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Research Paper

Dynamical Behavior of Droplet Diffusion Flame of Blended Castor Oil with Metal Based Liquid Catalyst

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Abstract The tests revealed the exceptional combustion properties of a blended fuel consisting of castor Article Info oil and rhodium liquid (Rhl) as a highly effective homogeneous combustion catalyst. Our Submitted: findings indicate that castor oil's unique molecular structure makes it an ideal fuel component, 06/06/2024 and the catalyst interacts with the fuel's triglycerides to enhance fuel properties and facilitate Revised: ignition. These findings support the pivotal role of the synthetic catalyst Rhl, which effectively 25/07/2024 reduces the binding forces within the triglyceride chain through polarization interactions. As Accepted: a result, molecular bonds become more flexible, providing electrons with greater freedom of 26/07/2024 movement. Synthetic catalysts induce significant modifications in the triglyceride structure, Online first: increasing electron energy levels and enhancing the reactivity of fuel molecules, ultimately 18/09/2024 leading to improved fuel combustion efficiency. Integrating the Rhl synthetic catalyst also enhances fuel performance by reducing ignition duration and increasing the combustion rate. The elevated combustion temperatures of the fuel droplets highlight the effectiveness of promoting environmentally sustainable combustion processes. Keywords: Castor oil; Synthetic catalyst; Droplet combustion; Molecular structure; Flame characteristics

1. Introduction

The use of synthetic catalysts in castor oil combustion is a complex and unexplored area. Castor oil is a promising alternative energy source but faces challenges due to its high viscosity and flash point [1], [2], which affect combustion efficiency [3] and lead to environmental issues [4]. Research suggests that employing combustion catalysts can improve fuel performance, diesel engine power [5], and thermal energy production by breaking down complex fuel molecules for more efficient combustion [6]. This results in increased calorific value and reduced fuel consumption [7]. The combustion reaction can occur more easily and quickly with a lower activation energy [8]. Moreover, catalysts produce high combustion temperatures because catalysts help achieve more complete combustion by reducing the formation of by-products such as carbon monoxide and unburned hydrocarbons [9]. This complete combustion not only increases fuel efficiency but also the combustion temperature because more fuel is burned into CO₂ and H₂O, and, at the same time, produces environmentally friendly exhaust emissions [10]. They found that combustion catalysts can reduce or convert toxic gases resulting from combustion, such as CO, HC, and NOx, into harmless gases, such as CO₂, N, and O₂ before being released into the air. Based on previous studies, it is also known that rhodium is used as an automotive catalytic converter, to produce hydrogen fuel [11], and improve fuel economy [7]. This allows rhodium to function efficiently over a longer period, thereby

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saving fuel use. Apart from that, it was also found that the rhodium catalyst was able to increase the combustion stability because it is able to survive high-temperature conditions [12], remaining active and effective even when exposed to extreme temperatures. In addition, rhodium results in a faster rate of heat release and higher peak cylinder pressure [13], thus enhancing fuel combustion efficiency [14] and saving fuel consumption rates [15].

Previous study have successfully enhanced the efficacy of castor oil by incorporating Rhl as a homogeneous combustion catalyst [16]. A catalyst increases electronegativity between itself and the carbon chain, enabling precise adjustments in bond angles of fuel molecule [17]. This breakthrough to has led а remarkable improvement in the reactivity of fuel molecules, resulting in a highly combustible fuel. Although understanding the intricacies of Rhodium liquid's effectiveness as a catalyst in multi-component biooil like castor oil is still challenging, researchers continue to make notable progress in this area, especially from atomic and molecular perspectives. On the other hand, studies on the use of rhodium catalysts are becoming increasingly attractive because it has also been proven that rhodium is a very effective electron donor in producing hydrogen, which can be used as hydrogen fuel [18]. They further discovered that Rhl can reduce the mass of other carbon chain compounds close to it. This is possible because they found that with a large enough proton energy, Rhl can attract other atoms around the fatty acid's carbon chain, such as carbon, hydrogen, and oxygen. Moreover, previous researcher [19] stated that rhodium also acts as an electron acceptor because the molecular structure of rhodium liquids shows that the presence of oxygen allows rhodium to bind two hydrogen atoms to produce water molecules (H2O), which have a critical role in the process of making biodiesel (transesterification) through a separate mechanism glycerol from three fatty acids [20], [21]. Unfortunately, previous research that revealed synthetic catalysts' role in changing triglycerides molecular geometry and their impact on fuel combustion performance is very lacking. Although previous studies have performed a droplet combustion experiment using synthetic catalysts in normal gravity conditions to streamline the issue and many things have not been revealed [22]. Thus, more data is needed to understand how the different components in castor oil affect combustion characteristics from a molecular perspective. Therefore, all this suggests that it is advisable to conduct a study on a way to overcome these difficulties can be studying how changing atomic structures and interactions affect castor oil combustion is essential. The research findings will help develop a fuel that is efficient and cost-effective for actual application use.

