

Homework 13

Ch En 263 – Numerical Tools

Due: 01 Dec. 2025

Instructions

- Complete the problems below and submit the following files to Learning Suite:
 - Excel portion: submit a workbook named `LastName_FirstName_HW13.xlsx` where each worksheet tab is named “Problem_1”, “Problem_2”, etc.
 - Python portion: submit a *single Jupyter notebook* named `LastName_FirstName_HW13.ipynb`.

Problems

1. Use the symbolic math engine in Python to find the four possible partial derivatives ($\partial f_0/\partial x_1$, $\partial f_0/\partial T$, $\partial f_1/\partial x_1$, $\partial f_1/\partial T$), of the vector function in residual form

$$\mathbf{f}(x_1, T) = \begin{bmatrix} x_1 10^{A_1 - B_1/(T+C_1)} - p_1, \\ (1 - x_1) 10^{A_2 - B_2/(T+C_2)} - p_2 \end{bmatrix} = \mathbf{0}$$

where A_1 , B_1 , C_1 , A_2 , B_2 , C_2 , p_1 and p_2 are known constants. Be sure to display these expressions in the notebook.

2. Recall that the enthalpy of gaseous CO_2 is given by

$$h(T) = h(298.15) + \int_{298.15}^T c_p(T) dT.$$

The units of h are J/mol. The heat capacity (J/mol K) is given by

$$c_p(T) = R_g(a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4),$$

where $R_g = 8.314$ J/(mol K), and $a_1 = 2.275724$, $a_2 = 0.009922$, $a_3 = -1.04091 \times 10^{-5}$, $a_4 = 6.86669 \times 10^{-9}$, $a_5 = -2.11728 \times 10^{-12}$. Also, $h(298.15) = -393549.1$ J/mol.

In Lab 16, we solved for the temperature when $h(T) = -362828$ J/mol. We did this by evaluating the integral by hand, and then we used `root` to solve the resulting non-linear equation. This time, use `quad` in Python to do the integral and `root` to solve for T . Be sure to print the value of T in the notebook.

Hint: You will need to set up a function to pass to `root` that uses `quad` inside of it. Also, you may want to compare the answer you get here with the one you found in Lab 16.