CHEN 364 HW7

April 10, 2023

[ ]:
```
import matplotlib.pyplot as plt
import numpy as np

from scipy.integrate import solve_ivp, odeint

import matplotlib_inline
%matplotlib inline
matplotlib_inline.backend_inline.set_matplotlib_formats('png', 'pdf')
```

1 Problem 1

Mole balances:

$\frac{dF_A}{dV} = -r_1 v_0 - r_2 v_0$

$\frac{dF_B}{dV} = -2r_1 v_0$

$\frac{dF_C}{dV} = 2r_1 v_0 - r_2 v_0$

$\frac{dF_D}{dV} = 2r_2 v_0$

Reactions:

$r_1 = k_1(T) C_A C_B^2$

$r_2 = k_1(T) C_A C_C$

Temperature:

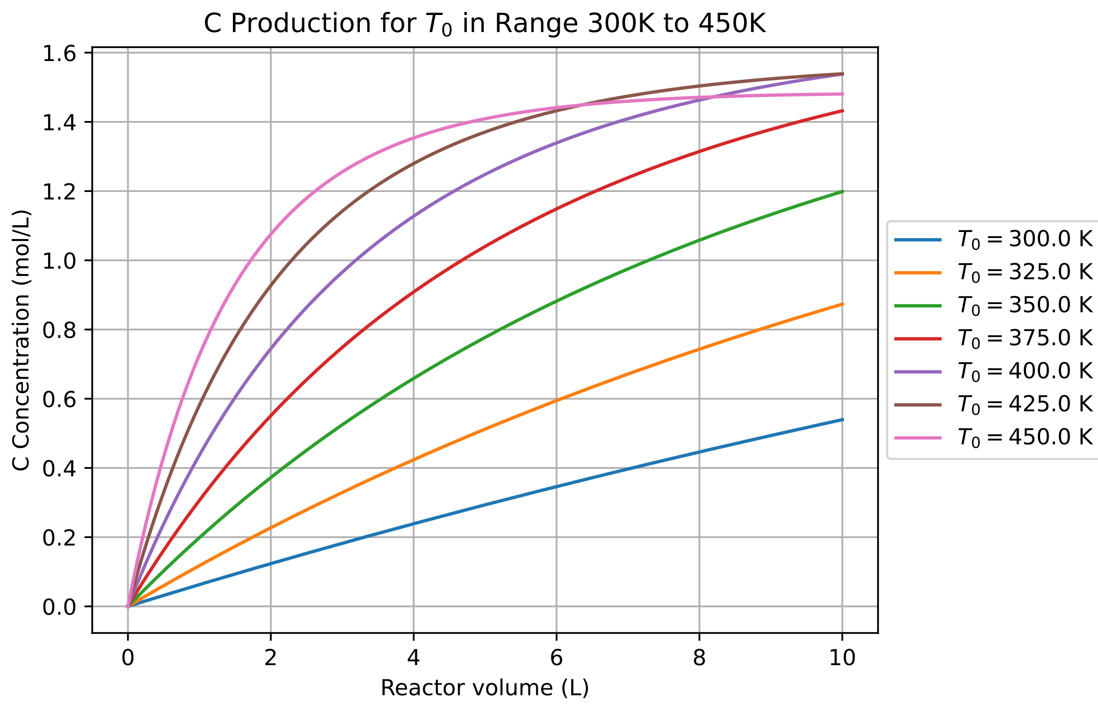
Adbiabatic $Q_r = 0$

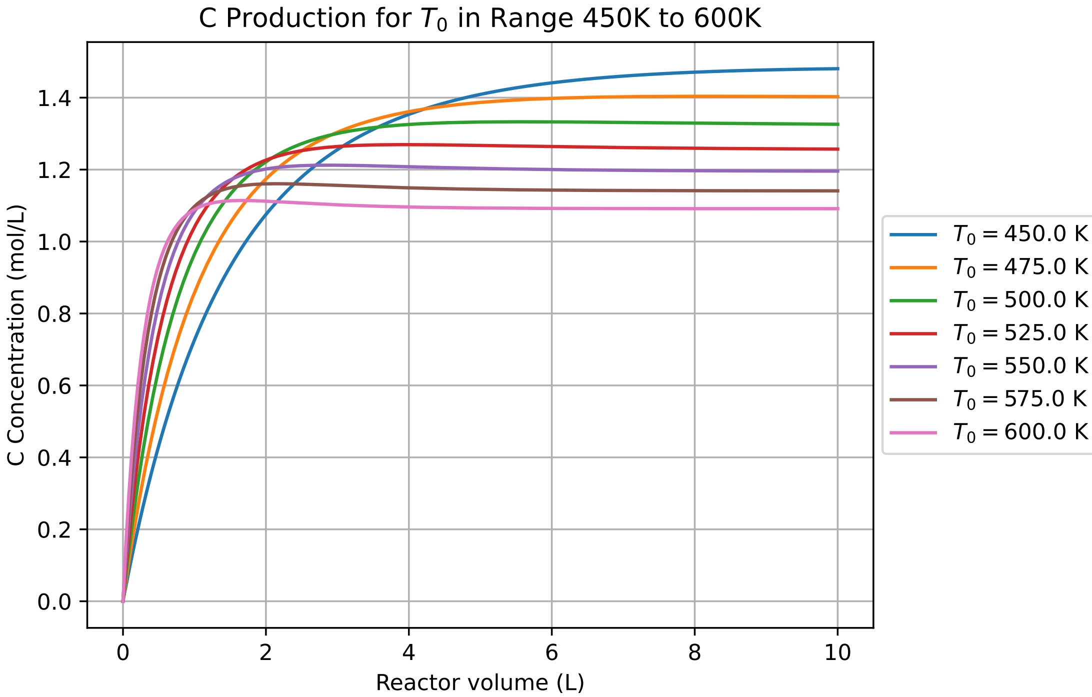
$\frac{dT}{dV} = \frac{r_1 \Delta H_1 + r_2 \Delta H_2}{F_A C_{P,A} + F_B C_{P,B} + F_C C_{P,C} + F_D C_{P,D}}$

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

def p1_ode(t, y):
    f = y*0
```

```
    F_A = y[0]
    F_B = y[1]
    F_C = y[2]
    F_D = y[3]
    T = y[4]

    v_0 = 10
    C_PA = 20
    C_PB = C_PA
    C_PC = 60
