Mathematical Methods in Chemical Engineering
CHE 5355/PETE 5355
Fall 2022

Project #1
Due: Friday, 12/16/2022

Three-Member Team Project

1. Select from an appropriate journal an ordinary differential equation representing a boundary-value problem (ODE-BVP) or a set ordinary differential equations representing an initial-value problem (ODE-IVP). The article selected should pertain to a phenomenon in chemical or petroleum engineering and should be published within the last ten years. Include reference(s).

2. Clearly indicate the physical phenomena examined/model assumptions. How was the model equation(s) derived?

3. List the ODE(s) and boundary condition(s).

4. Clearly list and define all variables (what do they mean physically).

5. Completely classify the model equation and boundary conditions. Write NA if a given classification is inappropriate.

    a. Dependent and Independent Variables
    b. Linear or Nonlinear
    c. Homogenous or Non-homogenous
    d. Order
    e. Steady State or Non-Steady State
    f. Deterministic or Probabilistic
    g. Microscopic, Multiple Gradient, Maximum Gradient, or Macroscopic and Why
    h. Boundary Conditions:
        - Robin, Cauchy, Dirichlet, or Neumann
        - Linear or Nonlinear
        - Homogenous or Non-homogenous

6. Write the ODE(s) in non-dimensional form. If already in non-dimensional form, write the original dimensional ODE(s).

7. Solve the ODE(s) with the following ODE-IVP methods: Euler, Runge-Kutta 4^{th} order, and Adams 2^{nd} order closed formula or ODE-BVP methods: Matrix, Shooting, and Successive Over-relaxation (SOR). Compare the benefits/disadvantages of each method.

8. What is an appropriate step size/interval size for the solution methods? Compare the effect of step size/interval size on the solution. Relate to the Stability and Accuracy of the Numerical Methods with the ODE(s).

9. Determine the analytical solution to the ODE(s) and compare to the numerical solutions. If no analytical solution exists, describe why.

10. Compare the modeling results to experimental data and describe how the experimental data was obtained. If no experimental data exists, describe the type of experiment(s) that would be used to obtain data.

* You may use any available software, algorithms, subroutines, etc.

For the Progress **Memo due on October 29**, write a brief memo (2–4 pages) describing the completion of the **first six items listed above**. Include any calculations/ derivations in attachments.

For the Final Report due on December 14, prepare a written report in journal style format describing all of the required items for the modeling project (see attached guidelines).

Group Project Grade Distribution:

Progress Memo:	10%
Final Report:	
Technical	70%
Communication:	20%
Total	**100%**