Homework 11

Ch En 263 – Numerical Tools

Due: 8 Apr. 2024

Instructions

- Complete the problems below and submit the following files to Learning Suite:
  - Excel portion: submit a workbook named `LastName_FirstName_HW11.xlsx` where each worksheet tab is named "Problem_1", "Problem_2", etc.
  - Python portion: submit a *single Jupyter notebook* named `LastName_FirstName_HW11.ipynb`.

Problems

1. Evaluate the integral

$$I = \int_{-50}^{50} x^2 f(x)\,dx$$

   using the data contained in the file `HW11_Prob1_Data.csv` with the trapezoidal rule. The first column of the data file contains x, the second column contains $f(x)$. Make sure you print the value of I to the console.

2. In reaction engineering, the average residence time $\bar{t}$ is the amount of time an element of fluid spends in a reactor and is related to the amount of substance present in the system. The easiest method to determine $\bar{t}$ is via a pulse stimulus, where a small amount of a tracer is put into a reactor operating under steady state and the effluent concentration measured over time. The average residence time is calculated as

$$\bar{t} = \frac{\int_0^\infty tC dt}{\int_0^\infty C dt}$$

t (s)	C (ppm)
0	0
100	20
200	20
300	16
400	10
500	7
600	5
700	3
800	1
900	0

   Given the data in the table, write a Python program to:

   (a) Find and plot a cubic spline which interpolates the function $C(t)$, and

   (b) Calculate the residence time $\bar{t}$ via the composite trapezoidal rule.

   Hint: There are two integrals in part (b): one in the numerator and one in the denominator.

3. 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

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

   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.

4. 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

$$c_p(T) = R_g(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4),$$

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 my want to compare the answer you get here with the one you found in Lab 16.*