    C_PD = 80
    H_1 = 20000
    H_2 = -10000

    k_1 = 0.001 * np.exp(5000 * 4.184 / 8.314 * (1 / 300 - 1 / T))
    k_2 = 0.001 * np.exp(7500 * 4.184 / 8.314 * (1 / 300 - 1 / T))

    r_1 = k_1 * F_A / v_0 * (F_B / v_0)**2
    r_2 = k_2 * F_A / v_0 * F_C / v_0

    f[0] = (-r_1 - r_2) * v_0
    f[1] = -2 * r_1 * v_0
    f[2] = (2 * r_1 - r_2) * v_0
    f[3] = 2 * r_2 * v_0
    f[4] = (r_1 * H_1 + r_2 * H_2) / (F_A * C_PA + F_B * C_PB + F_C * C_PC + 
 ↪F_D * C_PD)

    return f

T_range = np.linspace(300, 600, 13)

p1_sols = []

for i, val in enumerate(T_range):
    ode_args = (
        p1_ode,
        [0, 10],
        [20, 40, 0, 0, val],
    )
    p1_sols.append(solve_ivp(*ode_args, **ode_kwargs))

for i in range(0, 7):
    plt.plot(p1_sols[i].t, p1_sols[i].y[2]/10, label=rf"$T_0=${T_range[i]} K")

plt.xlabel("Reactor volume (L)")
plt.ylabel("C Concentration (mol/L)")
plt.title(r"C Production for $T_0$ in Range 300K to 450K")
```

