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Work-in-Progress: Visualizing Bubble Formation on Pt2Al3 Surface during Dibenzyltoluene (DBT) Dehydrogenation

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Abstract

Dibenzyl Toluene (DBT) has emerged as a highly promising Liquid Organic Hydrogen Carrier (LOHC) for efficient hydrogen storage and transfer. The critical role of a catalyst in the DBT dehydrogenation process necessitates studying bubble formation on the catalyst's surface. This research project, conducted by a sophomore undergraduate student under the supervision of an advisor, aims to develop a procedure to simulate bubble formation on the Pt2Al3 catalyst. The project involves designing an experimental setup to visualize bubble formation on the catalyst's surface effectively. Additionally, a custom MATLAB code, utilizing image processing techniques, was developed to measure the total volume of bubbles generated during experiments. Due to the absence of established safety protocols regarding hydrogen use at the author's institution, bubble formation simulations on Pt2Al3 surfaces were performed using water as a safe alternative to DBT. The research successfully visualized bubble formation on the surface of the catalyst, and the custom MATLAB code measured bubble volumes. The promising results obtained with water as a substitute offer a foundation for future research using DBT. Suggestions were made to simplify the procedure to be easily used in lab class settings. It is expected that performing this lab procedure will help students understand that hydrogen is considered a future energy source, as well as its limitations.

1. Introduction

Scientific data has indicated that climate change is ongoing. The average global temperature continues to rise, and sea levels are steadily increasing [1], [2]. Climate change leads to extreme weather events such as flooding, droughts, intense rainfall, and heatwaves [3]. One proposed solution to address this issue is reducing fossil fuel usage. However, implementing such reductions in fossil fuel consumption presents significant challenges in reality. Consequently, there is a need to explore alternative energy sources that are more sustainable. Hydrogen is considered one of the most promising sustainable energy sources. However, its storage and transportation present challenges due to its low density and high diffusivity, requiring a large volume of space. Hydrogen is typically compressed to between 5,000 psi and 10,000 psi for storage in a hydrogen charging station, significantly higher than atmospheric pressure [4]. Another method under consideration is liquefaction, which significantly reduces the volume of hydrogen gas for storage. However, the liquefaction temperature of hydrogen is below -253°C (-423°F), consuming a significant amount of energy [5]. Therefore, alternative methods for storing and transporting hydrogen are being intensively studied.

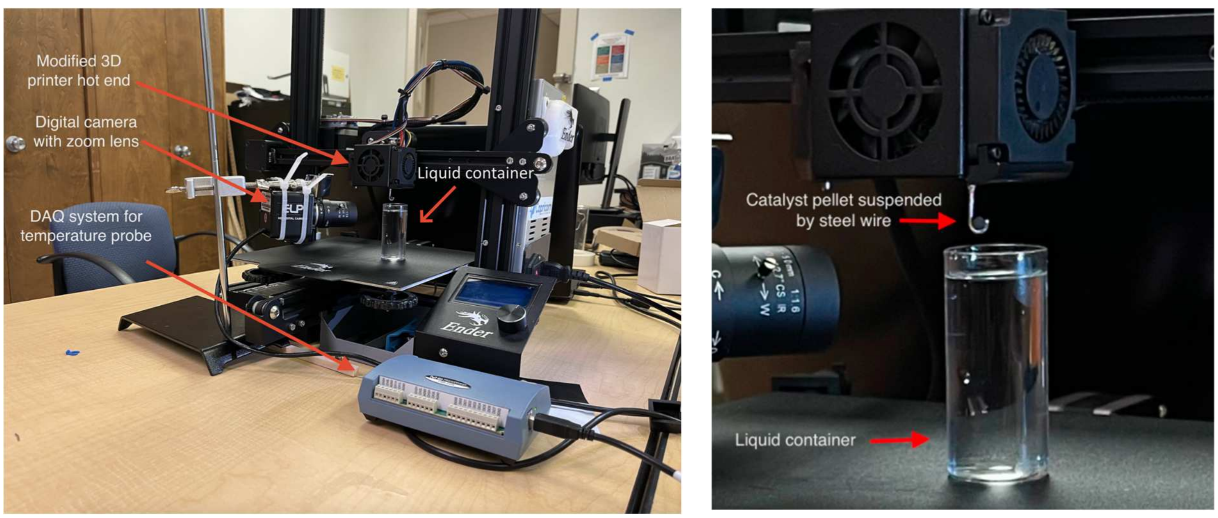
Liquid Organic Hydrogen Carriers (LOHCs) are organic compounds capable of absorbing and releasing hydrogen through chemical reactions. They are regarded as highly promising materials for storing and transporting hydrogen due to their high energy density and ease of handling. Among the various LOHCs, Dibenzyltoluene (DBT) holds advantages as a hydrogen storage material due to its physical properties and availability [6]. Remaining in a liquid state at room temperature and ambient pressure, DBT facilitates convenient storage and transportation. Moreover, it has a history of use as a heat transfer liquid in industries, ensuring ready availability. However, challenges hinder DBT from widespread use as a hydrogen storage medium. Notably, the hydrogenation and dehydrogenation of LOHCs necessitate expensive catalysts [7], prompting a need to minimize catalyst usage. To explore methods for reducing catalyst dependency, studying the formation of hydrogen bubbles on catalyst surfaces during the dehydrogenation process is crucial. Visualizing bubble formation through a visualization study stands as an effective approach to this study.

