Term Project Report ESC113M
Group-2

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1 Problem Statement

The reaction to produce Nitrogen Dioxide (NO_2) has been well established as a third-order homogeneous reaction. This gas-phase oxidation, has two steps :

$$\mathrm{NO + NO \underset{k_2}{\overset{k_1}{\rightleftharpoons}} (NO)_2}$$

$$\mathrm{(NO)_2 + O_2 \xrightarrow{k_3} 2\,NO_2}$$

This reaction, like most third-order reactions, is not termolecular but rather a combination of an equilibrium followed by a subsequent bimolecular step.

Our objective is to use different computational and numerical methods to solve real life-problems related to the field of Chemical Engineering, and to understand the differences between different computational methods when categorized on the basis of their accuracy and error.

2 The Kinetics

$$\frac{d[NO]}{dt} = -k_1[NO]^2 + k_2[(NO)_2]$$

$$\frac{d[(NO)_2]}{dt} = k_1[NO]^2 - k_2[(NO)_2] - k_3[O_2][(NO)_2]$$

$$\frac{d[O_2]}{dt} = -k_3[(NO)_2]$$

$$\frac{d[NO_2]}{dt} = k_3[(NO)_2][O_2]$$

3 Assumptions

Though the first step of the reaction (Formation of $(NO)_2$) is a very fast process we assume it to be of a significantly observable pace in this hypothetical system to ease our analysis and to achieve a more efficient solution.