2. Material and Methods

Figure 1 setup is designed to suspend the oil droplet precisely at the thermocouple intersection. The ImageJ software was used to measure the droplet's diameter precisely and meticulously prepared using a syringe for utmost accuracy. Additionally, ImageJ was utilized to measure both the height and width of the droplet flame, ensuring thorough and precise data collection for analysis. High-speed photography was used to analyze the ignition process of castor oil droplets and their combustion characteristics with great precision. The experiment took place under normal gravity and room temperature conditions, with 57-62% humidity. A camera recorded ignition and burning times, while a thermocouple connected to a laptop captured the temperature evolution of the droplets.

A process was conducted to enhance fuel quality by blending 150 mL of castor oil with a catalyst having a concentration of 10 ppm. The mixture in the test tube was analyzed using gas chromatography to determine fuel properties, including composition. The catalyst's influence on castor oil's properties was simulated using Avogadro chemical software. The results from these tests are summarized in **Table 1**, demonstrating the effectiveness of the catalyst.

3. Results and Discussions

3.1. The Role of Synthetic Catalyst on the Ignition Phenomenon

The initial step in elucidating the role of synthetic catalysts in the ignition characteristics of castor oil is to conduct physical properties testing. The results, as detailed in **Table 1**, unequivocally demonstrate the significant positive impact of the synthetic catalyst on fuel performance. Notably, there is a marked decrease in viscosity, density,



Captions:

- 1. Personal computer.
- 2. Data logger.
- 3. High-speed photography.
- 4. 6V power supply.
- 5. Electric coil heater.
- 6. Thermocouple wires.
- 7. Oil droplet.

Figure 1. The schematic of the droplet combustion experiment

Table 1. Physical properties of castor oil

Fuel parameters	Without synthetic catalyst	With synthetic catalyst
Kinematic viscosity at 40 °C (cSt)	36.02	32.35
Density at 15 °C (gr/ml)	0.918	0.908
Flash-point (°C)	244	211
Caloric value (cal/gr)	9505	9027
Carbon residue (% Wt)	0.46	0.189

flash point, and carbon residue, while the calorific value experiences a substantial increase. These findings undeniably establish that the addition of synthetic catalysts substantially enhances the energy content of castor oil and has excellent potential to improve fuel performance.

Figure 2 clearly illustrates that, when paired with the catalyst, the castor oil droplet exhibits a notably reduced ignition time of approximately 1.3 seconds, as opposed to around 1.4 seconds without the catalyst. Furthermore, it can also be seen that in the initial stage, when the droplet receives heat from the coil heater, which is around 0.3 seconds, the diameter of the droplet without the catalyst expands more than the droplet with the catalyst, namely around 1.13 mm², while with the catalyst the droplet diameter expands to around 1.07 mm². This phenomenon shows that droplet fuel without a catalyst absorbs heat faster than droplet fuel with a catalyst in the initial stages. This is due to droplet fuel with a catalyst having a higher composition of fuel compounds, namely fatty acid and rhodium. Hence, droplet fuel molecules with a catalyst have slower expansion. On the other hand, droplet fuel without a catalyst has faster expansion because it only has the same constituent compound, namely the fatty acid carbon chain. From Figure 2, it can also be seen that from the 0.4th second, both fuel droplets have the same trend until they ignite. The difference is that both fuels ignite at different times, sizes, and temperatures, where it can be seen that droplet fuel with a catalyst ignites faster at smaller diameters and temperatures than droplet fuel without a catalyst. These results show that the catalyst accelerates the fuel in absorbing heat and igniting.