In this project, three objectives are targeted. Firstly, the aim is to develop an experimental procedure to effectively visualize bubble formations on the surface of a catalyst. During the dehydrogenation process, bubbles formed on the catalyst's surface may impede direct contact between the catalyst and hydrogenated Dibenzothiophene (DBT), potentially reducing efficiency. Therefore, visualizing how hydrogen bubbles may form on the catalyst's surface is deemed valuable. Secondly, the goal is to devise an image processing technique to measure the volume of hydrogen produced from DBT during the dehydrogenation process. In the experimental process, the volume of hydrogen produced from the dehydrogenation of LOHC can be commonly measured by capturing it in a container. However, using an image processing technique for measurement eliminates the need to capture hydrogen, making the process more convenient. Thirdly, the objective is to simplify the experimental procedure for easy adaptation in a laboratory class setting. While solar and wind energy are widely recognized as sustainable energy sources, the public is less aware of hydrogen as a sustainable energy source, including newly admitted engineering students [8], [9]. An effective way for students to learn about hydrogen as a sustainable energy source is through hands-on experiments [10], [11], [12]. To be applicable in a lab class environment, the experimental procedure should not demand expensive or complex devices and processes. Hence, this project aims to develop a relatively simple experimental procedure that does not require expensive equipment.

2. Method

Fig. 1 shows the experimental setup developed in this study. A 5mm-long pellet of Pt2Al3 with a diameter of 3mm was used as the catalyst for the studied bubble formation. The pellet was suspended by a 2mm diameter steel wire connected to a heating element. The heating element consisted of the modified hot-end of a Creality Ender 3 3D printer, which provided precise control over the position of the catalyst as well as the temperature. A thermistor probe was attached to the wire and connected to a computer to measure the temperature of the catalyst. Using the 3D printer to control the vertical positioning of the catalyst, the pellet was lowered into a small beaker of water. While submerged, the water was allowed to reach the desired temperature for 5 minutes, after which a 5-minute period of bubble formation was observed. This process was repeated 4 times with the catalyst's temperature measured at 70°C, 80°C, 90°C, and 100°C.

It is worth noting that water was used to simulate hydrogenated dibenzothiophene (DBT). Hydrogenated DBT was intended to be used in this study; however, it is not commercially available. Although it can be prepared in a laboratory, this process requires a high-pressure hydrogen tank capable of delivering compressed hydrogen gas at a minimum of 3 MPa [13], and a high-temperature, high-pressure reactor to synthesize the hydrogenated DBT from dehydrogenated DBT. Due to the absence of safety protocols for handling hydrogen at the authors' institution, water was utilized as a substitute for hydrogenated DBT. Although hydrogenated DBT and water do not behave identically in all respects, it is known that their bubble formation behavior on the surface of Pt2Al3 is very similar. This knowledge arises from the understanding that vapor bubbles develop in small crevices of a surface upon water contact. In a similar process, hydrogen bubbles are produced on the catalyst's surface when it comes into contact with hydrogenated DBT. It remains unclear, however, whether hydrogen bubble formation is limited to the catalyst's crevices like the water vapor bubble formations, though it is plausible to assume so. This is because hydrogenated DBT in crevices would likely reach the necessary dehydrogenation temperature faster than on flat surfaces. Thus, it seems reasonable to surmise that water's bubble formation behavior on this catalyst closely resembles that of hydrogen bubble formation on the same surface. While variations in the speed of bubble formation may occur due to the distinct properties of water vapor and hydrogen gas, these differences are not relevant to the aims of this study. The primary objective here is to develop an experimental setup, not to measure the actual volume of hydrogen bubbles.



