Combustion Kinetics of Gasoline with Commercial Nanoparticle: Analysis Using Artificial Neural Network

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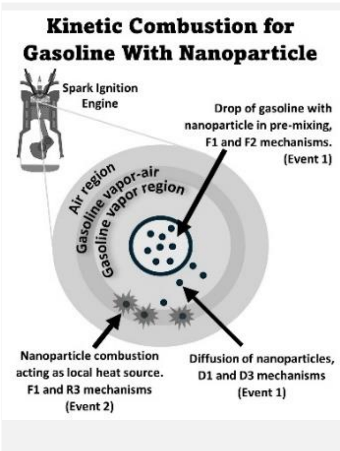

This work studied the impact of a commercial nanoparticle added to regular Brazilian gasoline in the combustion process. The tests were carried out in a Single Cylinder Research Engine (SCRE) operating at a fixed indicated mean effective pressure (IMEP) of 7 bar at three engine speeds (1900, 2200, and 3000 rpm). From the Mass Fraction Burned data (MFB), an artificial neural network methodology was used to determine the kinetics. The correlation between the study of nanoparticles in gasoline and advanced oxidation technologies (AOTs) lies in the enhancement of reaction rate and efficiency. In the study, the addition of commercial nanoparticles to Brazilian gasoline was found to act as a local heat source, contributing to combustion by increasing the rate constant. The rate constant is one of the most important kinetic parameters, which can be related to engine performance. A fuel with a superior rate constant is favorable because it reduces heat loss to the cylinder walls, allowing enhanced combustion efficiency parameters and reduced consumption, verified by the indicated specific fuel consumption for the samples.

Introduction

Liquid fuels derived from petroleum are the main source of power for internal combustion engines (ICEs). However, the industry faces a demand for change driven by economic, political, and environmental factors. Change is necessary to guarantee energy security, regulate gas emissions, and improve local air quality. New criteria for cleaner energy are crucial for reducing pollution. However, fossil fuels will still power most vehicles due to their ready availability and distribution. Effective technologies to boost energy efficiency are essential to shift this fuel to cleaner energy. Adding catalyst nanoparticles to fossil fuels could make internal combustion engines more eco-friendly [1].
Mixing nanoparticles (NP) with liquid fuels aims to improve fuel quality and combustion performance. Desirable properties of these nanoparticles include reduced ignition delay in burners, lower fuel consumption and pollutant emissions, increased oxygen concentration in the combustion chamber, and enhanced air-fuel mixture burning velocity [2].
This work studies the combustion process of commercial regular Brazilian gasoline, with and without the addition of commercial nanoparticles in a Single Cylinder Research Engine (SCRE).

Material and Methods

Experiments were performed on an AVL 0.45 L spark-ignited (SI) SCRE fueled with Brazilian commercial gasoline with 0.01%v/v and without nanoparticles.The nanoparticles used have a patent-protected formulation. The aim of this study is to study their influence on the combustion kinetics in engines. All the tests were performed at a fixed indicated mean effective pressure (IMEP) of 7 bar at three different engine speeds: 1900, 2200, and 3000 rpm. These operating points were selected because they represent typical conditions for vehicle commercial engines operating in urban driving cycles.
The chemical kinetics was studied from the Mass Fraction Burned (MFB) data as a function of the crank angle position (°CA) with constant engine operation speed, $\beta = d(°\mathrm{CA})/dt$. It was determined the activation energy (Ea), frequency factor (A), and mechanism of reaction $(f(\alpha))$ throughout the combustion process using artificial neural network. The multilayer perceptron (MLP) neural network provides the contribution of all kinetic models adopted to describe the experimental data of MFB as a function of the crankshaft angular position. The neural network's architecture is based on Araujo et al. [3].

Results and Discussion

A priori test of compensation effect [3] must be performed. In this test, the logarithm of frequency factor is correlated with activation energy, following Arrhenius equation as $ln(A) = ln(k) + Ea/RT$.The system should present a linear correlation, assuming the process occur in a major macroscopic event with simultaneous reactions. Break in linearity represents a strong change in the global mechanism, with consecutives events.
After the compensation effect test, two events were involved in the combustion of the samples. For regular gasoline, it is verified that the second event

starts after 30% conversion. The second event starts later in the system with commercial nanoparticles after 80% conversion.

