Project Overview

ESC 113 TERM PROJECT BY GROUP 3

Term Project ESC 113

Team Participants.

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We have analyzed the decomposition reaction of hydrogen peroxide H2O2 by stimulating the reaction at a fixed temperature. We determined the concentration of reactants and product species with respect to time by solving ODE IVP using Euler's method and the Range-Kutta method. The reaction got analysed for 40 seconds and we plotted concentration vs time plot for reaction species. We observed minor differences in results provided by both of these methods. The problem statement and analysis of the project are as follows.

PROBLEM:- The decomposition of hydrogen peroxide is represented by the equation:
$2H_2O_2 \rightarrow 2H_2O + O_2$.
The reaction follows first-order kinetics with a rate constant of **k.** Simulate the decomposition reaction **using Euler's method or Runge-Kutta** with a **time step size of dt = 0.01 s**, starting from an **initial concentration of 2.0 M of hydrogen peroxide** (H2O2). Perform the simulation for a total time of 40 seconds. **Calculate the value of k from the given data(** Ea=75000 J/mol ,A=1.2*(10^11)sec^-1, R=8.314J/mol) **at T = 333K**
Write a MATLAB script to simulate and **plot the concentration of the product as well as the reactant over time** using Euler's method / Runge-Kutta at T = 333K

- ## Balanced Reaction

Hydrogen peroxide decomposes to form water and oxygen

$$2\,H_2O_2 \longrightarrow 2\,H_2O + O_2$$

The rate of decomposition increases with rise in temperature

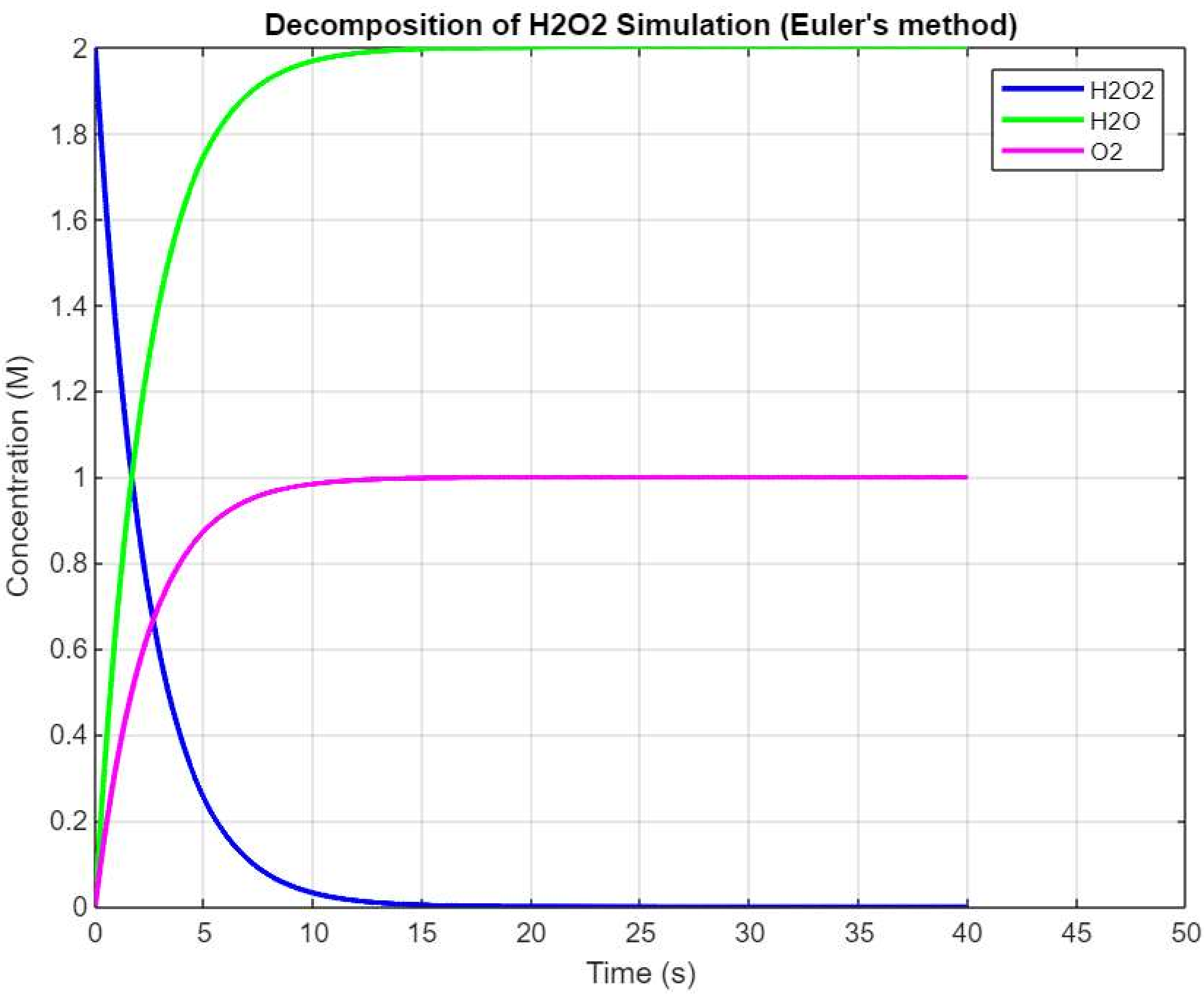
For analysis since we know that rate constant k is temperature dependent and we can find it through Arrhenius equation.

We will use k = 0.2072 s^-1 for our simulation which is at 333 K.

