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Full Length Article

On the determination of cetane number of hydrocarbons and oxygenates using Adaptive Neuro Fuzzy Inference System optimized with evolutionary algorithms

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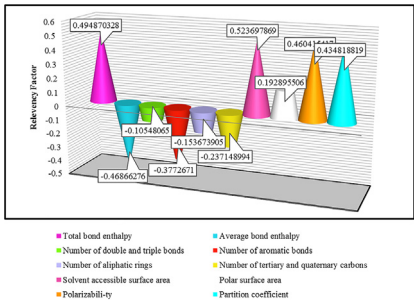
GRAPHICAL ABSTRACT



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ABSTRACT

Prediction of the cetane numbers (CN) of hydrocarbons and oxygenates was considered using the Adaptive-network-based fuzzy inference system (ANFIS) based on the quantitative structure-property relationship (QSPR) approach. In order to construct a general model, descriptors of pure compounds were selected regarding their applicability to all kinds of compounds and ability to provide an accurate knowledge about combustion and evaporation process of fuels inside compression-ignition engines. The predictive capability of optimized ANFIS models based on the Back Propagation (BP) algorithm, Particle Swarm Optimization (PSO), Genetic Algorithm (GA), Differential Evolution (DE), and Ant Colony Optimization (ACO) have been evaluated for estimating CN. In this regard, an extensive databank containing almost all available single-compound CN data of 204 hydrocarbons and 292 oxygenate was gathered from the literature. Obtained results indicated that the PSO-ANFIS approach has the most satisfactory prediction of all considered approaches. Furthermore, an outlier analysis was applied to enhance the model accuracy and detect suspected data points. The statistical coefficients of R-squared (R^2), Mean Squared Error (MSE) and Mean Relative Error (MRE%) were obtained for testing data set as 11.49 & 2.95, 12.53 & 3.28, 25.7 & 7.77, 34.35 & 9.92 & 47.43 & 14.1 for the PSO-ANFIS, GA-ANFIS, ACO-ANFIS, BP-ANFIS, and DE-ANFIS models, respectively. Accordingly, the PSO-ANFIS strategy appeared to be a great tool for estimating CN.

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Table 1
Assigned descriptors for construction of QSPR model.

Type of descriptors	Name of descriptors
Evaporation Relevant	Solvent accessible surface area
	Polar surface area
	Polarizability
	Partition coefficient
Combustion Relevant	Total bond enthalpy
	Average bond enthalpy
	Number of double and triple bonds
	Number of aromatic bonds
	Number of aliphatic rings
	Number of tertiary and quaternary carbons

1. Introduction

Recently, in order to overcome the bad effects of traditional fuels emissions on the environment and human health, tremendous efforts have been focused on developing and utilizing the carbon-neutral renewable fuels. One of the mainstream forms of renewable energy is biomass, which processing of it through several kinds of techniques including the transesterification, fermentation, and pyrolysis, produces most of the renewable fuels such as biodiesel, ethanol, and another complex oxygenates [1]. The majority of components of fossil fuels is hydrocarbons; while the renewable fuels are usually composed of oxygenates including alcohols, fractions of fatty acid methyl esters (FAMEs) and derivatives of furan [2,3]. Oxygenates are usually added to biodiesel in order to enrich the oxygen content tending to decrease the particulate matter emissions [4,5]. However, developing and screening of green alternatives to fossil fuels are still subject to challenges. Because of different chemical and physical characteristic of the renewable fuels, application of them on traditional fuels engines is not directly possible [2].