```
plt.legend(loc="right", bbox_to_anchor=(1.3, 0.5))
plt.grid(which='both', axis='both')
plt.show()

for i in range(6, len(p1_sols)):
    plt.plot(p1_sols[i].t, p1_sols[i].y[2]/10, label=rf"$T_0=${T_range[i]} K")

plt.xlabel("Reactor volume (L)")
plt.ylabel("C Concentration (mol/L)")
plt.title(r"C Production for $T_0$ in Range 450K to 600K")
plt.legend(loc="right", bbox_to_anchor=(1.3, 0.5))
plt.grid(which='both', axis='both')
plt.show()
```





An optimal inlet temperature is one between 400K and 425K. Both 400K and 425K inlet temperatures have about the same rate of production of C.

2 Problem 2

$\epsilon = \frac{1}{2} - 1 = -\frac{1}{2}$

Concentrations in terms of X

$C_A = C_{A0}\left(\frac{1-X}{1-\frac{X}{2}}\right) p\frac{T_0}{T}$

$C_C = C_{A0}\left(\frac{X}{1-\frac{X}{2}}\right) p\frac{T_0}{T}$

Rate law

$r_A = -\left(k(T)C_A^2 - \frac{k(T)}{K(T)}C_C\right)$

$k(T) = 0.1 \exp\left[\frac{8000}{8.314}\left(\frac{1}{450} - \frac{1}{T}\right)\right]$

$K(T) = 10000 \exp\left[\frac{-20000}{8.314}\left(\frac{1}{450} - \frac{1}{T}\right)\right]$

Design equation:

$\frac{dX}{dW} = \frac{r_A}{F_{A0}}$

Pressure drop

$\frac{dp}{dW} = -\frac{\alpha\left(1-\frac{X}{2}\right)}{2p}\frac{T}{T_0}$

Energy balance

$\frac{dT}{dW} = \frac{r_A \Delta H_{\mathrm{Rx}} - Ua(T - T_a)}{F_{A0}(\sum \Theta_j C_{p,j} + X \Delta C_P)}$

$\sum \Theta_j C_{p,j} = C_{P,A} = 40$

$\Delta C_P = \frac{1}{2} \cdot 20 - 40 = -30$

$\frac{dT}{dW} = \frac{r_A \Delta H_{\mathrm{Rx}} - Ua(T - T_a)}{F_{A0}(40 - 30X)}$

Adiabatic case

$\frac{dT}{dW} = \frac{r_A \Delta H_{\mathrm{Rx}}}{F_{A0}(40 - 30X)}$

Changing T_a case

Parallel flow:

$\frac{dT_a}{dW} = \frac{Ua(T - T_a)}{\dot{m}_c C_{P,c}}$

Countercurrent flow:

$\frac{dT_a}{dW} = -\frac{Ua(T - T_a)}{\dot{m}_c C_{P,c}}$

[ ]:
```
C_A = lambda X, p, T: 1.9 * (1 - X) / (1 - X / 2) * p * 450 / T
C_C = lambda X, p, T: 1.9 * (X) / (1 - X / 2) * p * 450 / T
dpdW = lambda X, p, T: -0.005 * (1 - X / 2) / 2 / p * T / 450
k = lambda T: 0.1 * np.exp(8000 / 8.314 *( 1 / 450 - 1 / T))
K = lambda T: 10000 * np.exp(-20000 / 8.314 * ( 1 / 450 - 1 / T))
r_A = lambda C_A, C_C, T: -k(T) * C_A**2 + k(T) / K(T) * C_C
F_A = lambda X: 5 * (1 - X)
F_C = lambda X: 5 * (X / 2)
```

[ ]:
```
def p_2_adiabatic_ode(t, y):
    f = y*0

    X = y[0]
    p = y[1]
    T = y[2]

    f[0] = -r_A(C_A(X, p, T), C_C(X, p, T), T) / 5
    f[1] = dpdW(X, p, T)
    # f[2] = -20000 * r_A(C_A(X, p, T), C_C(X, p, T), T) / (F_A(X) * 40 +
 ↪F_C(X) * 20)
    f[2] = (-20000 * r_A(C_A(X, p, T), C_C(X, p, T), T)) / (40 - 30 * X) / 5

