Kinetic study of gasoline combustion in Research Engine: Chemical and mechanical strategies to improve performance

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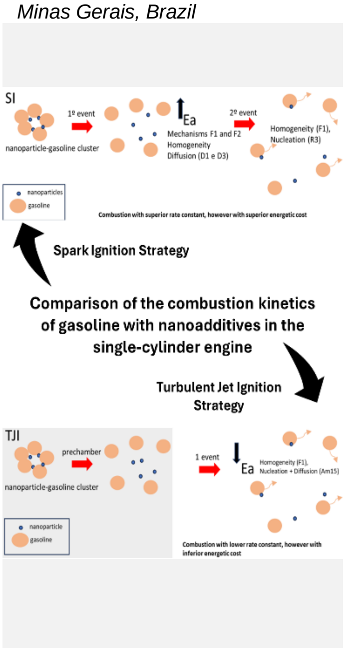

This work investigated the effects of adding nanoparticles to Brazilian commercial gasoline and the impact on combustion in two different engines, which were modified to improve advanced oxidation technologies. The methodology includes experimental tests on a Single Cylinder Research Engine (SCRE) operating with spark ignition (SI) and Turbulent Jet Ignition (TJI). Mass Fraction Burned (MFB) data were used to determine combustion kinetics using artificial neural networks. In the SI engine, the results showed that nanoparticles promote an increase in intermolecular interaction with the fuel, requiring more energy for combustion and vaporization, which is confirmed by the high values of activation energy at the beginning of the process. However, the molecularity is also enhanced, which promotes higher values of the rate constants. For the TJI engine, the prechamber contributes to the initial dissociation of gasoline and nanoparticles cluster and combustion occurs with lower activation energy values. The combustion process of nanoparticles is more exothermic than pure fuel. In this way, they contribute to greater combustion efficiency, with higher rate constants. The TJI engine promoted a more efficient combustion process, with a single event, unlike the SI engine, which presented two events. These results provide information about the oxidation processes in engines and highlight the impact that advanced technological modifications, performed in engines, have had on the combustion process, corroborating modelling and simulation of AOTs.

Introduction

Projections point to continued use of gasoline as an energy source in the coming decades and call for initiatives that increase its conversion efficiency and reduce the environmental impact. In the transportation sector, which is mostly dependent on internal combustion engines, the use of catalyst nanoparticles and combustion prechambers have been highlighted as viable alternatives that make the use of gasoline more attractive from an economic and environmental point of view [1,2]. In this sense, this work investigates the effects of adding nanoparticles to gasoline, based on experimental tests on a SCRE operating in TJI and SI combustion mode. In addition to analysing the engine performance data, an understanding of the combustion chemical kinetics is sought through a neural network assessment based on MFB curves [3].

Significant advances in engine efficiency can be achieved with advanced combustion technologies, such as TJI. This technology allows engines to operate with leaner mixtures, increasing efficiency and reducing the need for pollutant treatment systems. Furthermore, the use of nanoparticles has shown potential to improve the performance of internal combustion engines, accelerating combustion and reducing pollutants, which contributes to its sustainable development.

This work aims to evaluate the feasibility of reducing total operating costs and environmental gains by adopting advanced combustion strategies with both, chemical and mechanical technologies.

Material and Methods

Experimental tests were carried out on the SCRE on a dynamometer bench with commercial gasoline added with nanoparticles (NP). The NP used are commercial, with a patent-protected formulation. However, this study does not aim to characterize it, but to highlight its influence on the combustion process in engines. The combustion process was evaluated for the SI and TJI combustion strategies. The AVL SCRE engine was used at the Indicated Mean Effective Pressure (IMEP) of 7.0 bar at engine speeds of 1900, 2200 and 3000 RPM. From the experimental MFB data obtained, it was possible to study the combustion kinetics, determining the activation energy (Ea) and frequency factor (A) throughout the process. Using Artificial Neural Networks, it was possible to determine the set of kinetic models, f(α), that best fits the experimental data.

