ESC113 Group 9

Formation of NO_2F

Simulating the stages that contribute to the production of NO_2F, its concentration as time goes by, the impact of other chemicals, and the graphical representation of the reaction using the MATLAB software

Team

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Introduction

Nitryl Fluoride (NO_2F) is a strong oxidizing agent that is used as a fluorinating agent and has been considered as an oxidizer in rocket propellants. Nitryl fluoride can be used to prepare organic nitro compounds and nitrate esters as well. Therefore, it is crucial to examine how it is produced and how its concentration changes with time.

The overall reaction looks like:

$$\mathbf{F_2 + 2NO_2 \rightarrow 2NO_2F}$$

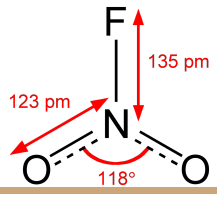
The mechanism involves the following two steps:

Step 1 - $\mathbf{F_2 + 2NO_2 \rightarrow NO_2F + F + NO_2}$ (Rate constant k_1)

Step2 - $\mathbf{F + NO_2 \rightarrow NO_2F}$ (Rate constant k_2)

Any process that breaks the strong F-F bond is likely to be rate limiting, and the atomic fluorines that follow will react with other odd-electron species rapidly. So, Step 1 will have a smaller value of the rate constant compared to Step 2, which is comparatively faster.

Structure of NO_2F →



Problem Statement

$$\textbf{Rate (1)} = k_1 [F_2] ([NO_2])^2$$

$$\textbf{Rate (2)} = k_2 [F] [NO_2]$$

$$-d[F_2]/dt = k_1 [F_2] ([NO_2])^2$$

$$d[F]/dt = k_1 [F_2] ([NO_2])^2 - k_2 [F] [NO_2]$$

$$d[NO_2F]/dt = k_1 [F_2] ([NO_2])^2 + k_2 [F] [NO_2]$$

The initial condition for the concentration of F_2 is a_0 and concentration of NO_2 is b_0 throughout the reaction

To analyze the precision and computation complexity of the Problem Statement, we will be deploying the Explicit Euler's as well as the Runge-Kutta (Order 4) Methods.

Solution

Parameters

The simulation parameters provided are as follows:
Initial NO_2 concentration = 1 M
Initial F_2 concentration = 1 M
Initial NO_2F concentration: 0 M
k_1 = 38 dm^(3)mol^(-1)s^(-1) at T = 300K
k_2 = 400 dm^3()mol^(-1)s^(-1) at T = 300K
These parameters are used in the simulation code to calculate the changes in F_2 and NO_2F concentrations over time.

Simulation time and time step

- Total simulation time = 0.2 seconds
- Time step = 0.0001 second
- Number of time steps = 2000

These values specify the simulation's time frame and the level of detail at which the concentrations are updated.

Numerical Methods

The simulation of NO_2F production is carried out within this section of the code. The changes in F_2 and NO_2F concentrations at each time step are calculated iteratively over the time steps.

- Arrays are initialized and initial conditions are set for time zero
- The rates of change for F_2 and NO_2F concentrations are computed based on the specific growth rates and the given equations.
- The Explicit Euler and Runge-Kutta (Order 4) algorithms are implemented for the specific growth rates.

[Explicit Euler : Using Euler's method, which multiplies the rates of change by the time step and adds them to the concentrations at the previous time step, the concentrations at the current time step (i) are updated.]

[Runge-Kutta (Order 4) : $y_{i+1} = y_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$

This particular approach strikes a good balance between the quantity of functional evaluations and the overall accuracy, which is O(h^4), and is very effective. This particular fourth-order Runge-Kutta method is commonly referred to as "RK4".]

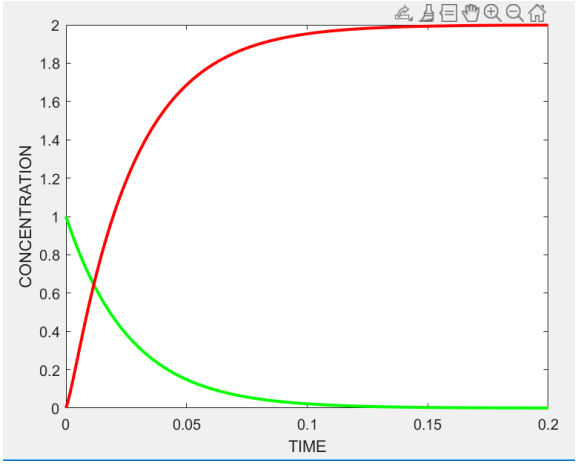
- By iterating over the time steps and updating the concentrations using the specific growth rate and rate equations, the simulation calculates the changes in F_2 and NO_2F concentrations over time.

Plot the concentrations

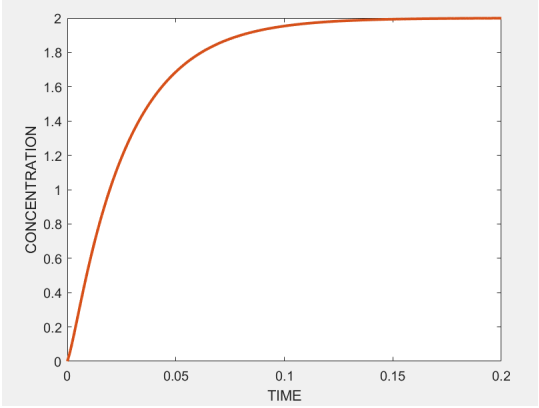
The plot function is used to visualize the concentrations over time.

- The concentrations of F_2 and NO_2F are plotted on the same graph using the 'plot' function. The time values are plotted on the x-axis, and the corresponding Concentration values are plotted on the y-axis. The concentration values are represented by different colors to distinguish them.

The plot for concentration of NO_2F and F_2 vs time looks like this -



Where concentration of NO_2F is denoted in red which is shown to increase by both the algorithms we have used and concentration of F_2 is denoted by green color.
The plot for concentration of NO_2F by both methods looks like this -



The graph for both the methods overlap each other showing the accuracy of the time step as well as the algorithm chosen

Conclusion

In conclusion, this study investigated the formation and concentration of NO_2F over time, specifically examining the reaction between NO_2 and F_2. The main focus was to analyze the numerical aspects of the simulation using Explicit Euler's method and the Runge-Kutta 4

algorithm. Throughout the investigation, both numerical methods proved to be effective in approximating the concentration of NO_2F at different time intervals. However, several key observations emerged when comparing their performances.

Explicit Euler's method, although straightforward and computationally efficient, exhibited some limitations when applied to this system. It demonstrated a tendency for significant numerical errors and inaccuracies, especially when the time step was large. This resulted in a less precise estimation of NO_2F concentrations, particularly over extended time periods.

On the other hand, the Runge-Kutta 4 algorithm, renowned for its accuracy and stability, showcased superior performance in this study. By employing a more sophisticated approach that involved evaluating multiple intermediate steps, it provided more precise approximations of the NO_2F concentrations. It is worth noting that while the Runge-Kutta 4 algorithm demonstrated superior performance, it also incurred higher computational costs compared to the Explicit Euler's method.

In conclusion, this study sheds light on the formation and concentration of NO_2F over time, emphasizing the numerical aspects of the simulation process. The comparison between Explicit Euler's method and the Runge-Kutta 4 algorithm highlighted the importance of accurate and stable numerical methods in obtaining reliable results.