    return f

def p_2_const_T_a_ode(t, y):
    f = y*0

    X = y[0]
```

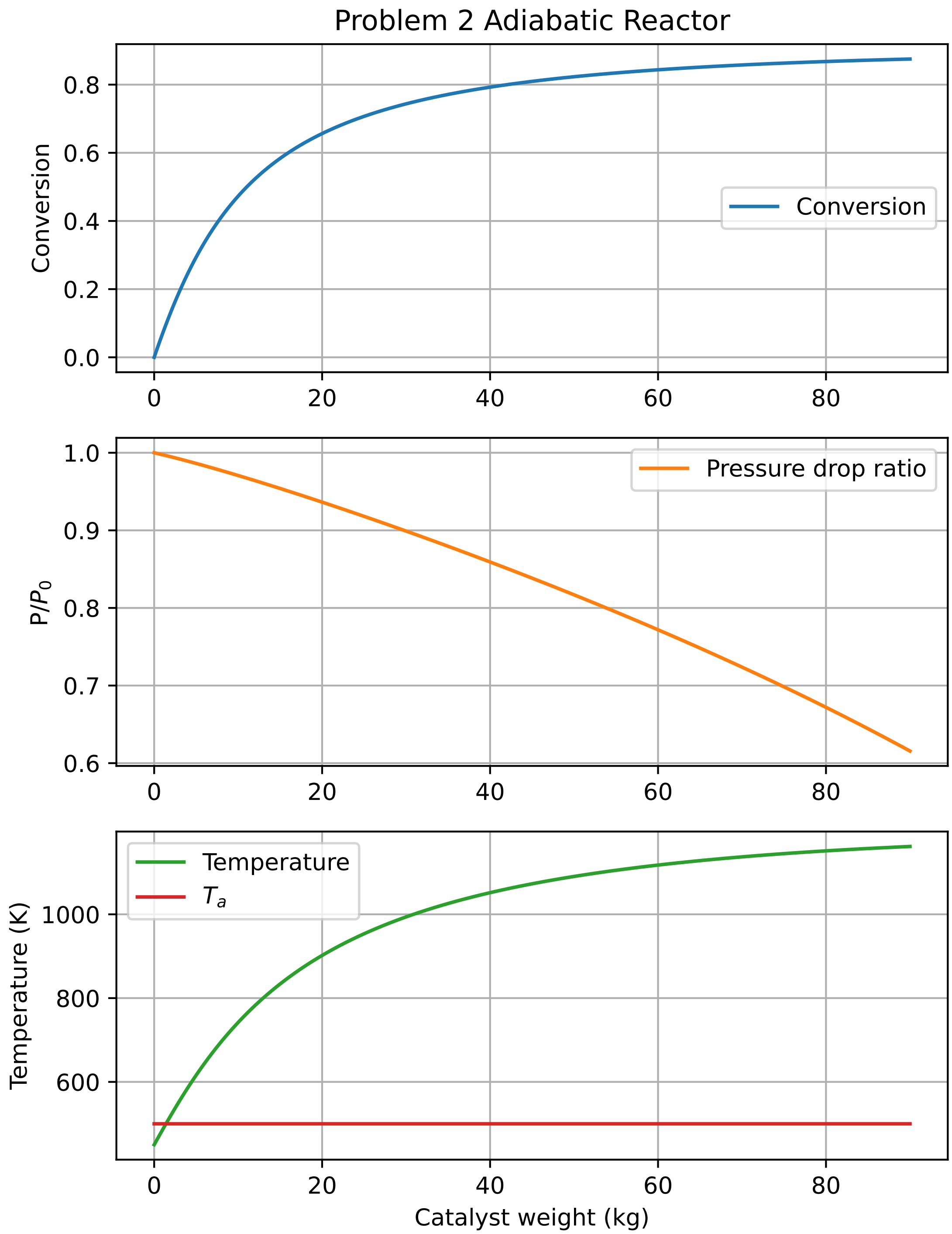
```python
    p = y[1]
    T = y[2]

    r = r_A(C_A(X, p, T), C_C(X, p, T), T)

    T_a = 500

    UA = 0.001 * 3600

    f[0] = -r / 5
    f[1] = dpdW(X, p, T)
    f[2] = (-20000 * r - UA * (T - T_a)) / (40 - 30 * X) / 5

    return f

def p_2_parallel_ode(t, y):
    f = y*0

    X = y[0]
    p = y[1]
    T = y[2]
    T_a = y[3]

    r = r_A(C_A(X, p, T), C_C(X, p, T), T)

