Final Term Project Report

Kinetic Modelling and Optimisation of Series Reactions.

Group 7

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Introduction

Our project emphasises on the kinetic modeling and optimization of a series reaction comprising two consecutive steps (A → B → C) and an additional parallel step (B → D). Kinetic modeling is a very powerful tool used in chemical engineering which plays a fundamental role in understanding and optimizing chemical reactions.

By mathematically describing the rate of reaction and concentrations of species over time. kinetic models provide insights into reaction mechanisms and enable prediction of reaction behavior under various conditions and design efficient chemical processes.

From this project we aim to estimate the solution to this kinetic system by solving a set of ordinary differential equations that regulates the rate of change of reactants and products involved in the given series reaction. The ODEs provide a mathematical representation of the reaction kinetics, by allowing us to measure the variations of concentrations of species A, B, C, and D as a function of time.

Problem Statement :

Determine the solution to the kinetic system :

- $A \longrightarrow B \longrightarrow C$
- $B \longrightarrow D$

where the reaction rates are k_1, k_2, and k_3 (in the order written here).The corresponding ODEs that you need to solve are :

- $\mathrm{dA/dt} = -k_1 A$; $\mathrm{dB/dt} = k_1 A - k_2 B - k_3 B$; $\mathrm{dC/dt} = k_2 B$; $\mathrm{dD/dt} = k_3 B$

Initial Conditions : $A(t = 0) = A_0$; $B(t = 0) = 0$; C(t=0) = 0; D(t=0) = 0;

1) Write a MATLAB program that plots the solution up to $t = 10$ for $k_1 = 2$, $k_2 = 0.5$, $k_3 = 0.3$, and $A_0 = 1$.

2) Now write a MATLAB program that use methods to solve the system.

3) Pick a time step so that the solution is stable and the error is small. Our program should plot the numerical solution and the analytical result together.

Results

Explicit Euler's Method :

- This is the simplest numerical approximation method for IVPs, in which we approximate the derivative with a forward finite difference. This method calculates the next point in the solution by taking a small step (h) in the direction of the derivative at the current point, using this algorithm : $y_{i+1} = y_i + \mathrm{hf}(x_i, y_i)$.
- Here, we choose h=0.1 initially for better approximation of solution. After that we increment the value of h by 0.1 and find out the value of $h_c = 0.4$ above which the numerial instability occurs.
- This method has a local truncation error of $\sim \mathbf{O}(h^2)$.

Implicit Euler's Method :

- This is the numerical approximation method for IVPs , in which we approximate the derivative with a backward finite difference. This method uses this algorithm
  : $y_{i+1} = y_i + \mathrm{hf}(x_{i+1}, y_{i+1})$.
- y_{i+1} cannot be calculated analytically (explicitly). So we have made the residual's equation given by : $\mathrm{R}(y_{i+1}) = y_{i+1}$ - y_i - $\mathrm{hf}(x_{i+1}, y_{i+1}) = 0$
- We have aplplied an iterative numerical method **Newton Raphson Method** which require the calculation of the Jacobian matrix. The Jacobian matrix, denoted as J, is defined as the matrix of partial derivatives of the residual function with respect to the components of y_{i+1}. So basically this iterative process is performed using Jacobian and Residual at each time step to obtain the solution at the next time step.
- Here, we choose h=0.1 initially for better approximation of solution.After that we increment the value of h by 0.1 and find out the value of hc=0.4 above which the numerial instability occurs.
- This method has a local truncation error of $\sim \mathbf{O}(h^2)$**.**

Runge-Kutta 4 Method :

- The RK-4 method is a higher-order method that provides improved accuracy compared to the Euler methods.
- It is a widely used numerical analysis method that involves four stages of calculation to approximate the solution at the next point. The method calculates four intermediate slopes (k_1, k_2, k_3, k_4) using derivatives at different points within the time interval 0 to 10 sec and then combines them to obtain the next point in the solution using algorithm mentioned below.

- $y_{i+1} = y_i + (\mathrm{h}/6)*(k_1 + 2k_2 + 2k_3 + k_4)$, where
  $k_1 = \mathrm{f}(x_i, y_i)$;
  $k_2 = \mathrm{f}(x_i + h/2, y_i + k_1 h/2)$;
  $k_3 = \mathrm{f}(x_i + h/2, y_i + k_2 h/2)$;
  $k_4 = \mathrm{f}(x_i + \mathrm{h}, y_i + k_3 \mathrm{h})$;
- Here, we again choose h = 0.1 initially for better approximation of solution. After that we increment the value of h by 0.1 and find out the value of h_c = 0.4 above which the numerial instability occurs.
- The RK-4 method has a local truncation error of $\sim \mathbf{O}(h^5)$

Plot Explanation :
A is exponentially decreasing from initial time to final time.
B is increasing till 0.7 secs and decreasing till 10 secs.
C is increasing till 4.5 secs and then almost constant till 10 secs.
D is increasing till 3.2 secs and then almost constant till 10 secs.

Conclusion

- During working on this project we have applied three methods (**Explicit Euler's**, **Implicit Euler's** and **RK-4 method**) in MATLAB to solve the ordinary differential equations that governs the rate of change of reactants and products involved in the given problem statement.
- We have matched the solutions obtained by the above mentioned methods analytically with the help of **ode45 method** to check the closeness of solutions with the accurate one.
- We came to conclusion that **RK-4** is more accurate than **Explicit Euler's method** and **Implicit Euler Method** as it involves multiple calculations of derivatives at different concentrations within each time step.
- One common thing for all the methods is choosing of step size(h). Accuracy is ***inversely proportional*** to step size which means that smaller step sizes will give more accurate solution.
- **Implicit euler's method** is unconditionally stable, while **Explicit euler's method** and **RK-4 method** is conditionally stable.
- Overall we conclude that kinetic modeling and optimization of series reactions contribute to improved process efficiency, product quality, and safety in chemical engineering .This helps engineers in making informed decisions regarding reactor design, operating conditions, leading to cost-effective and sustainable chemical processes.