Cetane number (CN), a widely used parameter by compression-ignition (CI) engineers, is one of the main properties of a fuel to affect its utilization [4]. CN describes the fuel ignition characteristics based on the combustion quality and ignition delay after injection of the fuel in CI-engine. A higher CN value of a fuel refers to the better ignition properties of the fuel, i.e. shorter ignition delay [6]. The diesel fuels show CN in the range of 50 to 58 [7], where the renewable fuels compounds possess CN in a wide range of −5 to 110 [8]. The experimental determination of CN is economically challenging because of expensive and time-consuming procedures. Based on ASTM (American Society for Testing and Materials) D613 standard, where an expensive single-cylinder cooperative fuel research engine is required, approximately 1 L of the sample is needed along with cetane (n-hexadecane) and *iso*-cetane (2,2,3,3,6,8,8-heptamethylnonane) as Ref. [9]. Requiring a large amount of sample fuel, being time-consuming and having high reproducibility error are main disadvantageous of this method [10]. Hence, developing the alternative experimental-based methods to replace the ASTM D613 method attracted attention. A favored and feasible example is ASTM D6890-08 where an Ignition Quality Tester (IQT) is used to measures the ignition delay of the fuel and calculate the derived cetane number (DCN) [11]. The benefits of this method are its lower cost and requirement of less amount of sample (< 50 mL) [10]. It has been shown that its results are precise, having a repeatability of 0.7 for CNs between 33 and 60, and the derived DCN is in a good correspondence with the engine ASTM D613 measured CN [12]. Another American standard test, the ASTM D4737 uses four variable equations for estimation CN from the bulk physical properties of the fuel including density and distillation recovery temperatures measurements [13]. The current version of this standard is ASTM D4737-10 and is applied as a complementary tool in the case that the cetane improver and is not utilized and the results of Test Method D613 are not available [14].

Besides the experimental approaches, supplementary methods can be performed for calculation CN, such as modeling and simulation-based techniques which take advantage of empirical equations for predicting fuel blends CN based on physical properties of the blend including aniline point, density, boiling point, and viscosity. Ladommatos and Goacher tested 22 equations for prediction CN of diesel fuels and figured out that only 8 equations are capable of predicting CN and have standard errors less than 1.91 [15]. But, these equations are applicable in the absence of cetane improvers and generally valid for traditional diesel fuels rather than renewable fuels. For estimating the effects of cetane improver on CN, a molecular composition-based model has been presented in [16], which showed the correlation of the model to CN enhance using a simple empirical correlative equation and resulted in the prediction of CN boost with a standard error of ± 0.8 CN. Furthermore, CN values are derived using the data provided by experimental instruments. For instance, Williams has calculated the correlation between Near-IR Fourier-transform (FT) Raman data and CN of fossil fuels with CN in the range of 42 to 51 [17]. As another study, in [18], Yang et al. used neural networks to predict and correlate the CN and density of diesel fuel determined by chromatography methods. Also, artificial neural network (ANN) models have been developed to estimate the CN of biodiesel employing the

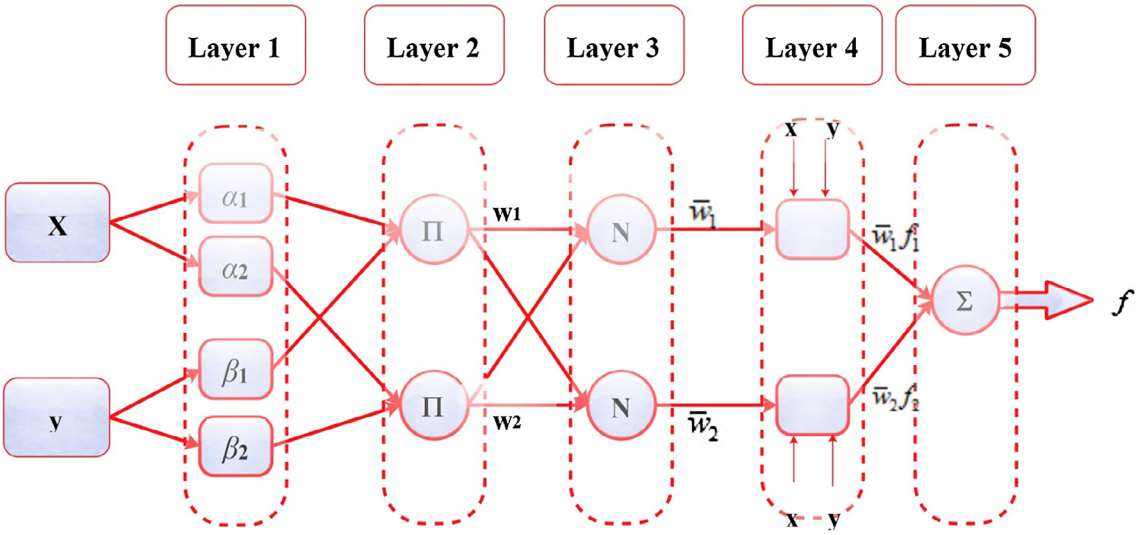

Fig. 1. Schematic diagram and functionality of ANFIS modeling.