# Shedding light on ethanol combustion in spark ignition engines: determining the kinetics using artificial neural networks

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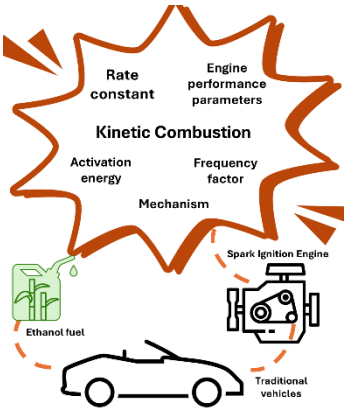


This study aims to determine the combustion kinetics of commercial hydrated ethanol in a Single Cylinder Research Engine (SCRE) with spark ignition. The experimental data were obtained at the indicated mean effective pressure (IMEP) of 7 bar, at speeds of 1900, 2200 and 3000 rpm. An artificial neural network (Multilayer Perceptron – MLP) was applied in Mass Fraction Burned (MFB) data to characterize the combustion kinetics. The results demonstrate increasing behaviour for activation energy values, indicating that the combustion of hydrated ethanol in the engine is not an autocatalytic process. The combination of mechanisms in the process highlights the Avrami-Erofeev models (order 1.5 and 2) and the first order model (F1). The determined rate constants did not vary significantly with engine speed, which explains the experimental results of efficiency parameters and specific fuel consumption of the engine in these different speeds.

## Introduction

The global electrification of automobiles is required to reduce $CO_2$ emissions, with public policies and vehicle manufacturers mobilizing to reduce or even discard the use of fossil fuels. However, the effectiveness of electrification depends on the renewable origin of electrical energy. It is necessary to consider the entire life cycle, that is, not only operation, but also production, maintenance, and residue disposal. The traditional vehicle using fully renewable fuel is environmentally competitive, if not superior, compared to the electric configuration also using renewable sources throughout its life cycle.

In Brazil, the widespread use of flex-fuel vehicles and hydroelectric generation place the country in a unique position in terms of renewable energy matrix. Ethanol emerges as a sustainable and economically viable solution, while ethanol-enriched gasoline serves as a transitional solution, requiring engines with optimized efficiency to minimize environmental impact [1].

Studies of combustion kinetics are essential to understand and optimize the fuels in engines. In this work, it was presented the results using Artificial Neural Networks that use experimental data of Mass Fraction Burned (MFB) to determine the kinetic parameters of combustion in engines, relating the kinetics to engine performance parameters [2].

## Material and Methods

For experimental tests, a SCRE with spark ignition (SI) from the AVL was used. The Artificial Neural Networks methodology [2] was used to determine the kinetic triplet, consisting of the activation energy (Ea), pre-exponential factor (A) and reaction mechanism f(α) which were obtained from MFB data in 3 engine speed, 1900, 2200 and 3000 rpm with load (IMEP) of 7,0 bar. This experimental condition was chosen as it represents urban operating conditions for engines of this type.

The MFB data are used to characterize combustion in engines and the respective performance parameters (combustion efficiency, conversion efficiency and indicated specific fuel consumption (ISFC).

## Results and Discussion

Figure 1 presents the MFB data for the experimental engine conditions. From these data it was possible to calculate the kinetic triplet of ethanol combustion in the engine. The activation energy was determined by isoconversional methodology [2] and ranged from 10 to 24 kJ $mol^{-1}$, with lower values at the beginning of the process and a maximum value at 70% of conversion. The increasing behaviour for activation energy values suggests that the combustion of hydrated ethanol in the engine is not an autocatalytic process, that is, energy must be continuously supplied up until this degree of conversion. Frequency factor values were also obtained throughout the process and the behaviour was like the activation energy. The variation in activation energy and frequency factor can be seen in Figure 2.

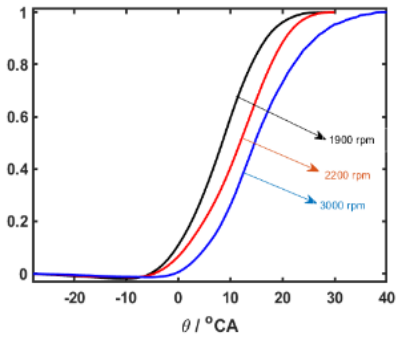


**Figure 1.** MFB data for ethanol combustion in SCRE at 3 engine speeds, 1900 rpm (black line), 2200 rpm (red line) and 3000 rpm (blue line).

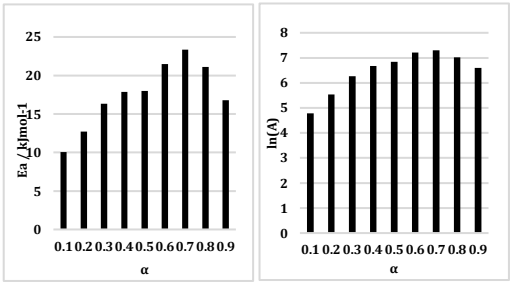


**Figure 2.** Activation energy and Frequency factor along the combustion process.

The combustion mechanism is calculated through the neural network methodology and is given by the combination of kinetic models, which describes the global ethanol combustion process in a more appropriate way, since the MLP residual error for adjustment is lower than that of the individual models. The Avrami-Erofeev models (order 1.5 and 2) and the first order model (F1) presented higher contribution values, with the Avrami-Erofeev models indicating that the process occurs with a nucleation step followed by diffusion and the F1 model indicates that for the complete combustion of ethanol, the system must be homogeneous. The nucleation step can be related to the chemical potential of ethanol in the liquid phase, which becomes greater than the chemical potential of ethanol in the vapor phase in the combustion region.

With the kinetic parameters determined along the process, the rate constant can also be determined using the Arrhenius equation [2]. It can be seen in Figure 3 that the speed constants did not show significant variation when changing the engine speed. This result can be correlated with engine performance parameters such as combustion efficiency and conversion efficiency values, as well as ethanol consumption (ISFC). These also did not show significant deviations between the 3 engine speeds, since the rate constants of the combustion process also did not show significative deviations. This result is in line with evidence from the literature [3], which correlates combustion speed with engine performance parameters.

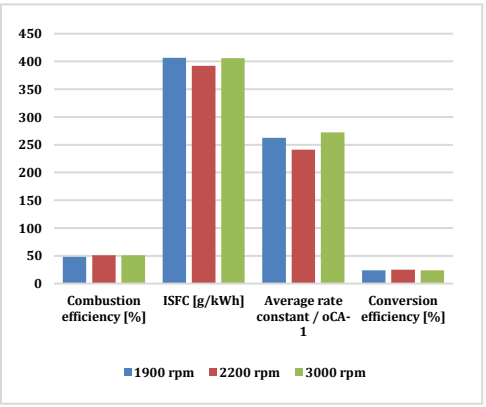


**Figure 3.** Engine performance parameters and kinetic rate constant correlation to ethanol combustion in SCRE.

## Conclusions

This study used Mass Fraction Burned (MFB) data to determine the kinetic triplet of ethanol combustion in a single-cylinder research engine. Artificial neural network adjusts the kinetic models with high precision. The activation energy increased along the combustion process, indicating that the process is not autocatalytic. The kinetic rate constants remained stable at different engine speeds, reflecting the consistency of the engine performance parameters. The methodology allowed a detailed analysis of ethanol combustion and its influence on engine performance parameters, which supports the future proposal for changes in fuels and engines, to make them more efficient.

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