COMPUTATIONAL MODELING OF A SYSTEM FOR THE APPLICATION OF PURE AMMONIA IN INTERNAL COMBUSTION ENGINES OF THE OTTO CYCLE

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ABSTRACT

Ammonia and hydrogen hold great potential as carbon-free fuels, with promising applications in energy systems. Hydrogen, in particular, has generated high expectations as an enabler of a carbon-free economy, but issues related to storage, distribution, and infrastructure deployment are delaying its full implementation. Ammonia, on the other hand, stands out as a highly efficient energy carrier, offering high energy density and an already established acquisition, storage, and transportation infrastructure capable of mitigating the main disadvantages presented by hydrogen. However, there are some counterpoints regarding its implementation in internal combustion engines, among them its slow combustion process. In this context, the main objective of this article is to propose the use of a flame-jet ignition system as a solution and to verify through computational simulations (CFD) the effectiveness of using a pre-combustion chamber to overcome significant existing constraints in the application of pure ammonia as a fuel in internal combustion engines with a spark ignition system. Many researchers in this field are developing strategies to optimize ammonia combustion, such as dual- fuel injection to overcome impasses related to its application. However, the use of pure ammonia depends on mechanical adaptations in the engines to speed up its combustion. A possible solution is the use of a pre-combustion chamber. This system is generally applied in engines operating on the diesel cycle and functions as a turbulence generator in its volume, thus increasing the interaction between the air-fuel mixture molecules, which in turn leads to an increase in the combustion propagation speed.

1. INTRODUCTION

Due to the concerning current climatic and environmental situation globally, significant debates have arisen regarding power generation, whether for population mobility or energy generation purposes. Currently in Europe, transportation stands as the largest source of carbon emissions, responsible for over a quarter of all greenhouse gas (GHG) emissions, approximately 27%, and it is the only sector to have seen an increase in GHG emissions since 1990 (Navas-Anguita et al. (2019)). With the current momentum favoring the phasing out of fossil fuels, if European Union (EU) leaders intend to fulfill the Paris Agreement, much more compelling measures must be endorsed to meet climate targets.

Meanwhile, various alternatives are being considered, including electrification, hydrogen, and ammonia, all of which hold significant potential as solutions for reducing GHG emissions in the mobility sector. However, each faces substantial challenges that hinder their widespread adoption. For instance:

Electromobility: Despite potentially generating up to 68% more emissions during manufacturing (Lototskyy *et al.* (2014)), electric

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vehicles still emit far fewer GHGs and atmospheric pollutants over their lifespan compared to gasoline or diesel counterparts. Yet, significant obstacles remain concerning battery range, recharge time, charging infrastructure, and the environmental impact of lithium.

Unconventional fuels: Hydrogen has generated high expectations as a potential enabler of a carbon-free economy (Cardoso *et al.* (2021)). However, challenges such as storage, distribution, and infrastructure deployment have delayed its full implementation.

It is widely acknowledged that energy storage is a crucial step towards reducing reliance on natural resources and increasing the share of renewable energy in the capacity of energy generation. Solutions like lithium batteries are unlikely to provide the necessary capacity for large-scale energy storage. Chemical storage, on the other hand, offers a more flexible and cost-effective solution, allowing large amounts of energy to be stored for extended periods and in various locations (Valera-Medina *et al.* (2018)).

However, significant improvements and paradigm shifts are still needed even for the most optimistic projections of current low-carbon solutions, such as biofuels and hydrogen (Apostolou and Xydis (2019)). In this context, nitrogen- based fuels like ammonia emerge as a short-term attractive solution, circumventing user concerns about charging and the need for extensive investments in infrastructure or sophisticated technologies to mitigate CO effects, leading to significant logistical savings and environmental benefits.