The experiment unequivocally demonstrates the inherent challenges in expanding, evaporating, and igniting castor oil droplets without catalysts. Fuel droplet ignition time prolongation is caused by volatility, molecular mass, molecule chain shape, and carbon chain rigidity [23]. This leads to less reactive fuel molecules. The experiment shows that ignition time in castor oil is determined not only by fatty acid carbon chain length and C=C bond count but also by the rigidity of the molecule and bond angle [24]. This result is very reasonable because it is also supported by the results of the fuel properties test, which are listed in Table 1 It can be seen that without a synthesis catalyst, the viscosity of castor



Figure 2. Ignition phenomena of castor oil droplet

oil is 36.02 cSt, whereas with a synthesis catalyst is 32.35 cSt. These results show that the catalyst can reduce the bonds between carbon chains, causing the viscosity to decrease and causing the fuel to ignite in a shorter time. Moreover, **Table 1** also shows that with a catalyst, the fuel can reach a lower flash point, around 0.908 °C, whereas without a catalyst, the fuel has a higher flash point, around 0.918 °C.

3.2. The Role of Synthetic Catalyst on the Flame Shape

Meanwhile, the information presented in **Figure 3** to **Figure 4** indicates that as the heating time and temperature increase, the droplets' size increases, which is clarified by the results of the flame height and width measurements shown in **Figure 5** to **Figure 6**. This phenomenon occurs due to the catalyst's influence on the reactivity of the molecules [25]. The catalyst achieves this by creating a difference in electronegativity between the carbon chains of the triglycerides, which weakens their molecular bonds and changes their overall geometry. The catalyst plays a significant role in enhancing molecule reactivity, resulting in lower flash points, faster-burning rates, and reduced droplet diameter [26].

Figure 5 to **Figure 6** shows that a catalyst makes a big difference in the height and width of a flame, and we found that sudden increases in the height and width of the flame happen because of microexplosions [20]. When the height goes up quickly, it is because of spike type micro-explosions [27]. Furthermore, when the width gets bigger suddenly, it is because of a bulge-type micro-explosion [28]. In Figure 4, we saw that the flame width without a catalyst got as big as 62 mm after about 0.5 seconds. However, with a catalyst, the width got to 86 mm in just 0.4 seconds.

In **Figure 6**, we saw that the flame height went up faster with a catalyst than without. It reached 100 mm in 0–0.17 seconds with a catalyst, while it took 0.21 seconds to get to a height of around 75 mm without one. With the catalyst, the flame went up to around 187 mm in only 0.48 seconds, but without one, it took 0.38 seconds to get to around 186 mm. Furthermore, **Figure 5** to **Figure 6** shows that longer flame evolution without catalysts indicates more rigid carbon chains with more muscular bond strength. Fuel viscosity is higher for castor oil without the catalyst (**Table 1**).

3.3. The Role of Synthetic Catalyst on the Combustion Phenomenon

Figure 7 shows droplets burn slowly without a catalyst due to the diverse castor oil composition. Catalysts balance the crude castor oil, allowing droplets to burn faster and more efficiently. The catalyst enhances electron reactivity, weakens carbon chains, and causes rapid breakdown, leading to a single-stage combustion process. The catalyst draws the weakest hydrogen bond position in the triglyceride chain, leading to intense micro-explosions [28], [29].

These recent findings have unequivocally confirmed that atoms that respond to infrared heat are rotatable molecular bonds. This phenomenon occurs due to a photochemical reaction induced by light, which causes the electrons to be more reactive and weakens the triglyceride chain. As a result, the molecules undergo bending vibrations, leading to significant alterations in the bond angles. These findings are strongly supported by the evidence presented in our previous studies [26], [30], which clearly illustrates that introducing a catalyst results in modifications to bond angles, thereby changing the triglyceride shape. These insights have opened up new avenues in molecular reactions and could serve as a vital foundation for future breakthroughs in the field.