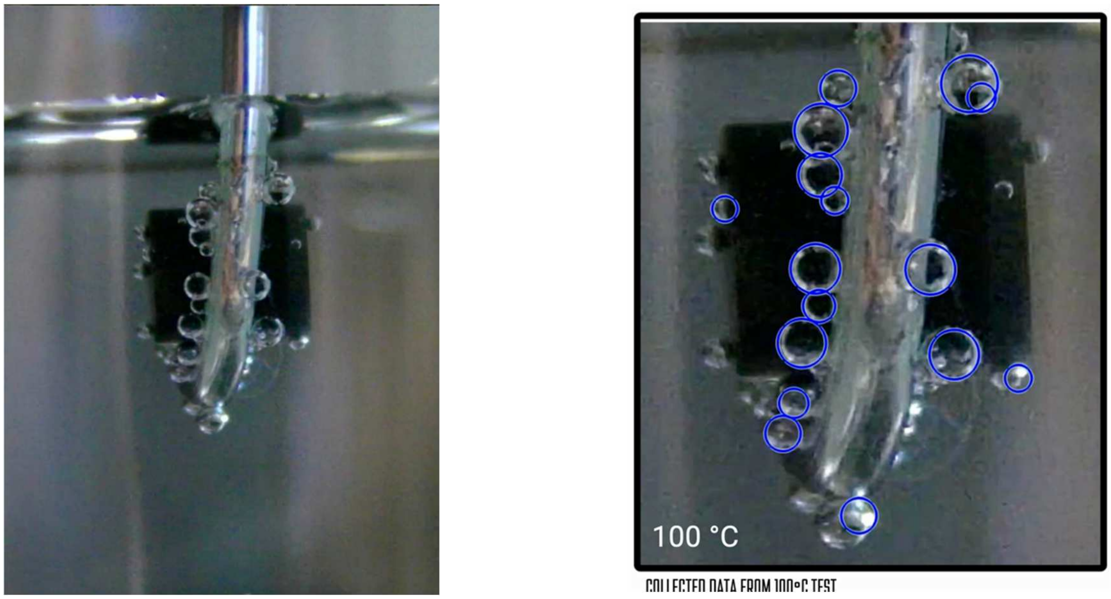
(a) (b)

Fig. 1 (a) Overall experimental setup, including the heating element (a 3D printer), a camera, a liquid container, and a DAQ system. (b) This shows a zoomed view of a portion in (a), featuring the Pt2Al3 pellet as a catalyst, a supporting steel wire that holds the pellet, and the liquid container.

A high-resolution digital camera with a zoom lens was utilized to capture footage of the bubble formation. Positioned within two inches of the glass beaker, the camera was focused at the position of the catalyst pellet. After 5 minutes of recording at 1080p, the file is automatically saved onto a connected computer in .mp4 format, where it is utilized by the MatLab code. The MatLab code employed for this project consists of several distinct sections that analyze the video input, detect formed bubbles, and determine their radius and volume. The first section of the code reads the video file and defines the functions, variables, matrices, and parameters for measuring the size and tracking the formation of the bubbles. Additionally, using pixel measurements of the catalyst in the video, a conversion factor was determined for each trial to convert the size of each bubble in pixels to millimeters. The subsequent major section of the code splits the video into separate frames and processes each frame through a set of filters aimed at eliminating video noise, smoothing the background, and highlighting the bubbles against the rest of the video. Once the frames have been filtered, the next section of code fits a circle around each detected bubble to determine its radius. A digital mask is placed over the area of the video that contains the wire, ensuring that any bubbles formed on the wire are not counted alongside those formed on the catalyst. Following this, the code identifies each circle in a given frame and tracks them compared to previous and subsequent frames to avoid tracking the same bubble multiple times, particularly in the case of a bubble floating off the pellet. Subsequently, the frames are overlayed with the circles used for measurement and recompiled into a video that visually displays the data. Additionally, a table is generated containing the radii data, as well as the calculated volume determined from those radii. The outcome of running the video through the MatLab code is a new video with the detected bubbles overlayed over the original image, alongside a table of data to be used for reporting the results of the experiment.

