Simulating the Creation of Kerosene Using Sunlight Water Vapor and Air

New Mexico

Supercomputing Challenge

Final Report

April 5, 2023

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Table of Contents

Executive Summary

Our team's goal is to model and simulate a recently developed method for creating kerosene which involves sunlight, water vapor, and air. An array of solar panels funnel into a solar tower that contains a concentrated amount of water and carbon dioxide, which react to produce hydrocarbon chains, a vital component in kerosene. Modeling this method using solar would require industrial-grade materials and a great deal of chemical engineering experience. Given these hiccups, our team decided to model the chemical process using Python and Pygame to test the efficiency and potential real-world applications of the method. Our code attempted to use the Gillespie Algorithm (a stochastic simulation of stoichiometry problems) to simulate the process, and Pygame helps visualize the reactions taking place. In our progress, the team has learned about solving stoichiometry problems, coding with Numpy for computational problems, and using Pygame and collision for graphics.

Report

The Problem

The constant rise of global emissions is a hazard to the environment and the overall health of the world. Transportation accounts for a large number of emissions, especially the commercial airline businesses and the aviation industry. Most commercial jets utilize kerosene for fuel due to its efficiency, but unfortunately, it is costly and environmentally impactful. Oil is a widely used resource that is only produced by a few major countries. Price changes can affect many industries in good and bad ways. The airfare for an average passenger will only increase every day. Every 10% that gas prices rise, the cost of operating an airline increases by around 3%. According to the US Environmental Protection Agency, 27% of emissions are transportation based, of which around 90% is petroleum [2]. A large amount of the economy is reliant on fossil fuels, which isn't guaranteed to be around in the near future. Other options such as solar, wind, and hydropower are still relatively new. There is a need for a more stable, efficient, and less harmful option that humanity can use while researchers discover more about eco-friendly alternatives.

The Solution

With gas prices increasing each year, an environmentally friendly and cheaper option is necessary to continue the commercial airline industry. Kerosene is typically made with oil and a mixture of petroleum [1]. However, scientists are developing a method to create Kerosene through solar power [4]. The composition of Kerosene

includes hydrocarbons, which can be made through water, sunlight, and carbon dioxide. The components are compressed from a gas into a liquid, creating liquid hydrocarbons, which can be used to make Kerosene more efficiently. The discovery is recent and the chemical process is complicated, which is why it can help to simulate the scientific process.

Progress

Our team initially attempted to use the Gillespie Algorithm, a stochastic chemical simulation [3]. However, we decided to go with a more simple stochastic model. We first started by creating a visualization of our model, however, due to time constraints we eventually decided to further develop our visualization rather than continue with the Gillespie Algorithm. This model is more simple and uses Pygame to simulate molecule collisions. We will use this model to calculate kerosene production.

How It Works

The molecules in the simulation randomly move in a confined space. The molecules are circular objects created in Pygame. The molecules then move by a random increment. If the molecule collides with another molecule and meets certain criteria, we record it as a collision and update our molecule count.

```
def collision(m1: Molecule, m2: Molecule):
    """
    Calculate distance between two molecules.
    (Accounts for each molecule's radius.)
    """
    dist = (m1.x - m2.x)**2 + (m1.y - m2.y)**2
    dist = math.sqrt(dist) - m1.r - m2.r
    return dist <= 0
```

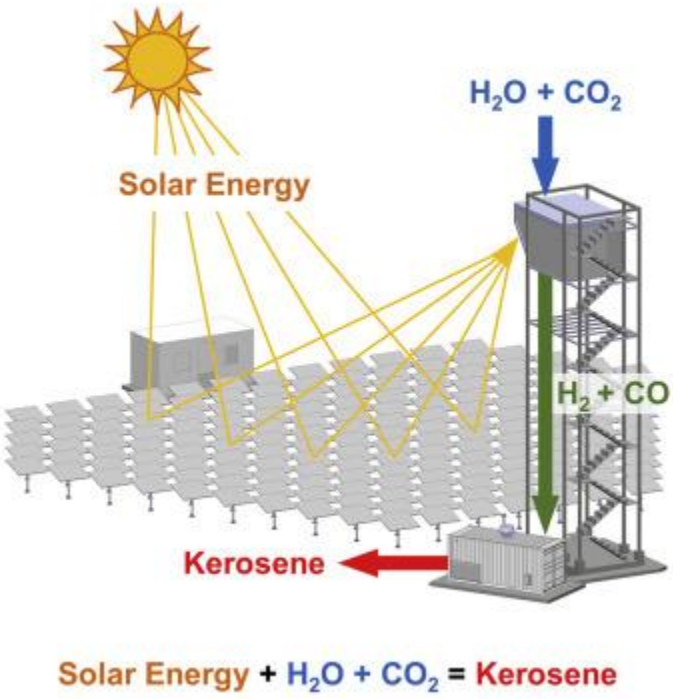
We track these collisions over a set period of time and use the data to determine kerosene products. We insert the H_2O and CO_2 molecules into the following equation to determine the amount of hydrocarbons that can be produced.

$$H_2O + CO_2 \rightarrow H_2 + CO + O_2$$

Future Work

So far we have completed the model and we want to test different types of values for time, molecules speed, reactivity levels, etc. We also want to graph results from multiple different simulations to get a more accurate answer.

Appendices



[5]

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