0.1 0.2 0.3 0.4 0.5 0.6 0.7 time (s)

Figure 6. The evolution of flame width

0 L

0.8



Figure 7. The droplet evolution at the burning stage

Meanwhile, Figure 7 unequivocally demonstrates that adding catalysts to castor oil droplets can significantly reduce the temperature at which they burn around 4.48%, requiring only around 223 °C instead of 243 °C without catalysts. The presence of catalysts also allows castor oil droplets to reach a considerably higher maximum combustion temperature of around 590 °C compared to approximately 556 °C without catalysts. This is because catalysts help the droplets absorb heat faster and reduce heat loss, significantly reducing the amount of soot formed during combustion. These findings align strongly with previous studies [30]. Furthermore, the all results presented prove that adding a synthetic catalyst as a homogeneous combustion catalyst has improved the performance of castor oil. The data in Figure 3 demonstrates that a catalyst's presence reduces the castor oil's ignition time. Additionally, it is evident that during the initial stage, when the coil heater heats the droplet, the diameter of the droplet without the catalyst expands more than the droplet with the catalyst, while with the catalyst, the droplet diameter expands. This observation indicates that the droplet fuel without a catalyst absorbs heat more rapidly than the droplet fuel with a catalyst in the early stages. Furthermore, Figure 3 also shows that the distinction lies in that both fuels ignite at different times, sizes, and temperatures. This indicates that the droplet fuel with a catalyst diameters ignites faster at smaller and temperatures than without a catalyst. These findings demonstrate that the catalyst hastens the fuel's heat absorption and ignition. This result is also confirmed in Figure 3 to Figure 4, and it can be seen that with the catalyst, the droplet flame has a higher peak at a faster time. On the other hand, although the width of the droplet flame with and without the catalyst is almost the same, it is clear that the catalyst requires a shorter time. These results prove that burning castor oil fuel can be more efficient because the fuel breaks down more easily into combustion products. This analysis is in accordance with previous research using coconut oil and sunflower oil, which stated that with a catalyst, droplet flames produce more even heat and increase the energy distribution in the flame, thereby influencing the width of the droplet flame [31]. In addition, this phenomenon is also clarified from Figure 7.

Furthermore, **Figure 7** shows that the fuel ignites at a lower temperature than fuel without a catalyst and can produce the highest combustion

temperature compared to fuel without a catalyst. These results indicate that the synthetic catalyst has excellent properties in distributing atoms on its surface, allowing the chemical combustion reaction to take place more quickly. It is accompanied by a large energy release, as evidenced by the higher combustion temperature [32].

In general, the results presented can be discussed more deeply from a molecular perspective to discover the fundamental causes of this phenomenon. Based on Figure 8, the carbon chains in these triglycerides can be classified into two categories based on their ability to rotate. The capacity of atomic bonds to rotate directly affects molecular reactivity. Upon analyzing castor oil, it is found that there are 110 no rotatable atomic bonds present. These bonds consist of 4 C–C, 102 C–H, and 4 C–O. Additionally, 52 rotatable molecules consist of 48 C–C and 4 C–O (see Appendix 1 for details). It is worth noting that

monounsaturated castor oil has lower flexibility than saturated oils. Overall, this detailed analysis of the composition of castor oil's triglycerides provides valuable insights into the properties and characteristics of this unique oil.

The liquid rhodium is highly effective in accommodating up to 12 hydrogen bonds [20]. Additionally, studies indicate that it can attract carbon chains to its surface, as shown in Figure 9. The higher proton count of the Rhl makes it more appealing to the carbon chain, resulting in an electronegativity contrast that facilitates their interaction. The catalyst interacts more with double bonds of triglyceride chains where electrons and nucleus are distant, leading to imbalanced electron repulsion due to variations in surrounding hydrogen atoms. This characteristic renders the double bonds a vulnerability in the chain of tree fatty acids and glycerol. Catalyst weakens triglyceride structure, increasing reactivity and making fuel more combustible.



🛱 Bond Properties							
	Type	Start Atom	End Atom	Band Order	Rotatable	Length (Å)	-
Bond 1	C-0	a	08	1	Yes	113560	I
Bond 2	C-0	a	02	2	No	1,32985	1
Bond 3	C-C	0	G	1	Ves	1,29055	4
Bond 4	сн	C2	H2	1	No	1.0576	
Bond 5	641	a	101	1	No	1,05883	
liond 6	c-c	a	0	1	Nes	1,22773	
Bond 7	сн	3	нв	1	No	1.058	
Bond 8	C-11	a	102	1	No	1.0073	
Bond 9	6-C	CI .	a	1	Nec.	1.2523	
Rend 10	сн	C4	H4	1	No	1.0328	
Bond 11	C-H	CH .	HD3	1	No	1.00/61	
Sond 12	c-c	65	a	1	Vec	1,27585	
Rend 13	сн	CS	HS	1	No	1,00855	
Bond 14	C-H	0	HDA	1	No	1.00/3	
Sond 15	C-C	ca	σ	1	Vec	1.17927	
Bond 16	C-H	a	18	1	No	1,00854	

