CHE290 Programming for CHEs – Winter 2024
Homework 2
Due Monday, February 10, 2025

Instructions:

- Download the starter files.
- Put your name in the doc-strings next to "YOUR NAME: ".
- Use this document and the provided doc-strings to complete the problems. Each problem is contained in its own file.
- Upload all 3 files after you have completed the assignment. DO NOT change the file names.
- The work you submit must be your own. You must only use concepts and syntax that have been explicitly covered in this course. Any use of syntax that has not been introduced in this course will be considered academic misconduct because the assumption is that the submitted work is not your own.

Problem Statements:

1. Complete and submit `05_practice_problem_2` from Day 15.

2. The following gas-phase reaction occurs in a plug flow reactor:

$$A + B \rightarrow C$$

where the reaction rate is given by:

$$r = kC_A C_B$$

and the rate constant is given by:

$$k = 5\exp\left(-\frac{1800\ \text{K}}{T}\right)[=]\frac{\text{L}}{\text{mol}\cdot\text{s}}$$

The feed is 25% B, 50% A, and 25% inerts. The process is isothermal at 445 K and isobaric at 1.25 atm.

(see the next page for the additional information needed to solve this problem)

The following are the governing equations for this problem:

- $\dfrac{dX}{d\tau} = \dfrac{kC_A C_B}{C_{B0}}$

- $C_A = \dfrac{C_{A0} - C_{B0}X}{1+\delta X}$

- $C_B = \dfrac{C_{B0}\left(1-X\right)}{1+\delta X}$

where $\delta = -0.25$ and the initial concentrations are determined from the ideal gas law $\left(R = 0.08206 \dfrac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}\right)$.

Complete the file `02_variable_density_PFR` using these equations to complete the TODOs. A figure is included in the download for comparison.

3. The differential equation that describes the temperature distribution (i.e., $T(x)$) in a solid material that is generating thermal energy is:

$$\frac{d^2T}{dx^2} = -a$$

where a is a constant value that accounts for the material properties. We can use the following initial values to solve this equation:

$$T\left(0\right) = T_{\max} \qquad \text{and} \qquad T'\left(0\right) = 0$$

The analytical solution to this equation is:

$$T = -\frac{a}{2}x^2 + T_{\max}$$

Complete the file `03_heat_generation` using these equations to complete the TODOs.

4. The amount of work per mole (W/n) needed to compress a gas isothermally can be determined by:

$$\frac{W}{n} = -\int_{\underline{V}_i}^{\underline{V}_f} P d\underline{V}$$

The pressure-volume relationship for real gases (i.e., those that do not behave according to the ideal gas law) can be described by the Peng-Robinson equation of state. The Peng-Robinson equation of state takes the form:

$$P = \frac{RT}{\underline{V} - b} - \frac{a}{\underline{V}\left(\underline{V} + b\right) + b\left(\underline{V} - b\right)}$$

The appropriate value for the gas constant is $R = 8.314 \times 10^{-5}$. The units on the result after integration with the provided unit set is $\frac{\text{bar} \cdot \text{m}^3}{\text{mol}}$. You must perform the unit conversion to determine the work in Joules.

Complete the file `04_compression_work` using these equations to complete the TODOs. Test cases are included to check your work.