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Optimizing Engine Performance: A Kinetic Analysis by Neural Network of Bioethanol Combustion with Hydrogen Gaseous Mixture

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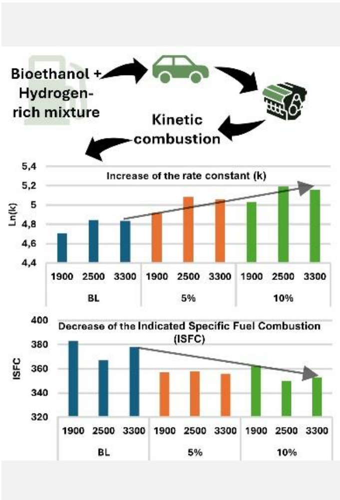

The combustion study focuses on the efficiency of burning bioethanol pure and with a Hydrogen Gaseous Mixture of 5%v/v and 10%v/v in a Single Cylinder Research Engine (SCRE). A kinetic study is calculated with a Multilayer Perceptron Neural Network based on the determination of the kinetic triplet: activation energy, frequency factor, and mechanism of reaction from the Mass Fraction Burned data (MFB). From these parameters, the rate constant of the process is obtained. The experiments indicate that increasing the concentration of the hydrogen mixture in the engine resulted in an increase in the rate constant, and this fact can be correlated to an improvement in fuel consumption and combustion efficiency. The kinetic study indicates the hydrogen-rich mixture acts as a local heat source within the combustion, increasing the activation energy but, more significantly, increasing the process's frequency factor, which has a more pronounced impact on the rate constant than the activation energy increment. Incorporating a hydrogen-rich mixture can be interpreted as an application of intensified oxidation. This addition enhances combustion efficiency, leading to an increase in the reaction rate constant.

Introduction

Although there is considerable interest in using pure hydrogen as a clean and renewable source, this practice presents some limitations. For example, its low density and high diffusivity can cause the substitution of the admitted atmospheric air for hydrogen on the intake manifold, leading to a decreased volumetric efficiency. Due to these limitations, hydrogen and/or its mixtures are suggested to be used as an additive for traditional fuels, contributing to the advanced oxidation technologies in internal combustion engines. [1].

In the short and medium term, implementing biofuels associated with high-purity hydrogen or hydrogen gaseous mixtures can be a sustainable solution to the energetic demands. Bioethanol, for example, presents an increased energetic density when used with gaseous mixtures containing hydrogen [2]. Therefore, studying the combustion kinetics of these systems in engines is necessary to understand their potential for commercial application and efficiency. The relationship between combustion efficiency and atmospheric emissions is quite significant. Combustion efficiency refers to a system's ability to convert fuel into useful energy with minimal losses. The more efficient the combustion, the smaller the amount of unburned fuel and, consequently, the lower pollutant emissions.

Material and Methods

The samples used in this study consist of bioethanol pure, as baseline (BL), and bioethanol with Hydrogen Gaseous Mixture (HGM) of 5%*v/v* and 10%*v/v*. Experiments were performed on an AVL 0.45 L spark-ignited (SI) Single Cylinder Research Engine (SCRE). All the tests were done at a fixed indicated mean effective pressure (IMEP) of 8 bar at three different engine speeds, β: 1900, 2500, and 3300 rpm. These specific points were chosen because they represent typical urban driving. More of the experimental methodology can be found in Amaral et al. (2024) [3].

The combustion study analyzes the Mass Fraction Burned (MFB) data as a function of the crankshaft angle (°CA). The kinetic equation can be represented as $d(MBF)/d(°CA) = K\beta^{-1}f(\alpha)$. Where k is the Arrhenius rate constant, β is the engine speed, and f(α) is the kinetic mechanism. For complex reactions, such as combustion, a single kinetic model usually fails to represent the multi-step reactions occurring in the process. For these cases, a multilayer perceptron (MLP) neural network can be used to calculate the contribution of different kinetic models to describe the experimental data. The neural network's architecture is based on Araujo et al. [4]. This methodology allows one to describe the macroscopic global mechanism of the combustion without the need to define the set of reactions as free radicals [5]. If a significant change in the contribution of the global mechanism occurs during the process, it is indicated by the kinetic compensation effect (KCE). The correlation of ln(A) X Ea shows that a major event is linear with simultaneous reactions. However, if there is a break in linearity, the kinetics study should be separated into consecutive multiple events.