Figure 8. The bond characteristics of castor oil carbon chain

Figure 9. Molecular interaction between carbon chain of castor oil and Rhl: (a) Monounsaturated carbon chain; (b) Polyunsaturated carbon chain

Furthermore, previous studies clearly shows that the introduction of a catalyst boosts the O-C-O bond angle from 84.6003 degrees to 120.4203 degrees, leading to a significant augmentation of bond angles in the triglyceride carbon chain [26]. This, in turn, causes the stretching of molecular chain bonds in castor oil, making them highly reactive and unstable, thereby increasing their kinetic energy. Moreover, stretching carbon chain bonds can enhance fuel performance by reducing viscosity, achieving easily attainable flash points, ensuring combustibility, and increasing the burning rate to generate greater power. The increased space for electrons in atoms intensifies their reactivity, making them more susceptible to reaction. Therefore, elongating carbon chain bonds can significantly enhance fuel performance.

Undoubtedly, due to hydrogen atom asymmetry, allylic and bis-allylic compounds weaken carbon chains, causing reduced bonding force. Consequently, these chains are highly susceptible to breakage, leading to shorter chains with lesser molecular masses. This analysis is in accordance with previous research that used ethanol as a synthesis additive and was discussed from a slightly different perspective [33]. Furthermore, when altering the bond angle weakens the atom bonds in the molecule. This leads to stretching, relaxation, and deformation of the molecule. The expansion of electron space causes this phenomenon, making electrons more energetic and likely to deviate from their orbits, which increases flammability. It is important to note that there is a significant decrease in oil viscosity (as shown in Table 1), which strongly supports this analysis.

Nevertheless, to fully maximize the efficacy of the rhodium synthesis catalyst as a homogeneous combustion catalyst, it is imperative to undertake further comprehensive research involving the utilization of various crude vegetable oils. This research should aim to delve into the unique properties and combustion characteristics of each type of oil in order to assess their potential as viable fuel sources. Additionally, an in-depth analysis of the behavior of crude vegetable oil spray upon impact with a wall is warranted as it serves as a simplified representation of the intricate interaction between the fuel and the combustion chamber wall during the injection process. Furthermore, an extensive comparative study of the rhodium synthesis catalyst with biocatalysts, which are derived from natural materials [34], is essential to gain a comprehensive understanding of their respective performance and potential applications in combustion processes.

4. Conclusion

A study on the effect of metal based liquid catalyst of Rhl on the combustion characteristics of bio-fuels from crude castor oil has been completed. Therefore, several significant findings can be concluded, including:

- a. The synthetic catalyst of Rhl is a very important factor as it effectively weakens the binding forces within the triglyceride chain through polarization interactions. As a result, molecular bonds become more flexible, and the increased space available enables electrons to move more liberally, where visible from qualitative or quantitative indicators of research results about the role of synthetic catalysts in the droplet ignition phenomenon.
- b. The synthetic catalyst has a significant role in triglyceride altering the structure and enhancing electron energy, leading to increased reactivity of fuel molecules and efficient fuel combustion, where with an indications of qualitative or quantitative indicators of research results about the role of synthetic catalyst on the role of synthetic catalyst on the flame shape of castor oil droplets.
- c. Adding the synthetic catalyst of Rhl significantly improves fuel performance by reducing ignition time and increasing combustion rate. The resulting high combustion temperatures for fuel droplets demonstrate its effectiveness in promoting environmentally friendly combustion, with an indications of qualitative or quantitative indicators of research results about the role of synthetic catalysts on the droplet combustion phenomenon.

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Author's Declaration

Authors' contributions and responsibilities

The authors made substantial contributions to the conception and design of the study. The authors took responsibility for data analysis, interpretation and discussion of results. The authors read and approved the final manuscript.

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Availability of data and materials

All data are available from the authors.

Competing interests

The authors declare no competing interest.

Additional information

No additional information from the authors.

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