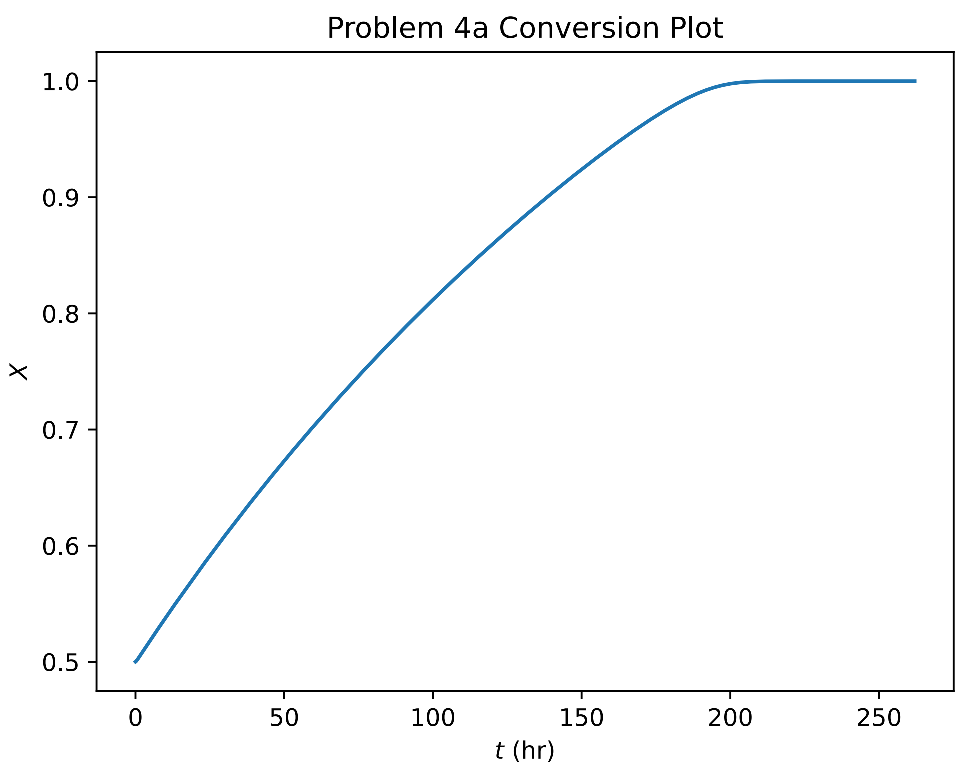
Concentrations and conversion are calculated from solution arrays.

$$
\begin{aligned}
C_j(t) &= \frac{N_j(t)}{V(t)} \\
C_A &= C_{A0}(1 - X) \\
X &= 1 - \frac{C_A}{C_{A0}} \\
X(t) &= 1 - \frac{\frac{C_A(t)}{V(t)}}{\frac{C_{A0}(t)}{V(t)}} \\
X(t) &= 1 - \frac{C_A(t)}{C_{A0}(t)}
\end{aligned}
$$

Output plots:

$C_C = C_D$




Code that creates the plots:

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

def ode(t, y):
    N_A = y[0]
    N_B = y[1]
    V = y[4]

    f = np.zeros(len(y))

    C_B0 = 1.5
    F_B0 = 6
    k = 5.1
    M_E = 44.0095
    rho_E = 1000
    v_0 = F_B0 / C_B0

    r = k * N_A * N_B / V**2

    f[0] = -r * V
    f[1] = F_B0 - r * V
    f[2] = r * V
    f[3] = r * V
    f[4] = v_0 - r * V * M_E / rho_E

    return f


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

N_A0 = 0.75*1500

initial_cond = [N_A0, 0, 0, 0, 1500]

solution = solve_ivp(ode, [0, 262], initial_cond, **ode_kwargs)

for i in range(4):
    plt.plot(solution.t, solution.y[i]/solution.y[4])

plt.legend([r'$C_A$', r'$C_B$', r'$C_C$', r'$C_D$'])
plt.xlabel(r"$t$ (hr)")
plt.ylabel(r"$C_j$ (mol/L)")
```

```python
plt.title('Problem 4a Concentration Plot')
print(solution.y[4][-1])
plt.show()

plt.plot(solution.t, 1 - solution.y[0]/solution.y[4]/1.5)
plt.xlabel(r"$t$ (hr)")
plt.ylabel(r"$X$")
plt.title('Problem 4a Conversion Plot')
plt.show()
```