3. Results and Discussions

The experiment was conducted multiple times to assess its effectiveness in determining the total volume of bubble formation on the catalyst's surface. Examples of bubbles formed on the catalyst's surface are depicted in Fig. 2 from the test conducted at a temperature of 100 °C. Utilizing the video data gathered from the experiment, the image processing code successfully detected the bubbles as they formed on the catalyst, as shown in Fig. 2 (b). In this figure, the bubbles are indicated by blue circles. The code also accurately measured the radius of each formed bubble and calculated the total volume of the bubbles formed. In studying the bubble formation on the catalyst's surface, it is imperative to exclude bubbles formed on the steel wire when calculating the total volume of bubbles. Although this figure illustrates that the Matlab code detects bubbles on both the surface of the steel wire and the surface of the catalyst pellet, masks were applied to the image data to ensure that the volume of the bubbles on the steel wire was not included in the total volume calculation.



(a) (b)

Fig. 2 (a) An example image that shows bubbles formed on the surface of the catalyst pellet. (b) An example image that shows the Matlab code detects the bubbles in the image.

Fig. 3 illustrates the volumes generated during the 5-minute period at temperatures of 70 °C, 80 °C, 90 °C, and 100 °C, calculated using Matlab code developed for this study. The data reveals a significant positive correlation between the temperature of the catalyst and the total volume of formed bubbles during each 5-minute period. This suggests that more bubbles are generated at higher temperatures in this study. These findings align with the intuitive understanding that higher temperatures lead to increased bubble formation. Therefore, it can be inferred that the algorithm developed in this study to calculate the volume functions effectively.

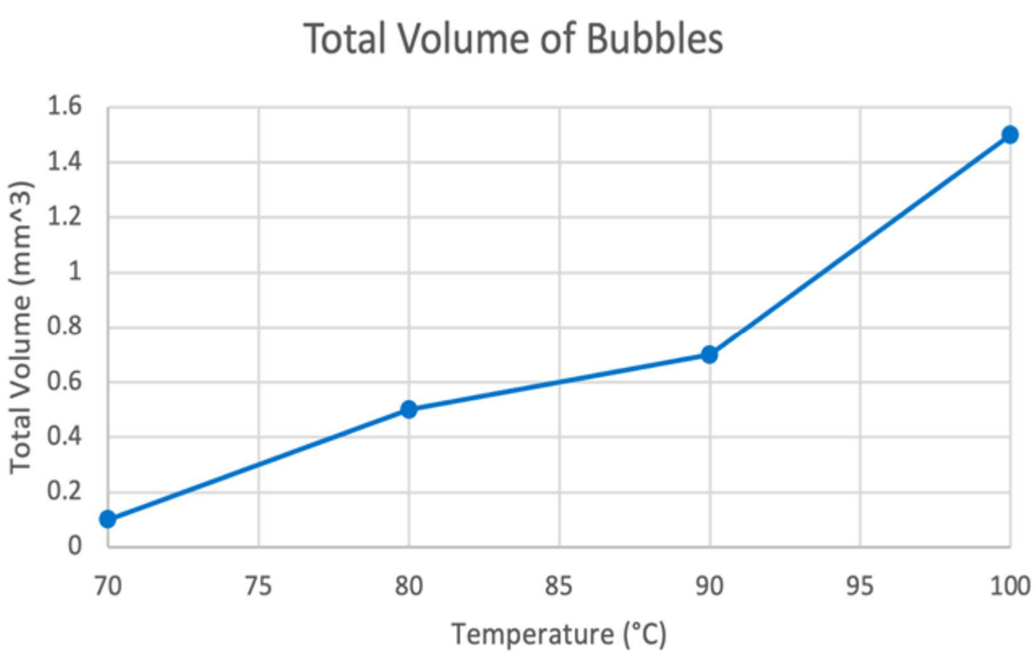


Fig. 3 Correlation between the temperature of the heating element and the total volume of the formed bubbles.