At the beginning of the process, it was interestingly verified that activation energy for the combustion of gasoline with commercial nanoparticles is greater than that for the combustion of regular gasoline. This result can be related to an increase in intermolecular forces between gasoline molecules and nanoparticles, which requires more energy to break the interaction, vaporization, and subsequent burning. After 60% conversion, but still, in Event 1, the Ea of the gasoline combustion process with the nanoparticle is lower than that of the regular gasoline. It is then suggested that the nanoparticle can act as a local heat source, [4] contributing to combustion and reducing the Ea of the process. In Event 2, although it is observed that the activation energy of gasoline with nanoparticles remains almost constant until the end of the process, it is always superior to the combustion process of regular gasoline, which suggests strong intermolecular interaction until the end of combustion. This activation energy of Event 2 can be attributed to the complete vaporization of the system. This result is corroborated by the type of mechanism the MLP neural network determines.

The combustion of gasoline with nanoparticles begins in Event 1 with first and second order (F1 and F2) and Diffusion (D1 and D3) mechanisms. Models F1 and F2 indicate that the process initially occurs in a homogeneous system, depending on the adequate dispersion of nanoparticles in gasoline, with reaction orders 1 and 2. Simultaneously, the process also depends on the diffusion of nanoparticles to the gasoline vapor-air region, where the combustion of these particles occurs. The two steps for the Event 1 mechanism can be called i) pre-mixing (models F1 and F2) and ii) diffusion (models D1 and D3). Considering the global process, after 80% of conversion, the mechanism is altered and Event 2 starts under the influence of model F1, predominantly dependent on the homogeneity of the system, followed by the contraction model (R3), which is related to the drop volumetric contraction in the vaporization process. The graphical abstract represents this schematic representation of the gasoline with the nanoparticle combustion process. The described mechanism is consistent with droplet combustion studies with nanoparticles [2,4], showing that this methodology can describe the kinetics using direct results from the research engine.

In the gasoline vapor-air region, nanoparticles work as local heat sources, contributing to combustion with a decrease in activation energy and an increase in molecularity, (or frequency factor), which consequently results in an increase in the rate constant (k) of the process, compared to regular gasoline. Figure 1 shows the comparison between the rate constants and combustion efficiency (η_c). It is also compared with the indicated specific fuel consumption (ISFC). It is noticed that when the nanoparticles were added to the gasoline, the combustion efficiency was improved 4.0% (1900 rpm), 5.1% (2200 rpm), 5.1% (3000 rpm), and the ISFC was reduced 3.00% (1900 rpm), 5.1% (2200 rpm), 2.5% (3000 rpm) compared to the pure commercial fuel. The difference between the rate constants of gasoline combustion with and without nanoparticles considering a global process was 18% (1900 rpm), 13.7% (2200 rpm), 15.6% (3000 rpm).

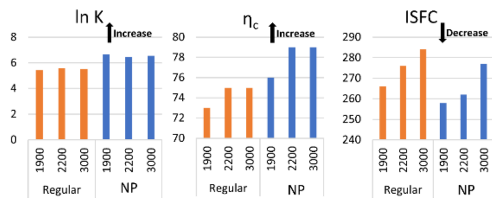

Figure 1. Correlation between the rate constants (lnK), combustion efficiency (η_c), and Indicated specific fuel consumption (ISFC) of the SCRE operating at 7 bar IMEP with common and catalyzed gasoline (NP).

Conclusions

This article presented a combustion kinetics study of Brazilian commercial gasoline, with and without the addition of nanoparticles, to investigate the effects on combustion. The work presented experimental tests carried out on a SCRE and a chemical kinetics study based on the application of neural networks. The validation provided by the SCRE tests constitutes a robust tool for describing combustion kinetics applied to real systems. In the context of AOTs, the principle of enhancing reaction rate can be analogously understood through the role of nanoparticles in the combustion study by providing localized heat that speeds up the combustion reaction and provides a more sustainable path for the current energy transition scenario. Fossil fuels are still likely to be the main source of energy in the coming years, and for this reason, alternatives that seek to increase the energy efficiency from their usage are in line with global decarbonization.

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