Abstract: A Computational Model Of Chemical Reactions

Authors: Miki Raz, Tomer Vered & Matan Friedenberg Hemda
Correspondent Author: Mr. Shlomo Rozenfeld, Hemda

Keywords: Reaction Rate, Closed System, Plastic Collision, Elastic Collision, Activation Energy, First Order Reaction

.

Introduction

Chemistry is all around us and chemical reactions occur every day in a lot of the processes we see and do on a regular basis. The simulation aims to simulate chemical reactions by using the microscopic properties of chemicals. In our study we tried to find the reaction rate of a certain chemical reaction in order to see if reaction rates can be simulated. We compared the results gained from the simulation to results we obtained from an experiment.

Method

Initially the program generates a closed system with chloride and bromine particles.
After the generation of the closed system the program executes the following steps:

1.The program finds the time of the next particle collision

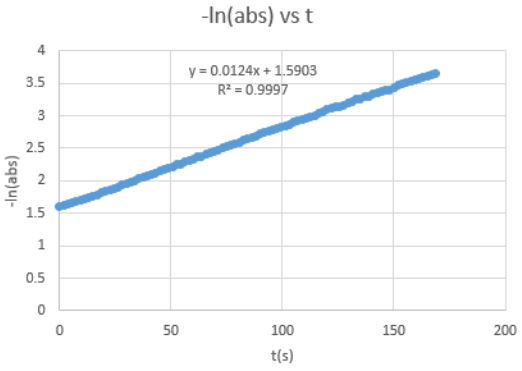
2. It simulates the particles movement until the next collision

3.It checks if a chemical reaction has taken place between the two colliding particles using the particle "type" and the total energy contained in the particles (The program compares the energy to the activation energy of the reaction).

4. if a chemical reaction took place the collision is treated as a plastic collision (And thus energy is removed from the system). If no chemical reaction took place the collision is treated as an elastic collision (Where energy is conserved).

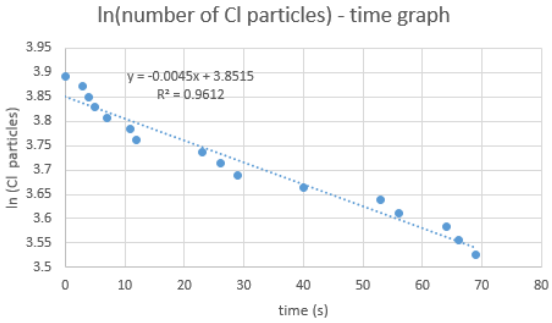
5.The program makes a list that marks the location of all the particles in each given time and it uses the coordinates to generate an animation of the system. In addition, it outputs a graph of the number of particles as a function of time (using some unit of time) and a graph of the natural log of the number of particles as a function of time (Can be used instead of Molar Concentration because the relationship between the two).

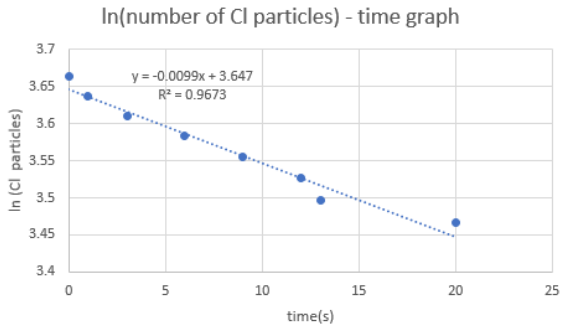
Results



Graphs from simulation

Graph from experiment





The results show that the reaction is a first order reaction.

Conclusion

We've created a model which can simulate the general behavior of a chemical reaction. Despite the limitations of the model, the results show that the reaction rate obtained from the simulation shows that the reaction is a first order reaction in concurrence with our predictions.

Discussion

While the model can simulate the general behavior of a chemical reaction the model makes many unrealistic assumptions about the behavior of particles in the system and does not account for:

1. Angles between the particles during the collision.
2. Intermolecular forces.
3. The rotational and vibrational energy of the particles.
4. States of matter.
5. Chemical Bonds

In summary, while the model was successful in simulating the general reaction rate of a chemical reaction, there are many improvements that can be made to the model.