A Comparison of Numerical Solutions to a Chemical Kinetic Model

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Abstract

In this project, we'll use computational methods to study hypothetical biomolecular reaction kinetics. The concentrations of five chemicals are modeled by a system of five coupled differential equations. It is important for any physical system to be simulated as accurately as possible. We will compare the numerical solution of the system using Euler's Method and the Runge-Kutta methods of orders two and four.

Introduction

Most physical processes are modeled by coupled differential equations. To see the outcome of the process, we need to simulate the mathematical model as accurately as possible. There are always errors in the simulation of any mathematical model due to the machine limitations. These are known as round-off errors and one cannot avoid round-off errors. We can delay the propagation of round-off error by choosing any efficient numerical algorithm. In this project, we simulate the following mathematical model using three algorithms.

Numerical Methods Used

Coupled Differential Equations:

$$\frac{dC_A}{dt} = -r_1 - r_2 = -K_1 C_A C_B - K_2 C_A C_C$$

$$\frac{dC_B}{dt} = -r_1 = -K_1 C_A C_B$$

$$\frac{dC_C}{dt} = r_1 - r_2 = K_1 C_A C_B - K_2 C_A C_C$$

$$\frac{dC_D}{dt} = r_1 = K_1 C_A C_B$$

$$\frac{dC_E}{dt} = r_2 = K_2 C_A C_C$$

Euler's Method:

$$y_{i+1} = y_i + hf(t_i, y_i)$$

Runge-Kutta Order 2:

$$y_{i+1} = y_i + \frac{h}{2}(k_1 + k_2)$$

$$k_1 = f(t_i, y_i)$$

$$k_2 = f(t_i + h, y_i + hk_1)$$

Runge-Kutta Order 4:

$$y_{i+1} = y_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = f(t_i, y_i)$$

$$k_2 = f(t_i + \frac{h}{2}, y_i + \frac{h}{2}k_1)$$

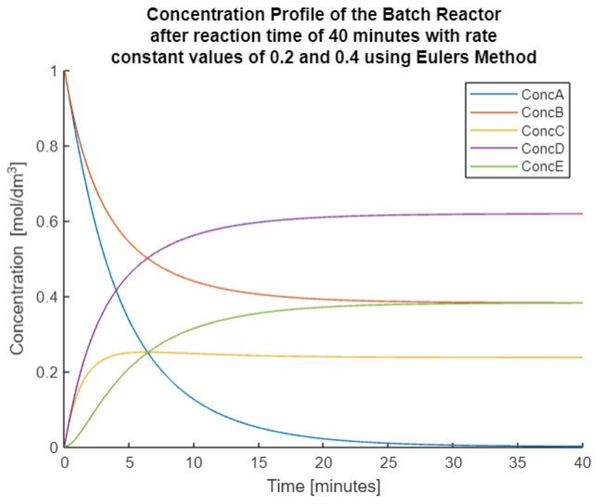
$$k_3 = f(t_i + \frac{h}{2}, y_i + \frac{h}{2}k_2)$$

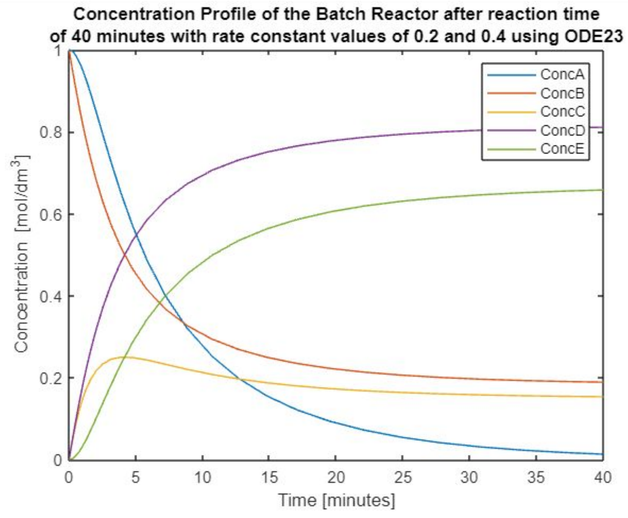
$$k_4 = f(t_i + h, y_i + hk_3)$$

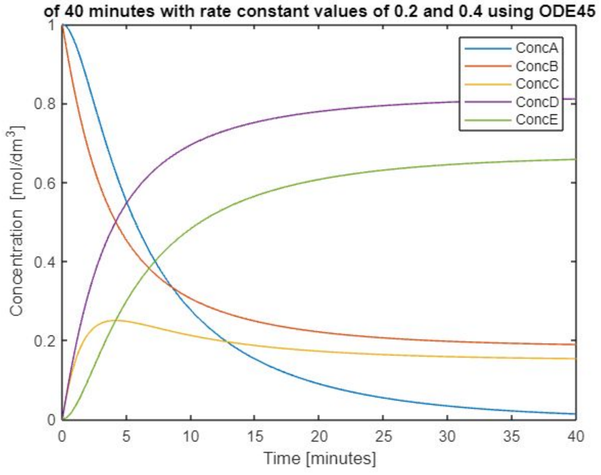
Methodology

The Chemical Kinetic model was simulated using three methods: Euler's Method and the Runge-Kutta methods of orders two and four. In addition to using the built-in MATLAB functions (ODE23, ODE45) for the Runge-Kutta methods of order two and four, a user defined function for Euler's Method will be used to calculate solutions for the five hypothetical coupled differential equations to the Chemical Kinetic model. Four live scripts and three functions were created. The three functions each corresponded to different k-values utilized in both ODE23 and ODE45. Utilizing the built-in MATLAB functions (ODE23, ODE45), separate files were created for each method of approximation. The third live script was a custom code for Euler's Method approximation. The main file graphed and compared the results of each method of approximation (Each method had the same defined step size to ensure comparable results). Each different concentration species at each k-value were graphed against each other to visibly display the differences and a table was created to define the error in five-minute intervals from 0 – 40 minutes.

Results







Conclusion

As seen in the models produced by Euler's Method, ODE23, and ODE45, the method which most accurately depicted the chemical reaction is ODE45. With a step size of 0.04, ODE45 simulates the most accurate model of this biomolecular chemical reaction.a

References

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