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Estimating gasoline performance in internal combustion engines with simulation metamodels

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HIGHLIGHTS

- Predictions of distinct gasoline effects on the behavior of an engine performance.
- Metamodels were generated using radial basis functions and kriging techniques.
- The "leave-one-out" cross-validation procedure was applied to select metamodels.
- Most of the prediction residuals were lower than 3%.

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ABSTRACT

The accurate simulation of fuel properties' influence in the performance of internal combustion engines is a very complex subject and combines many physical and chemical concepts such as combustion phenomena, chemical kinetics, fluid dynamics, turbulence and thermodynamics. In order to circumvent the complexity of these concepts, many of simulations packages for engine performance usually consider standard or surrogate fuels, which might not be enough for new fuel developments in some cases. This study aims to evaluate the influence of different formulations of gasoline on the behavior of a flexible fuel engine, relating the physicochemical properties of fuels with performance, efficiency and gaseous emissions. Based on an experimental dataset, metamodels were generated using different radial basis functions and kriging techniques in order to accurately predict torque, fuel consumption, specific fuel consumption, global efficiency and CO_2 emission with twelve blends of iso-octane, *n*-heptane, toluene and ethanol at different engine speeds and load conditions. The "leave-one-out" cross-validation procedure was applied to automatically select the best metamodel for each case. Metamodels were able to estimate the experimental results of five fuels within the 95% confidence intervals and most of the prediction residuals were lower than 3%.

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1. Introduction

Early in the history of fuel production, only a few requirements were specified to ensure that fuels were capable of running engines and vehicles with reasonable performance. The octane number was probably the most important property at that time [1]. From the 1970's onwards, with the growth of environmental concerns and implementation of emission regulations, other properties were added to the fuel specifications [2,3].

To meet regulatory metrics and achieve better performances, each new engine technology requires a corresponding improvement in fuel quality. Thus, the development of high-quality fuels for internal combustion engines has been widely expanded and has become a major research topic in the last decades for the world's leading oil and fuel companies.

In order to cover the key quality attributes of a new fuel, such as engine performance, fuel consumption, pollutant emissions, engine cleanliness and durability, developments usually require a large number of distinct experimental tests. This leads to

Abbreviations: RBF, radial basis functions; DACE, Design and Analysis of Computer Experiments; EAC, anhydrous ethanol; EHC, hydrous ethanol; LHV, lower heating value; AKI, anti-knock index; MON, motor octane number; RON, research octane number; SFC, specific fuel consumption; RAAE, Relative Average Absolute Error; RMAE, Relative Maximum Absolute Error.

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expensive laboratory arrangements, large amounts of different fuel formulations, vehicles, engines and specialized personnel that can result in huge budgets and schedules. A very attractive alternative to reduce costs and development time is the use of computational simulation during a first screening of fuels and/or additives formulations, optimizing the experimental effort [4–9].

Currently, several very powerful engine simulators [10–14] are commercially available and are widely used by the automotive industry to design and optimize new engines and vehicles. These packages are primarily dedicated to engines development and usually consider standard or surrogate fuels to evaluate performance for different engine setups. However, fuel development needs exactly the opposite configuration, setting the engine parameters and changing the compositions and properties of fuels.

Phenomenological approaches to simulate fuel performances related to their physico-chemical properties deal with very complex disciplines such as chemical kinetics, fluid dynamics, combustion, and thermodynamics [9,15]. The chemical kinetics of gasoline is under challenging research and it is not yet possible to completely model the combustion of gasoline. Calculations in this area require a large number of coupled equations with very high computational effort, which in fact are still not completely dominated [16–18].

Notwithstanding, the use of statistical techniques based on experimental data to evaluate the behavior of engines and fuels has been increasing in recent years. For example, Traver et al. [19] developed neural network metamodels to predict gaseous emissions of a Navistar T444 engine, related to combustion chamber pressure information. Sayin et al. [20] presented a neural network metamodel to predict specific fuel consumption, thermal efficiency, exhaust gas temperature and gaseous emissions from an engine running with four gasolines of different octane numbers.

In other studies, Najafi et al. [21] estimated the performance of an engine powered by different blends of ethanol and gasoline using a neural network metamodel; Colaço et al. [22] presented a hybrid optimization metamodel to evaluate the pressure inside the combustion chamber of an engine related to different blends of diesel and biodiesel; Abuhabaya et al. [23] used polynomial response surfaces to estimate performance and emissions of a diesel engine running with different biodiesel blends. In addition, other works present the use of metamodels as feasible computational alternatives to accurately predict the performance of engines and fuels [24–28].