Results and Discussion

Figure 1 presents the MFB data for the two engines and on the right are the kinetic compensation effect (KCE) curves, with the relationship between lnA x Ea, assuming the Arrhenius equation [3]. The system must present a linear correlation for processes that occur in a single event. For this test, the activation energy and frequency factor were determined considering the global event. As can be seen, the combustion of gasoline with nanoparticles in the SI engine occurs through a two-stage process, with the second stage starting after 80% of conversion. Therefore, the data must be separated into: Event 1 (10 to 70% conversion) and Event 2 (80 to 90% conversion). The straight-line equations and the correlation index (R^2) are highlighted in Figure 1. The data in the TJI engine presents a single curve, indicating that the process occurs in one step.

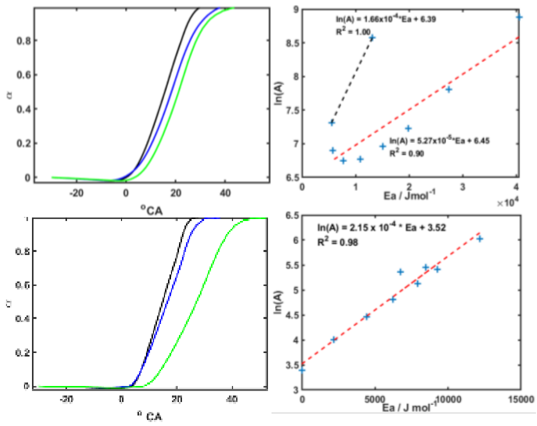

Figure 1. MFB data for gasoline with nanoparticles and KCE in the SI (top) and TJI (bottom) engine. Engine speed 1900 rpm (black), 2200 rpm (blue) 3000 rpm (green).

The Ea values throughout the combustion process show that the system with gasoline and nanoparticles in the TJI engine presented much lower activation energy values compared to the same fuel in the SI engine (1st and 2nd events). The reduction was significant, especially compared to the 2nd event in SI engine. The high energy values at the beginning of combustion in the SI engine suggest that the interaction between gasoline molecules and nanoparticles promotes the formation of an agglomerate that requires more energy to be broken and subsequently promote vaporization and burning. The prechamber in the TJI engine acts to previously dissociate this cluster, resulting in lower activation energy values for the combustion process in the chamber. The kinetics study with neural network provided insights into the combustion mechanism for both engines. Combustion of nanoparticle added to gasoline in SI engines begins requiring homogeneous system (F1 and F2 mechanisms) and diffusion mechanisms (D1 and D3), which depends on nanoparticle dispersion. For the 2nd event, the process occurs by the F1 and R3 (fuel vaporization) mechanisms. Combustion in TJI engines interestingly shows lower rate constants, due to the suppression of the initial exothermic stage, present in SI engines. In TJI, the prechamber facilitates combustion, but the dependence on molecular conformation, corroborated by the Avrami-Erofeev order n=1.5 (Am15) model, reduces the reaction rate. The exothermic step in the SI engines, which breaks the nanoparticle-gasoline cluster, increases the rate constant, an effect not observed in the TJI due to the prechamber. The graphical abstract presents a schematic representation. Traditional mechanisms to gasoline combustion are described by free radicals [4], but in this study, it is obtained the mechanism related to the macroscopic behaviour [3]. The reduction in activation energy in the case of the TJI engine is more effective in improving combustion parameters: greater combustion efficiency, conversion efficiency and lower indicated specific fuel consumption, (ISFC). The reduction in energy costs to break the nanoparticle-gasoline cluster causes greater efficiency and lower consumption in the TJI engine, although it has a lower speed constant.

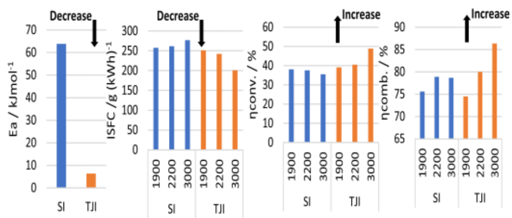

Figure 2. Relationship between combustion kinetic parameters (Ea) and engine performance parameters.

Conclusions

In this study, it was investigated the effects of adding nanoparticles to Brazilian commercial gasoline and the impact on the combustion in two engines. It was used experimental tests on a SCRE with SI and TJI combustion mode, in addition to chemical kinetics analyses with neural networks applied to MFB data. The correlation between kinetic parameters and engine efficiency parameters obtained through SCRE tests offers a robust tool for understanding the combustion mechanism and to propose new technologies to improve combustion efficiency in real systems.

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