    UA = 0.001 * 3600

    f[0] = -r / 5
    f[1] = dpdW(X, p, T)
    f[2] = (-20000 * r - UA * (T - T_a)) / (40 - 30 * X) / 5
    f[3] = UA * (T - T_a) / 0.05 / 4200

    return f

def p_2_counter_ode(t, y):
    f = y*0

    X = y[0]
    p = y[1]
    T = y[2]
    T_a = y[3]

    r = r_A(C_A(X, p, T), C_C(X, p, T), T)

    UA = 0.001 * 3600

    f[0] = -r / 5
```

```
    f[1] = dpdW(X, p, T)
    f[2] = (-20000 * r - UA * (T - T_a)) / (40 - 30 * X) / 5
    f[3] = -UA * (T - T_a) / 0.05 / 4200

    return f
```

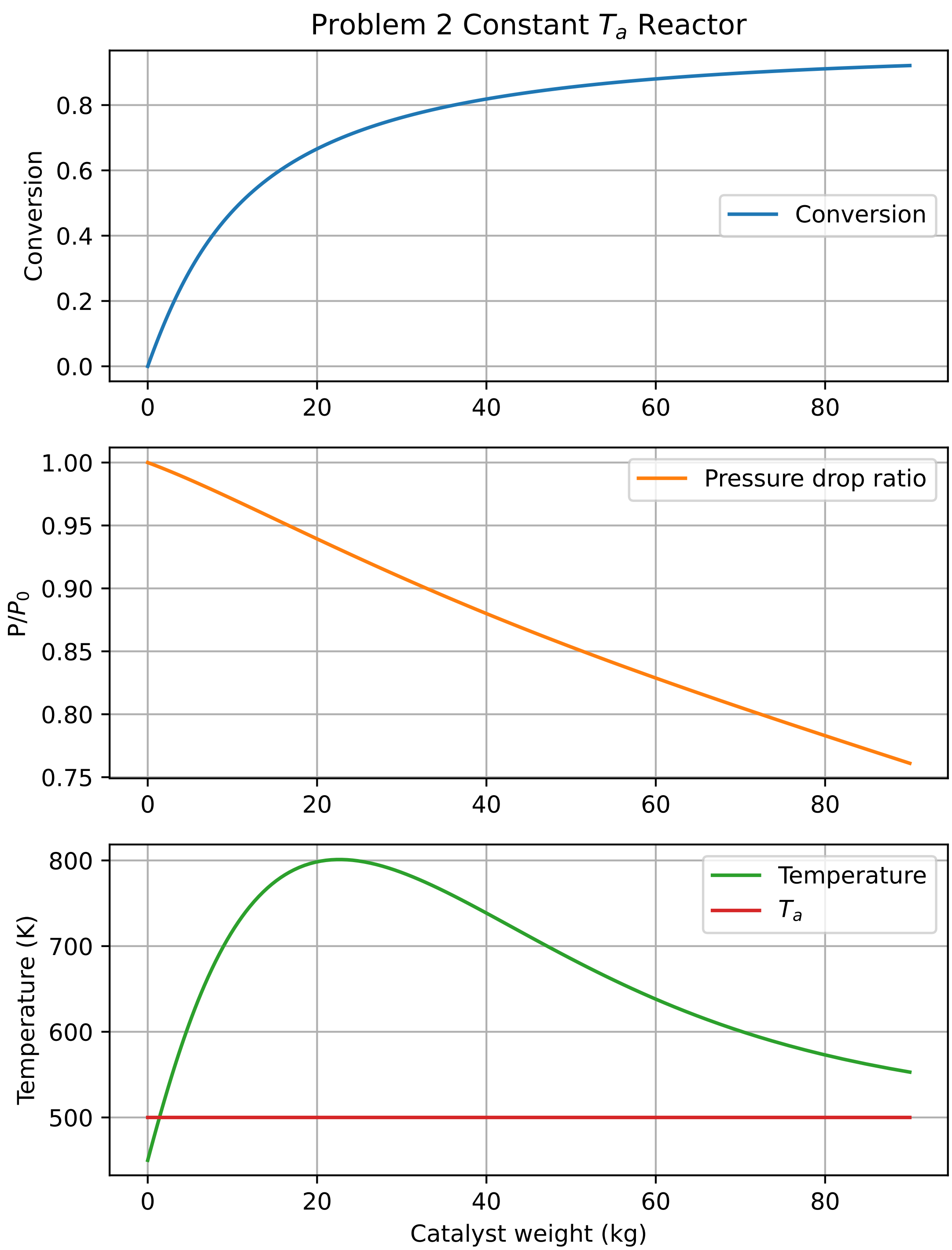
[ ]:
```
p2_options = {
    'Adiabatic': {
        'args': (p_2_adiabatic_ode, [0, 90], [0, 1, 450]),
        'kwargs': {
            'method': 'Radau',
            'atol': 1e-8,
            'rtol': 1e-8,
        }
    },
    'Constant $T_a$': {
        'args': (p_2_const_T_a_ode, [0, 90], [0, 1, 450]),
        'kwargs': {