Nevertheless, despite apparently not requiring a high level of technological development for storage or general use, the use of ammonia still faces hurdles due to its low laminar burning speed. Laminar burning speed refers to the speed at which unburned gases move through the combustion wave in a direction normal to the wave surface, which can be calculated using the power law relationship of Metghalchi and Keck (Metghalchi and Keck (1982)).

$$S_u = S_{u0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta}$$

Many studies on the laminar burning speed of ammonia have been conducted, mostly under ambient conditions for their development. However, a potential solution to overcome the current obstacle for application in internal combustion engines is believed to be increasing the turbulence level of the air/fuel mixture before and during its combustion to enhance interaction between the molecules in the mixture.

The solution found to increase turbulence involves adapting the use of a pre-combustion chamber already widely employed for this purpose, commonly found in diesel cycle engines. Each jet of the mixture from the pre-chamber represents a source of high energy for igniting the mixture within the main chamber. In engines equipped with flame jet ignition systems, combustion in the main chamber starts at several distinct points, which tends to promote increased combustion efficiency and the capability to safely and quickly ignite various fuels. (Rodrigues Filho (2014)).

2. METHODS

2.1 DEFINING ENGINE

The choice of the engine to be used as a reference model is crucial for the start of development. Therefore, a stationary Otto cycle engine with an indirect injection system has been selected. It is believed that the engine's characteristic of operating within a narrow range of rotation to achieve maximum efficiency will be of paramount importance in the initial development of parameters for the flame jet ignition system application.

2.2 DEFINING GEOMETRY

The pre-combustion chamber will be crucial for developing the application of ammonia in internal combustion engines. Clearly, it is necessary to follow some fundamental parameters for the system's efficiency, such as diameter, height, inlet orifice diameter of the pre-chamber, internal geometry, and the ratio between the cylinder piston volume and the pre- chamber volume. Based on the data from (Rodrigues Filho (2014)), we can determine the parameter values to be applied in the tests to be conducted, aiming to save computational cost in simulations and focus the solution on a specific part of the problem. The dimensions have been fixed as shown in Table 1.

Chamber Height (mm)	20
Chamber diameter (mm)	14
Inlet diameter (mm)	6
Inlet diameter (mm)	11.88
Angle	105°

2.3 DEFINING SIMULATION

To begin the simulations, the most crucial variable chosen is the lambda (λ) coefficient, which expresses the ratio between the stoichiometric air-fuel mixture and the actual mixture. Based on Graph 1, it has been decided that for a sufficiently large sample space, λ will vary between (0.9, 1.0, 1.1), while maintaining consistent geometry, definitions, models, and factors throughout the simulations.

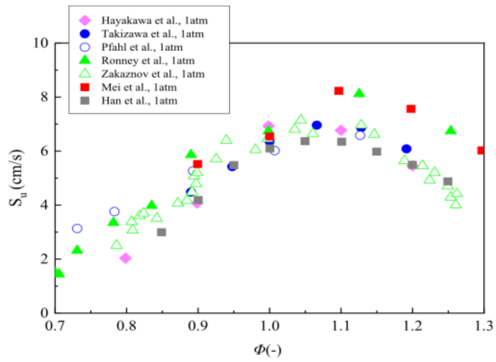


Figure 1. Laminar burning velocity of NH 3 flame with a function of equivalence ratio at 298 K and 1 atm, replotted from(Han *et al.* (2019); Kobayashi *et al.* (2019); Mei *et al.* (2019)).

Another assumption made to facilitate data acquisition was the use of dry air as atmospheric air, considering only the elements with the highest proportions, O2 and N2. Consequently, by performing chemical reaction balancing, the following formulas were derived for each coefficient λ.