One of the objectives of this study is to develop an experimental setup and methods that can be used for a lab class so that students realize that hydrogen is considered as an alternative energy source. Specifically, by observing bubble formation from the liquid, it is expected that students would understand that LOHCs store and release hydrogen. Additionally, by observing that bubbles are formed on the surface of the catalyst, which is Pt2Al3, it is expected that students would comprehend that dehydrogenation requires an expensive catalyst for releasing hydrogen. This would help students learn that storing hydrogen using LOHCs has limitations such as requiring expensive catalysts. Therefore, conducting this experimental procedure is expected to help students learn about hydrogen as an alternative energy source and its limitations for use as an energy source.

Based on the experiment using water as a hydrogenated DBT to simulate the formation of bubbles on the surface of a catalyst during the dehydrogenation process, a similar apparatus, code, and overall methods can be used to properly analyze the bubble formation during the dehydrogenation process of DBT. While it would be possible to use the apparatus and overall methods used in this study, there are some recommendations to make it convenient for use in a class.

Firstly, due to the lack of a hot plate, a 3D printer was used as a heating element for this study. Though it is creative to use a 3D printer as a heating element, it would be inconvenient to use it in a regular lab setting at a college. Therefore, it is recommended to use a hot plate that is regularly used in a chemistry lab. Secondly, Matlab code would need to be provided to students. It is assumed that most students would not know how to use Matlab, and especially, it would not be easy to learn and create a code to calculate the volume of bubbles from images. Therefore, it is recommended to provide a pre-made Matlab code to students.

In this study, water is used to simulate the dehydrogenation of DBT because hydrogenated DBT could not be produced due to the lack of safety features at the author's institution. Therefore, one might question whether the bubble formation behavior of water would be the same as that of hydrogenated DBT. Though this is a valid question, it is reasonable to consider that the bubble formation behavior of water would be similar to that of DBT. This is because hydrogen is extracted from hydrogenated DBT, not from a catalyst, similar to how vapor bubbles are extracted from water, not from the catalyst. Therefore, it is reasonable to use water for simulation purposes in educational settings. Although using water as an alternative to hydrogenated DBT serves educational purposes, it would be beneficial to use hydrogenated DBT if available.

Due to safety concerns, careful attention is required when using hydrogen for any experiments [14], [15]. For example, personal protective equipment should be defined before conducting this experiment, and it must be used during experiments. Instructors and students should be familiar with the basic properties of hydrogen regarding safety concerns, such as flammability and diffusiveness. Ventilation is required to prevent it from accumulating in a lab space. It is also necessary to avoid any ignition sources in the lab. For more details, it is necessary to consult staff who are in charge of lab safety concerns before designing and setting up any experiments related to hydrogen.

In this experiment, the student designed and tested the apparatus, code, and methodology required for the experiment to take place. With guidance from the mentor, the student first came up with a general idea for the basics of the experiment. A few hours every day over the course of the project were dedicated to designing the code and the apparatus. The majority of the project time was dedicated to developing the code in MATLAB first, then designing the full apparatus after. The project was completed then presented alongside other research projects at the institution.

4. Conclusions

An experimental procedure to effectively visualize bubble formation on the surface of Pt2Al3 during the dehydrogenation process of DBT was developed. Due to safety concerns, water was used as an alternative to hydrogenated DBT to simulate the dehydrogenation process. The developed experimental procedure successfully visualized vapor bubble formation on the surface of Pt2Al3. While a 3D printer was used as a heating element in this experiment, it is recommended to use a hot plate for simplicity and convenience. A MATLAB code to measure volumes of bubbles formed on the surface of Pt2Al3 was developed and successfully measured the volumes of the bubbles. Providing the MATLAB code to students is recommended due to the lack of knowledge of coding. It is expected that students will learn that hydrogen is used as an alternative energy source and understand its limitations regarding storage. Although this project initially began as an undergraduate research project, this experimental setup can be effectively used in a laboratory activity for students to learn the concept of LOHC, though the setup has not yet been used as a lab activity.

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