Results and Discussion

Three non-overlapping normalized MFB curves, α, were selected for the kinetic study. These data are presented in Figure 1. The KCE was calculated, revealing no significant deviations from linearity. Consequently, only one event was considered for each sample kinetic analysis.

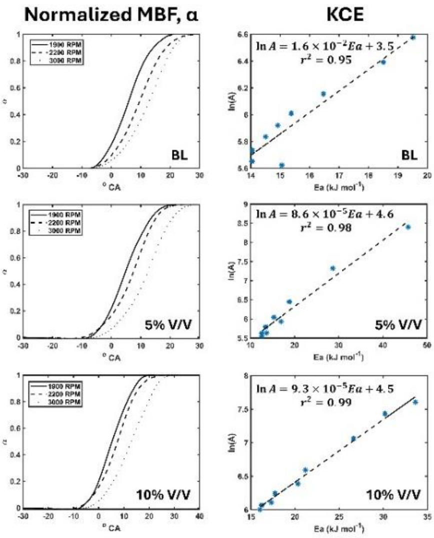

Figure 1. Experimental MFB data (left) to bioethanol baseline (BL) and with 5%v/v and 10% v/v Hydrogen Gaseous Mixture (HGM). KCE (right) for each sample.

The average values of Ea and ln(A) for the bioethanol combustion with a hydrogen-rich mixture are greater than for the baseline (BL) ethanol combustion. The mean values of activation energy for BL, 5%, and 10% are 15.8, 20.0, and 22.0 kJ mol^{-1}, respectively. The values for ln(A) are 5.9, 6.3, and 6.6.

The contribution of the kinetic models was calculated for the MLP neural network for all samples. The samples present a high contribution of the first order (F1) and Avrami-Erofeev with order 1.5 to 3 (Am1.5 to Am3) mechanisms. The F1 model also represents an Am1 mechanism; therefore, the combustion of samples follows the mechanism of nucleation followed by diffusion, which guarantees the system's homogeneity.

The high values to Ea for bioethanol with hydrogen-rich mixtures can be related to a high energy necessary to break the hydrogen bond, as it is a very stable molecule. Interestingly, once the process is initiated, the molecularity is increased, as the hydrogen (nucleation points) act as a local heat source [6], contributing to ethanol combustion. Consequently, this phenomenon promotes an increased behavior in the frequency factor, which has a bigger influence on the rate constant than the increase in activation energy.

The Graphical Abstract illustrates that increasing the hydrogen concentration in the bioethanol mixtures increases the rate constant and reduces the consumption under identical experimental setups. Also, it is observed that there is a direct association between a steady reduction in the engine's indicated specific fuel consumption (ISFC) and an improvement in combustion efficiency. HGM is distinguished by its minimal ignition energy, swift flame propagation speed, and extensive combustion range. These characteristics lead to a lowered specific fuel consumption when hydrogen is employed in spark-ignited combustion engines. Furthermore, the rapid flame spread of hydrogen enhances turbulence and guarantees a consistent flame distribution, which agrees with the noted rise in the rate constant.

Conclusions

The combustion kinetics of bioethanol and bioethanol with a hydrogen-rich mixture were studied using MFB data from SCRE tests. The methodology allows the explanation of the combustion kinetics in an internal combustion engine. In this work, samples of Bioethanol pure, and Bioethanol with Hydrogen Gaseous Mixture (HGM) of 5%v/v and 10%v/v were tested in steady-state conditions, considering urban driving operation points. The experiments indicate that increasing the concentration of the HGM implies an increase in the rate constant and an improvement of the combustion efficiency and ISFC reduction. In conclusion, the correlation between the combustion study and AOTs can be established through the concept of improving reaction efficiency. Our study highlights the potential benefits of HGM utilization in spark-ignited combustion engines, emphasizing its role in improving efficiency and reducing specific fuel consumption.

Acknowledgments

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References

[1] de Almeida L.Q., et al., *International Journal of Hydrogen Energy* 40 (2015) 6988.
[2] Ayad SMME, et al., *International Journal of Hydrogen Energy* 49 (2024) 744.
[3] Amaral LV et al., Case Studies in Thermal Engineering 57 (2024) 104316.
[4] Araujo NRS, et al., Thermal Science and Engineering Progress 36 (2022) 101490.
[5] Leplat, Nicolas, et al. *Combustion and Flame* 158.4 (2011) 705-725.
[6] Ooi JB, et al., *International Journal of Energy Research*. 41 (2017) 2258.