λ0.9:

$$0.236NH_3 + 0.16O_2 + 0.604N_a \Rightarrow 0.676N_2 + +0.303H_2O + 0.021NH_3$$

λ1.0:

$$0.217NH_3 + 0.163O_2 + 0.619N_2 \Rightarrow 0.69N_2 + +0.31H_2O$$

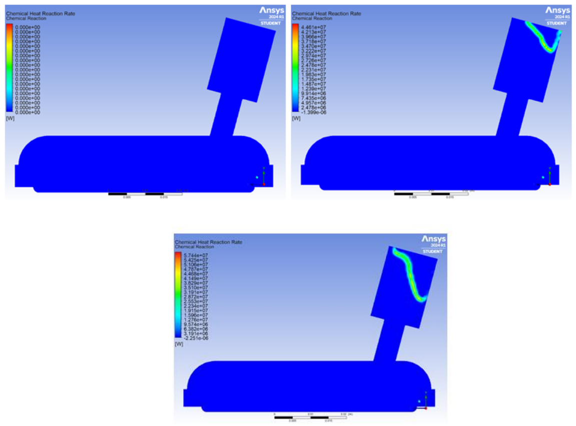
λ1.1:

$$0.202NH_3 + 0.166O_2 + 0.631N_2 \Rightarrow 0.697N_2 + 0.288H_2O + 0.014O_2$$

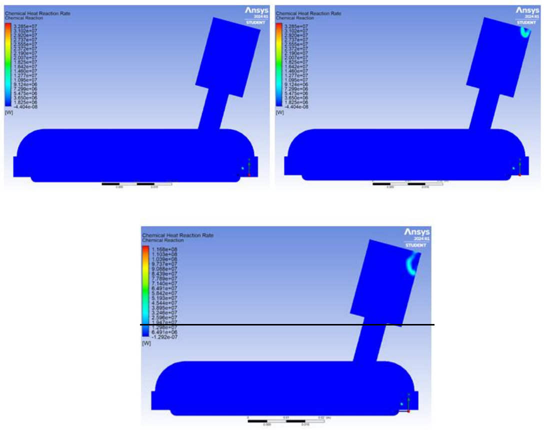
3. RESULTS

In this section, we can compare the results of the three simulations conducted for each time step, including their respective times and angles. This allows for the visualization of the combustion front development through the chemical reaction rate.

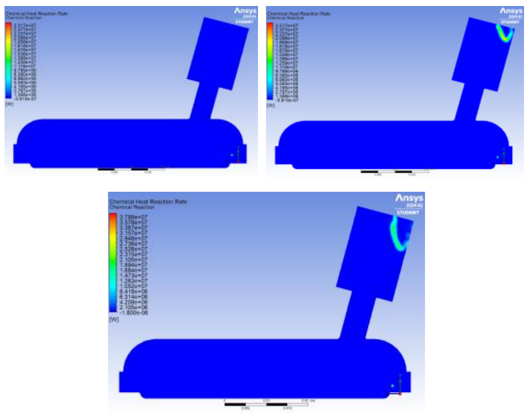
λ0.9:



λ1.0:



λ1.1:



4. CONCLUSION

Undoubtedly, the discovery of a new potential strategy to innovate the world we live in is fascinating to everyone. However, achieving comprehensive scientific development requires exploring numerous possible solutions. Overall, the current work fuels our hopes as it has shown increasingly visible advancements in the application of ammonia as an energy vector for use in internal combustion engines. Yet, further development is necessary to vary its volume, internal geometry, inlet orifice, and test the direct injection method in the pre-chamber to achieve greater precision regarding the air/fuel ratio within its internal volume.

Variation in these parameters is crucial to generate optimal combinations aimed at achieving more accurate results when validating the method through experimental work and subsequently in field trials, ultimately aiming for maximum efficiency of the system.

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6. RESPONSIBILITY NOTICE

This research had contributions from Bruno Lourenço de Souza: conceptualization, methodology, design and execution, formal analysis and writing. André Veríssimo Xavier: visualization and support execution. Marcio Ferreira martins and Flávio Lopes Francisco Bittencourt: conceptualization, theorical guidance, writing review, supervision, project ad- ministration.

The authors are solely responsible for the printed material included in this paper.