Process model formulation and solution, 3E4

Tutorial 5

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Tutorial objectives: solution of a single, nonlinear equation.

Note: All questions below will consider the following problem.

The heat of reaction for a certain reaction is given by $\Delta H_r^0(T) = -24097 - 0.26T + 1.69 \times 10^{-3}T^2 + \dfrac{1.5 \times 10^5}{T}$ cal/mol. Compute the temperature at which $\Delta H_r^0(T) = -23505$ cal/mol.

Question 1 [1]

Show the first 4 iterations of the bisection method to solve for T, justifying your choice for the initial bracket.

For iteration 2, 3, and 4, please also report these two relative errors:

$$\varepsilon_{\text{rel,x}}^{(k)} = \left| \frac{x_m^{(k)} - x_m^{(k-1)}}{x_m^{(k)}} \right| \qquad \varepsilon_{\text{rel,f}}^{(k)} = \left| \frac{f(x_m^{(k)}) - f(x_m^{(k-1)})}{f(x_m^{(k)})} \right|$$

Question 2 [1]

1. Derive a $g(x) = x$ function to use in the fixed-point algorithm.
2. Show the first 3 iterations of using the fixed-point algorithm, starting with an initial guess of $T = 380$ K.
3. Will the fixed-point method converge for this problem, using your $g(x)$?

Question 3 [1]

1. Write the Newton-Raphson iteration formula that you would use to solve this nonlinear equation.
2. Apply 3 iterations of this formula, also starting from $T = 380$ K, and calculate the error tolerances.

Question 4 [1]

Comment on the 3 approaches used so far. Are your calculations what you would expect from each method?

Bonus question [1]

A naive code for the bisection algorithm would evaluate the function $f(x)$ at the three points, $[x_\ell, x_m, x_u]$ in every iteration. Fewer function evaluations can be obtained though.

Write a function, in either MATLAB or Python, that implements the bisection method, that evaluates $f(x)$ as few times as possible. You should report the following 8 outputs in each iteration: $[x_\ell^{(k)}, x_m^{(k)}, x_u^{(k)}, f(x_\ell^{(k)}), f(x_m^{(k)}), f(x_u^{(k)}), \varepsilon_{\text{rel,x}}^{(k)}, \varepsilon_{\text{rel,f}}^{(k)}]$.

Use this code to find the solution to the above problem, within a tolerance of $\sqrt{\text{eps}}$ based on $\varepsilon_{\text{rel,x}}^{(k)}$.

END