Assignment 9

Q1. A chemical reaction takes place in a long cylindrical reactor. Heat is generated by the exothermic reaction and is dissipated through the reactor walls. The steady-state temperature distribution, $T(x)$, along the length of the reactor can be modeled by the following non-linear second-order differential equation:

$$\frac{d^2T}{dx^2} + \frac{Q}{k}(T^3 - T_a) = 0, \forall\, x \in [0, L]$$

where:

- $T(x)$ is the temperature along the reactor
- Q is the heat generation term
- k is the thermal conductivity of the reactor wall
- T_a is the ambient temperature outside the reactor
- L is the length of the reactor

Boundary conditions:

- $T(0) = 600$ K, the temperature at the inlet of the reactor,
- $T(L) = 400$ K, the temperature at the outlet.

Given parameters:

- $L = 10$ m,
- $Q = 2 \times 10^5\ \mathrm{W/m^3}$,
- $k = 50\ \mathrm{W/m \cdot K}$

Task:

1. Discretize the domain into $N + 1$ points and set up the finite difference approximation for the above equation.
2. Use an **iterative method** to solve the non-linear system of equations.
3. Implement a **Python program** to compute the temperature distribution along the length of the reactor.
4. Plot the temperature profile along the length of the reactor.
5. **Determine the temperature at $x = 7$ m.** Extract and report this value in your solution.

Q2. A catalyst pellet is modelled as a spherical shell where a chemical reaction occurs. The steady-state concentration profile, $C(r)$, of the reactant inside the pellet is governed by the following diffusion-reaction equation:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC}{dr}\right) = -kC^n, \forall\, r \in [r_0, r_1]$$

where:

- $C(r)$ is the concentration of the reactant inside the pellet
- k is the reaction rate constant
- n is the reaction order
- r_0 and r_1 are the inner and outer radii of the pellet respectively.

Boundary conditions:

- At the surface $r = r_1 (= 1 \text{ m})$, $C(r_1) = C_s (= 0.1 \text{ mol/m}^3)$ the concentration at the surface
- At the center of the pellet $r = r_1 (= 0 \text{ m})$, symmetry requires $\frac{dC}{dr}(r_0) = 0$

Given parameters:

- $k = 0.5 \text{ mol/m}^3$ and $n = 2$ (second-order reaction).

Task:

1. Use the shooting method to solve for the concentration profile $C(r)$ inside the pellet.
2. Implement a Python program to solve the system.
3. Plot the concentration profile $C(r)$ inside the catalyst pellet.
4. **Determine the concentration at $r = 0.5$ m.** Extract and report this value in your solution.