ESC113 PROJECT

(GROUP-2)

OBJECTIVE -

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.

PROBLEM STATEMENTS -

Nitrogen dioxide (NO_2) is an important atmospheric trace gas that is soluble in water. It has a reddish-brown color and is a strong oxidant. NO_2 is formed through the oxidation of nitric oxide (NO) in combustion processes such as diesel engines and coal, oil, gas, wood, and waste plants. Hence, it is important to analyze the production and behavior of their concentrations with respect to time .

In this project we are going to analyze the production of NO_2 such as its concentration at different times ,effect of other compounds and the graph of the reaction.

And we are going to stimulate the sequential reaction of formation of NO_2 in MATLAB.

$$2NO + O_2 \rightarrow 2NO_2$$

The reaction mechanism is mentioned below -

$$NO + NO \rightleftharpoons N_2O_2$$

(take k1,k2 is rate constant for forward and backward reaction respectively)

$$N_2O_2 + O_2 \rightleftharpoons 2NO_2$$

(take k3,k4 is rate constant for forward and backward reaction respectively)

Rate equations are-

$$d[NO]/dt = k_2[N_2O_2]-k_1[NO]^2$$

$$d[NO_2]/dt = k_3[N_2O_2] -k_4[NO_2]^2$$

(here O_2 is kept at a constant concentration so $[O_2]$ can be taken constant)

$$d[N_2O_2]/dt = -k_2[N_2O_2]+k_1[NO]^2+k_4[NO_2]^2-k_3[N_2O_2]$$

METHOD OF APPROACH -

In this project we shall apply Explicit Euler's method ,Implicit Euler's method and Predictor-Corrector Method and study the accuracy and computation complexity of the above processes through the above Problem Statement.

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