            'method': 'Radau',
            'atol': 1e-8,
            'rtol': 1e-8,
        }
    },
    'Parallel Flow': {
        'args': (p_2_parallel_ode, [0, 90], [0, 1, 450, 500]),
        'kwargs': {
            'method': 'Radau',
            'atol': 1e-8,
            'rtol': 1e-8,
        }
    },
    'Countercurrent Flow': {
        'args': (p_2_counter_ode, [0, 90], [0, 1, 450, 717.0987]),
        'kwargs': {
            'method': 'Radau',
            'atol': 1e-8,
            'rtol': 1e-8,
        }
    },
}
```

[ ]:
```
for key in p2_options:
    p2_sol = solve_ivp(*p2_options[key]['args'], **p2_options[key]['kwargs'])
    fig, ax = plt.subplots(3, figsize=[6.40, 4.80*1.8])
    ax[0].plot(p2_sol.t, p2_sol.y[0], 'tab:blue', label="Conversion")
    ax[0].set_ylabel("Conversion")
    ax[1].plot(p2_sol.t, p2_sol.y[1], 'tab:orange', label="Pressure drop ratio")
```

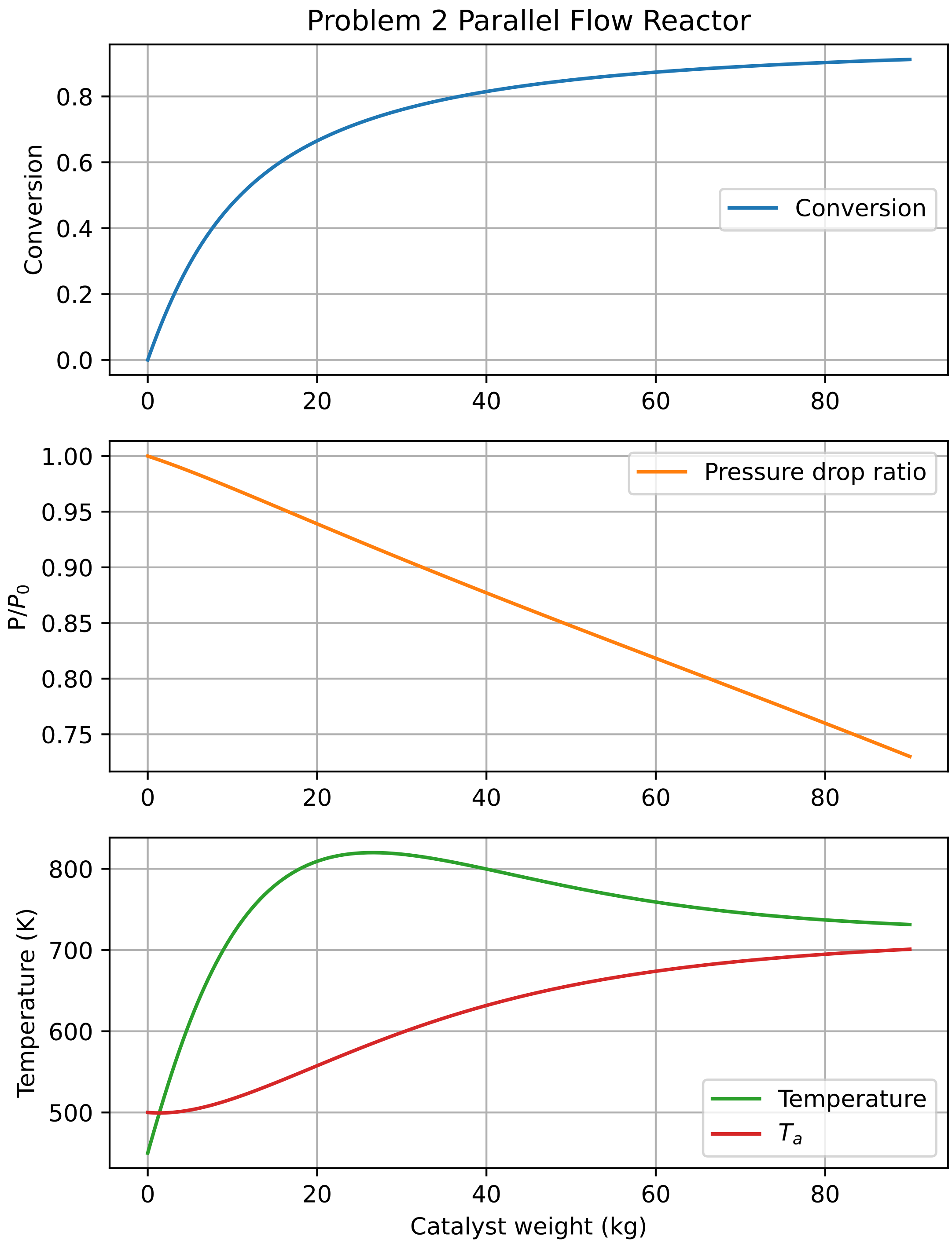
```
    ax[1].set_ylabel(r"P/$P_0$")
    ax[2].plot(p2_sol.t, p2_sol.y[2], 'tab:green', label="Temperature")
    ax[2].set_ylabel("Temperature (K)")
    try:
        ax[2].plot(p2_sol.t, p2_sol.y[3], 'tab:red', label=r"$T_a$")
    except:
        ax[2].plot(p2_sol.t, np.ones(p2_sol.t.shape[0])*500, 'tab:red',␣
↪label=r"$T_a$")
    for a in ax:
        a.legend()
        a.grid(which='both', axis='both')
    ax[0].legend(loc='right')
    ax[0].set_title(rf"Problem 2 {key} Reactor")
    plt.xlabel("Catalyst weight (kg)")
    plt.show()
```



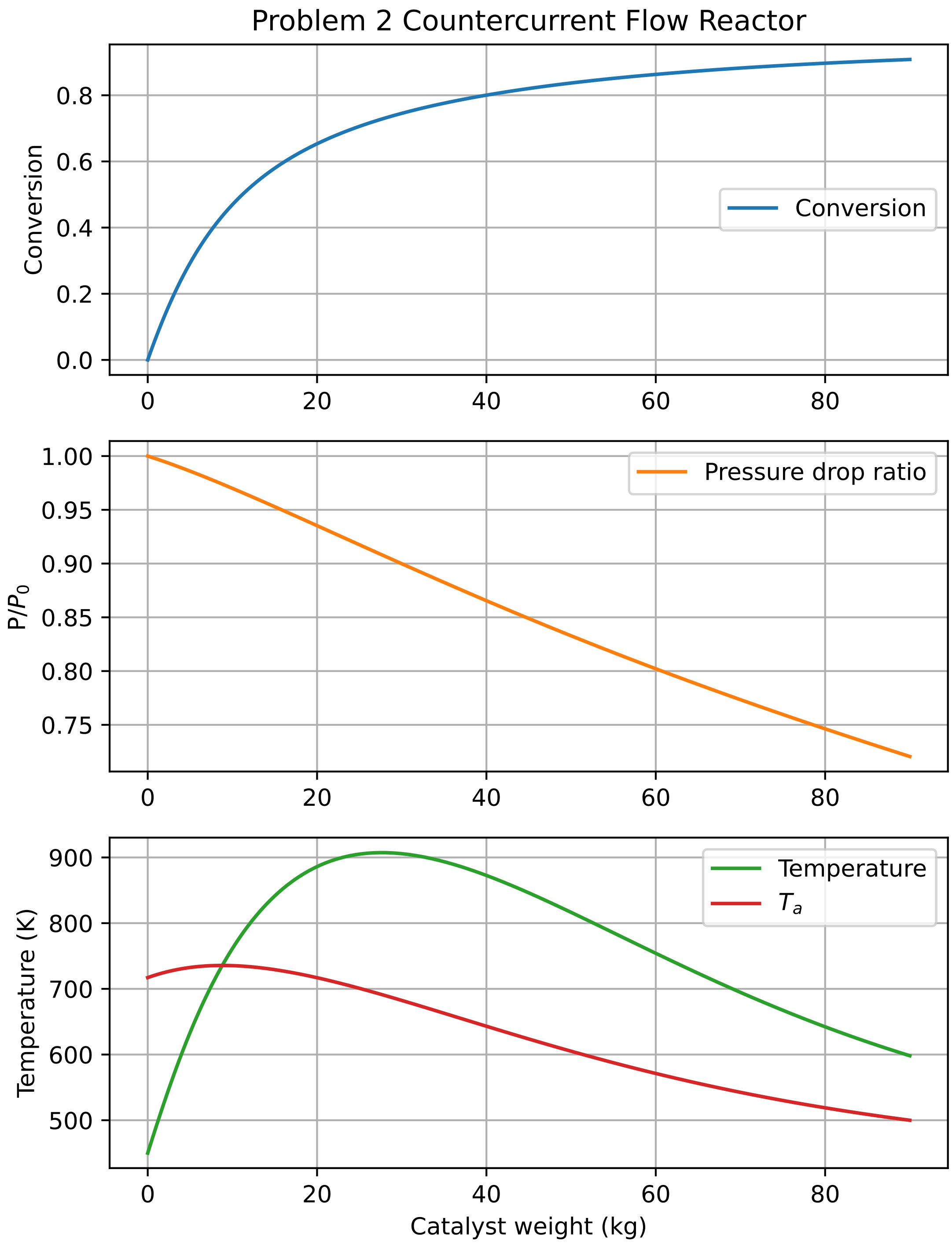
Problem 2 Adiabatic Reactor
Conversion
0.0
0.2
0.4
0.6
0.8
0
20
40
60
80
P/P_0
Pressure drop ratio
0.6
0.7
0.8
0.9
1.0
Temperature (K)
Temperature
T_a
600
800
1000
Catalyst weight (kg)



Problem 2 Constant T_a Reactor
Conversion
Conversion
0.0