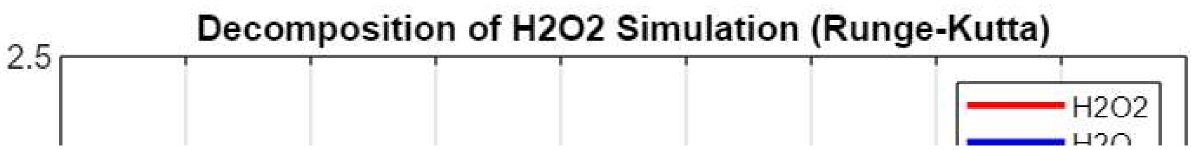
RESULTS

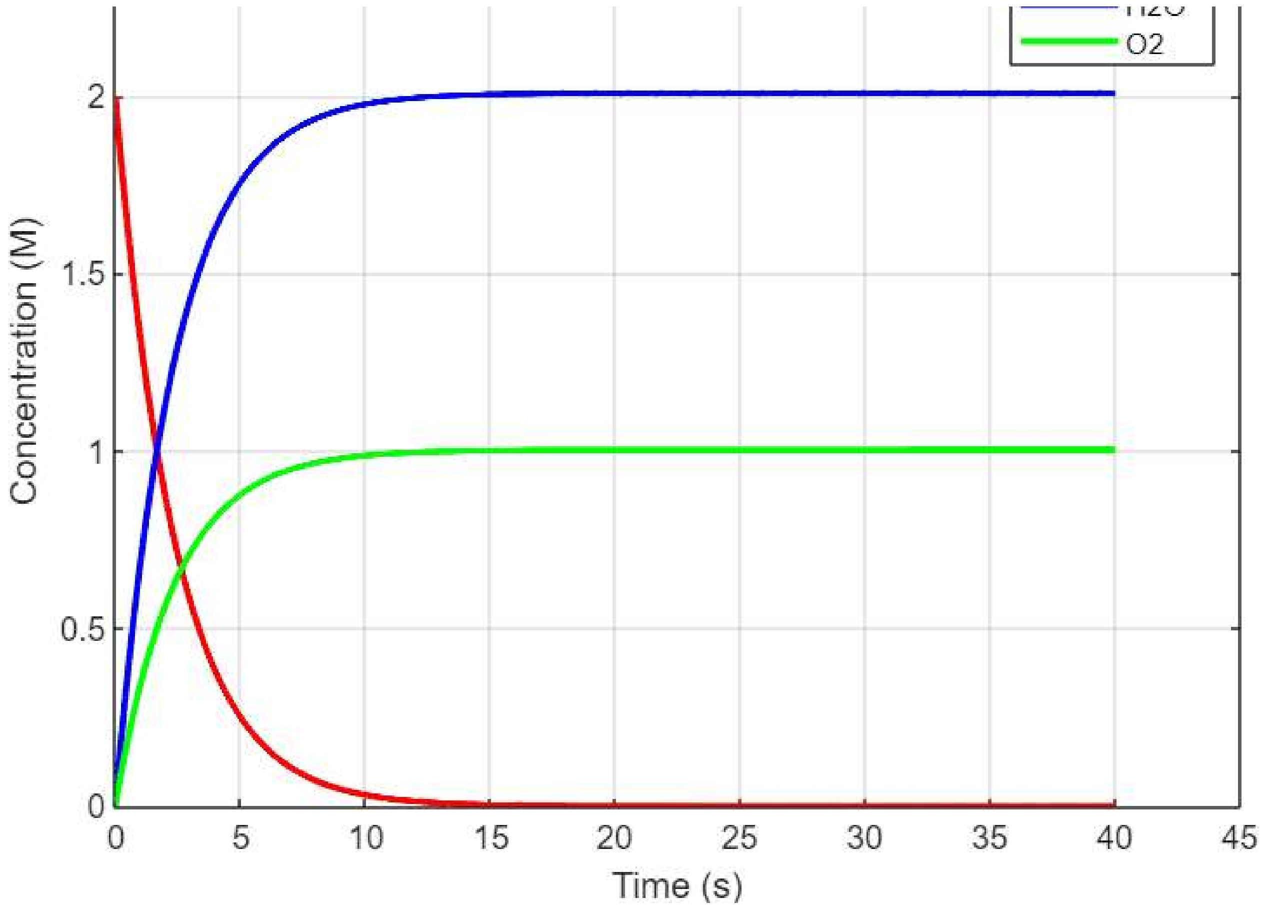
On performing the stimulation in matlab script we got following results.

Plot by Euler's method



Plot by Runge-Kutta method





Conclusion and review on usage of numerical methods.

- **Accuracy**: For complex systems or when the time step size is rather large, the Runge-Kutta approach that we employed is typically more accurate than Euler's method. Results are more accurate since more intermediate steps are taken into account during the calculation.
- **Efficiency**: When compared to the Runge-Kutta method, the Euler's method requires fewer computations. It is more effective for straightforward systems or when the time step size is minimal because it necessitates fewer calculations each time step.
- **Stability:** Euler's approach is less stable than the Runge-Kutta method in terms of stability. For some systems with huge time step sizes, the Euler's approach can display numerical instability, producing unreliable or oscillatory results. The Runge-Kutta approach is more reliable and less vulnerable to problems like these.
- **Implementation difficulty**: Since Euler's approach just requires a simple updating formula, it is simple to put into practice. The Runge-Kutta method is slightly more difficult to implement since it includes more computations and many steps..
- In our case, the time step size was 0.01 seconds, and the time period was 40 seconds, giving us a total of 4000 iterations for our display and analysis. As a result, both of our graphs are extremely accurate and show very small changes. We obtained virtually correct graphs for the reaction of H_2O_2 decomposing into H_2O and O_2 by using both approaches as the number of iterations per time period increased.

Thanking You

TEAM 3, ESC 113 TERM PROJECT 2022-2023

MATLAB