CHEN 364 HW7

April 9, 2023

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

from scipy.integrate import solve_ivp

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 $Q_r = 0$

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

[ ]:
```
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

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

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

p1_sols = []

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

for i in range(0, 7):
    plt.plot(p1_sols[i].t, p1_sols[i].y[2], 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.show()

for i in range(6, len(p1_sols)):
```

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    plt.plot(p1_sols[i].t, p1_sols[i].y[2], 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.show()
```

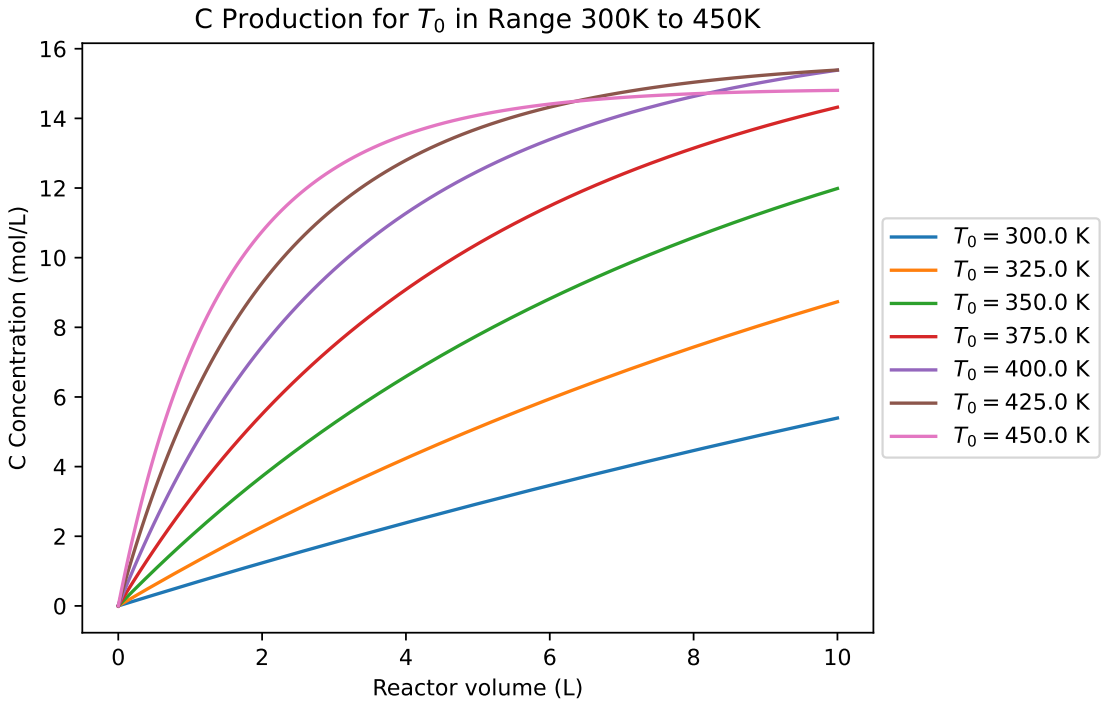

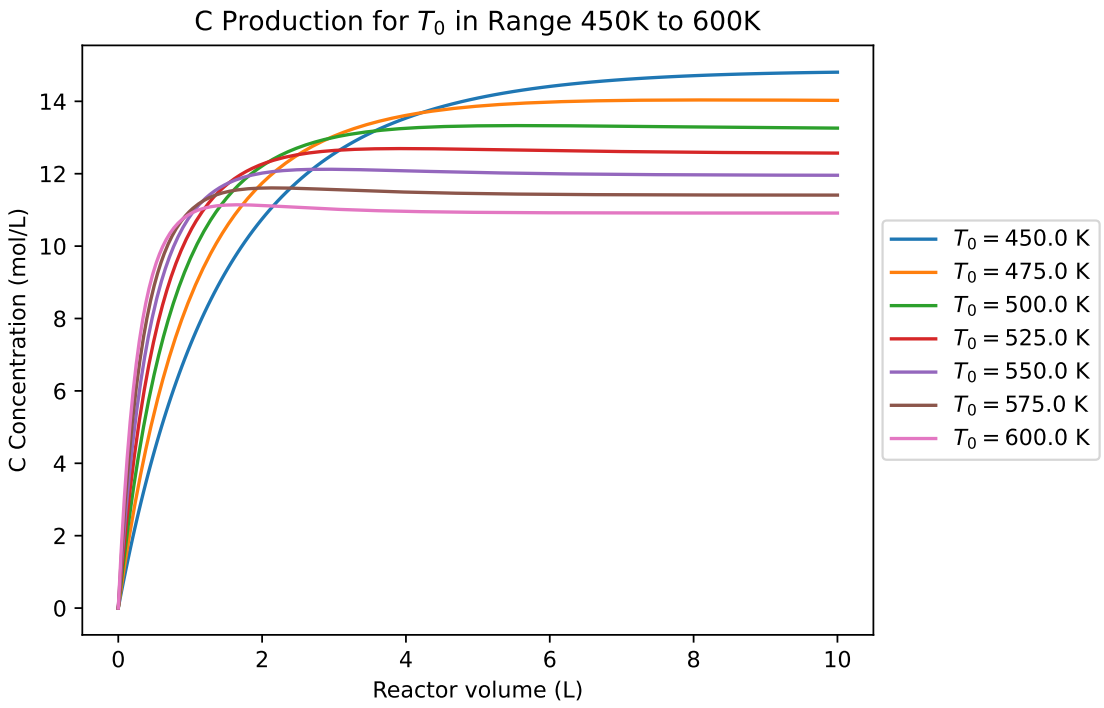
C Production for T_0 in Range 450K to 600K
C Concentration (mol/L)
Reactor volume (L)
0
2
4
6
8
10
12
14
$T_0 = 450.0$ K
$T_0 = 475.0$ K
$T_0 = 500.0$ K
$T_0 = 525.0$ K
$T_0 = 550.0$ K
$T_0 = 575.0$ K
$T_0 = 600.0$ K

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