This work proposes the use of response surface approaches, based on radial basis functions (RBF) and kriging [29–32] to predict the influence of different fuels on the performance of an engine. Prediction metamodels for performance, efficiency and gaseous emissions were generated from an experimental data set of a flexible fuel engine running in different operating conditions and using distinct surrogate fuel blends of isooctane, *n*-heptane, toluene and ethanol [4,5]. The validation results show that the proposed approach was able to accurately predict the performance of Brazilian gasolines under different engine operating conditions. This simulation algorithm has been successfully implemented in the Matlab® language and might become a helpful auxiliary tool in the development of new fuels.

This paper is organized as follows. Brief details on RBF and kriging techniques are presented in Section 2. Section 3 describes the experimental setup and also the configuration of implemented metamodels. Results of validation, prediction and metamodels accuracy are presented in Section 4. Finally, some conclusions are listed in Section 5, including proposals for future works.

2. Metamodels techniques

Metamodels or response surfaces are analytical models based on different mathematical and statistical techniques and used to approximate the behavior of complex phenomena or expensive simulation models in function of observed multidimensional data [33–36].

The general form of a metamodel can be represented by

$$y(\mathbf{x}) \approx Y(\mathbf{x}) = g(\mathbf{x}) + \varepsilon(\mathbf{x}) \tag{1}$$

where the estimative $Y(\mathbf{x})$ of the actual value of a quantity $y(\mathbf{x})$, at an observation point $\mathbf{x} \in \mathbb{R}^d$, $d > 0$, is described by a simplified model $g(\mathbf{x})$, plus an error $\varepsilon(\mathbf{x})$. The metamodel definition includes the identification of $g(\mathbf{x})$ and $\varepsilon(\mathbf{x})$.

Many techniques are available for generating metamodels [34], such as polynomial regression, splines, radial basis functions, neural networks, spatial correlations (kriging) and frequency-domain models.

In this paper, radial basis functions and kriging methodologies are investigated. Regarding kriging metamodels, two distinct approaches are applied. One is ordinary kriging that uses the adjustment of an experimental semivariogram to estimate covariances. Another is the so-called DACE method that describes a stochastic process. At last, a hybrid approach between RBF and kriging is also applied to estimate the variances of RBF predictions.

2.1. Radial basis functions

The generation of response surface based on Radial Basis Functions (RBF) was first proposed by Kansa [29], after the work of Hardy [37] on multivariate approximation for topography and other irregular surfaces. This technique is becoming an established powerful approach in recent years to interpolate multidimensional data and simulate different problems in many areas of engineering [25–28,38–40].

For a set of given observed values $y(\mathbf{x})$ associated to their respective spatial locations $\{\mathbf{x}_j;\ j = 1, \ldots, n\}$, the general form of a metamodel based on radial basis functions can be written as [29,41].

$$y(\mathbf{x}) \approx Y(\mathbf{x}) = \sum_{j=1}^{n} \alpha_j \phi(\|\mathbf{x} - \mathbf{x}_j\|), \quad \mathbf{x} \in \mathbb{R}^d, \quad y(\mathbf{x}) \in \mathbb{R} \tag{2}$$

where $Y(\mathbf{x})$ is the estimated value obtained by interpolation [42]. The kernel function $\phi : \mathbb{R}^d \to \mathbb{R}$ that builds the interpolator $Y(\mathbf{x})$ and uses the Euclidian norm $\|\mathbf{x} - \mathbf{x}_j\|$ is called a radial basis function centered at $\mathbf{x}_j$ [43,44]. This approximation is solved for the α_j coefficients from the following system of n linear equations:

$$\mathbf{\Phi a} = \mathbf{y}, \quad \mathbf{\Phi} \in \mathbb{R}^{n \times n}, \quad \mathbf{a}, \mathbf{y} \in \mathbb{R}^n \tag{3}$$

Radial basis functions can assume different forms such as linear, cubical, thin plate, spline, multiquadric, Gaussian, squared multiquadric, and cubical multiquadric [45,46]. In this work, the following forms of kernel functions are investigated:

1. Multiquadric:

$$\phi(\|\mathbf{x} - \mathbf{x}_j\|) = \sqrt{\|\mathbf{x} - \mathbf{x}_j\|^2 + c_j^2}, \quad i,j = 1, \ldots, n \tag{4}$$

2. Gaussian:

$$\phi(\|\mathbf{x} - \mathbf{x}_j\|) = \exp\left[-c_j^2 \|\mathbf{x} - \mathbf{x}_j\|^2\right], \quad i,j = 1, \ldots, n \tag{5}$$

3. Squared Multiquadric:

$$\phi(\|\mathbf{x} - \mathbf{x}_j\|) = \|\mathbf{x} - \mathbf{x}_j\|^2 + c_j^2, \quad i,j = 1, \ldots, n \tag{6}$$

4. Cubical Multiquadric:

$$\phi(\|\mathbf{x} - \mathbf{x}_j\|) = \left[\sqrt{\|\mathbf{x} - \mathbf{x}_j\|^2 + c_j^2}\right]^3, \quad i,j = 1, \ldots, n \tag{7}$$

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