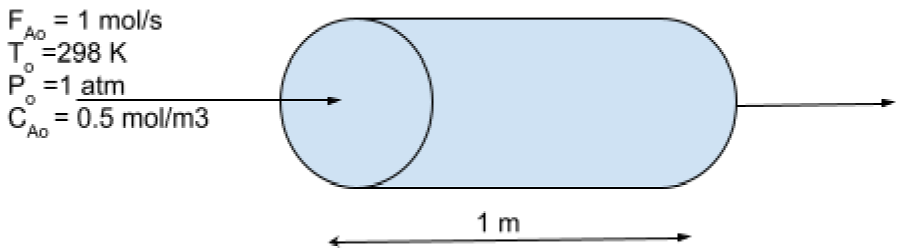
CL 249: Computational Methods Lab
Date: 01/10/24
Assignment 8

The Packed Bed Reactor Problem,



Consider a hypothetical situation in a packed bed flow reactor. Gas A flows through the catalyst bed, and on the surface, the following reaction occurs,

$$A \rightarrow B$$

With rate kinetics given as,

$$r' = -k.C_A$$

You are tasked to find the equilibrium conversion in this problem.
(Every information required to find the Conversion is provided in steps)

1. The initial temperature T_o is 298 K. For this particular reactor, the change in temperature is given by the following equation,

   $$\frac{dT}{dt} = T^3 - 581T^2 - 8870T - 29800$$

   The equilibrium is reached when the temperature reaches a **steady state** value. **Find the final equilibrium temperature (T)**.

2. The initial Pressure P_o is 1 atm. The pressure drop in the packed bed reactor follows the **Ergun equation**, which is a function of the density of the gas. For simplicity, the equation is modified to the following equation: **ΔP = (P_o - P)**

   $$\frac{\Delta P}{\Delta L} = A.\rho + B\rho^2 + C\rho^{-2} + D\rho^{-1}$$

   Where ρ is density equal to 0.8 kg/m^3
   And x = [A, B, C, and D] are constants that act as solutions of the following matrix.
   Mx =Y
   M = $\begin{vmatrix} 1 & 4 & 2 & 3 \\ 0 & 1 & 4 & 4 \\ -1 & 0 & 1 & 0 \\ 2 & 0 & 4 & 1 \end{vmatrix}$ Y = [1 2 3 4]^T

   Find the final pressure(P) at the reactor outlet. You can consider delta l to be 1 and units of pressure to be in atm.

3. There is one more factor, epsilon, ε, (unitless), which is related to the porosity of the bed. Now, you are given an equation that relates the epsilon with the length.

$$\boldsymbol{\varepsilon} = \int_{0}^{1} a.\,dl$$

For given various values for l and corresponding 'a' values. **Calculate the value of ε**

l (m)	0.1	0.2	0.3	0.6	0.9	1
a	4	1	4	0.5	1	3

4. Arrhenius's equation describes the Rate constant, but instead, you are given the rate constants at some of the temperatures:

T (K)	400	450	500	550	600	650
K (1/s)	0.1	3.2	10.4	20.8	25.5	32.3

Find the Rate constant (k) at equilibrium temperature (T).

5. Now, we come to the most important step:
The design equation of PBR is given as

$$\frac{dF_A}{dW} = r'$$

Where W is the weight of the catalyst bed in kg
Which, on further simplification, takes the form

$$F_{Ao}\frac{dx}{dW} = \left(\frac{W}{(1+W^2)^2}\right)\left[kC_{Ao}\boldsymbol{\varepsilon}(1 - x)\left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)\right]$$

Solve the differential equation and find the following**:**
(take the initial condition as x(0) = 0 and a step size 0.2)
   a. Plot the solution (Conversion vs Weight of catalyst)
   b. Find the equilibrium conversion
   c. The corresponding maximum efficient catalyst loading in the reactor and
   d. Write the pseudo-code for the 5th part of your submission.

6. Bonus: prove that the equilibrium conversion is reached.

— END of Problem Statement —

Write your answers here.

Conversion = ________________________

Weight of the Catalyst bed (kg) =_________________________