0.2
0.4
0.6
0.8
P/P_0
Pressure drop ratio
0.75
0.80
0.85
0.90
0.95
1.00
Temperature (K)
Temperature
T_a
500
600
700
800
0
20
40
60
80
Catalyst weight (kg)



Problem 2 Parallel Flow Reactor
Conversion
0.0
0.2
0.4
0.6
0.8
0
20
40
60
80
Conversion
P/P_0
1.00
0.95
0.90
0.85
0.80
0.75
Pressure drop ratio
Temperature (K)
800
700
600
500
Temperature
T_a
Catalyst weight (kg)



3 Problem 3

Rate law:

$r_A = k\frac{N_A}{V}$

Design equation:

$\frac{dN_A}{dt} = -r_A V = -kN_A$

Analytical solution:

$\int \frac{dN_A}{N_A} = \int -kdt$

$\ln \frac{N_A}{N_{A0}} = -kt$

$N_A = N_{A0}e^{-kt}$

For $\frac{dT}{dt} = 0$, energy balance must be $Q_g = Q_r$

$Q_g = r_A V \Delta H^\circ_{\mathrm{rx}} = kN_{A0}e^{-kt}\Delta H^\circ_{\mathrm{rx}}$

$Q_r = F_c C_{P,c}\left(T - T_0\right)$

$F_c = \frac{kN_{A0}e^{-kt}\Delta H^\circ_{\mathrm{rx}}}{C_{P,c}(T-T_0)}$

At 2 h

$F_c = 3.16$ lb/s