The rate constants are taken as,

$$k_1 = 0.1$$
$$k_2 = 0.001$$
$$k_3 = 0.001$$

The initial concentration of the compounds are taken as,

$$[\mathrm{NO}] = 1$$

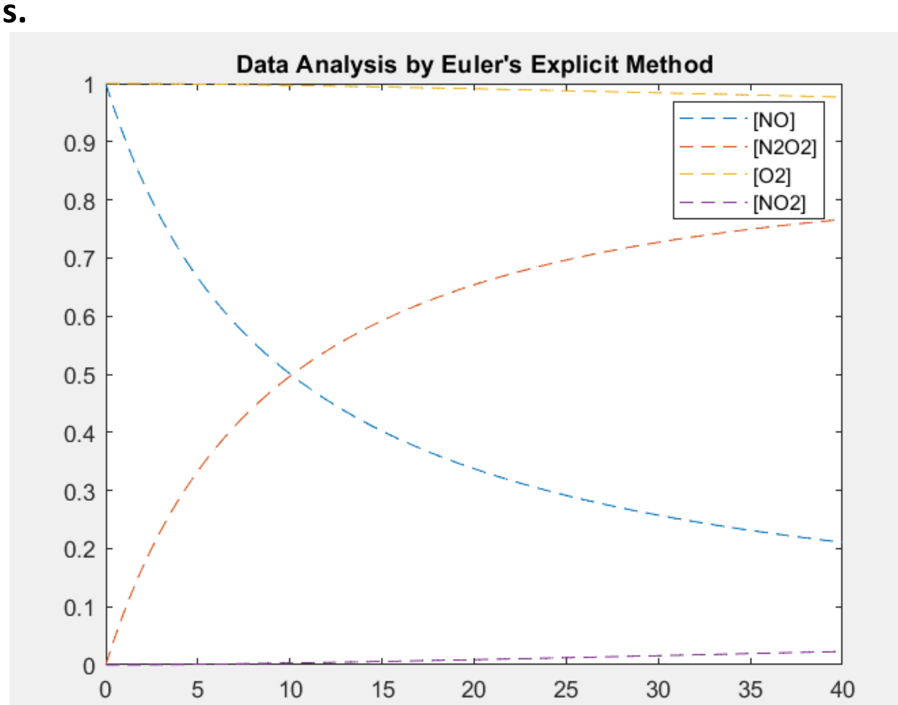
$$[(\mathrm{NO})_2] = 0$$

$$[\mathrm{O_2}] = 1$$

$$[\mathrm{NO_2}] = 0$$

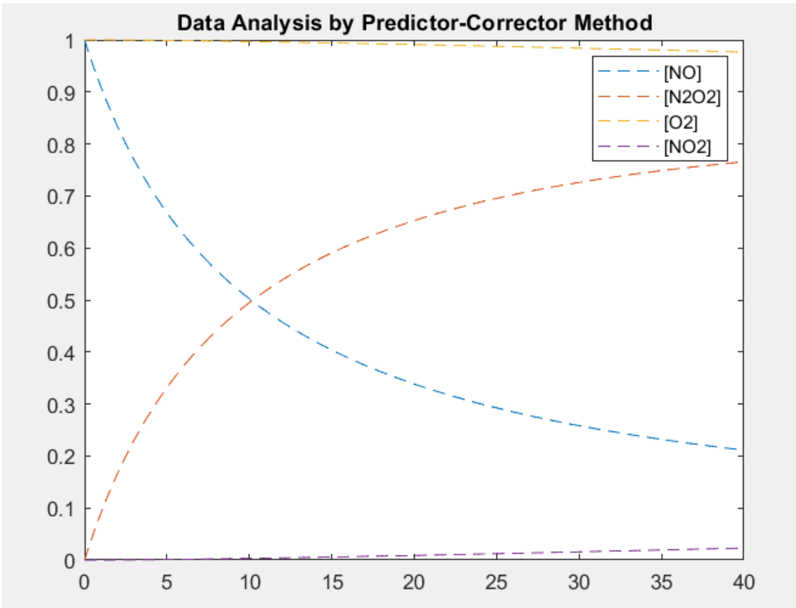
4 Explicit Euler Method.

We assume that the reaction is 40 seconds long and our **step size is 0.1 seconds.**



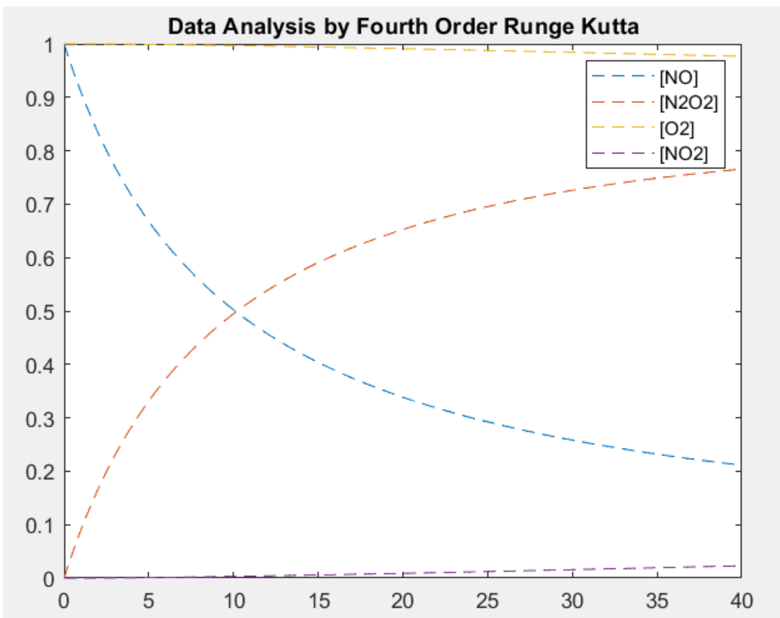
5 Predictor Corrector Method

We assume that the reaction is 40 seconds long and our **step size is 0.1 seconds.**



6 Fourth-Order Runge Kutta Method (RK4)

We assume that the reaction is 40 seconds long and our **step size is 0.1 seconds.**



7 Conclusion

Theoretically, it is mentioned that the ***<u>Fourth-Order Runge Kutta</u>*** Method Than the other two methods. Hence to Check the Accuracy of the other two methods we treated the **Runge Kutta** Method as the most accurate threshold, and in comparison to that we figured out which method was more accurate amongst the rest two we applied.

8 Result

In order to estimate accuracy of the methods we used the approximate time of 10^{th} second of the reaction and created a vector of the concentrations of the components at that time by different methods. And In calculating the error between theses vectors we used the "**computenorm"** function which gave us the following data.

*Error(Concentration(Explicit)-Concentration(RK4))=***<u>0.0010</u>**

Error(Concentration(Predictor-Corrector)-Concentration(RK4))= **<u>5.0454e-06</u>**

Hence In our computational analysis of the three methods we found out that In terms of accuracy:-

<u>Fourth Order Runge Kutta>Predictor-Corrector>Euler's Explicit Method</u>