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Development of Support Vector Regression-Based Model for Estimating Surface Tension of Methyl Esters Biodiesel

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ABSTRACT

Methyl esters perform similar function as petrodiesel in diesel engines and serve as potential alternative to non-renewable petrodiesel. Adoption of methyl ester as an alternative to petrodiesel is advantageous in the sense that it reduces the amount of greenhouse gases and eventually serves as a cleaner, renewable, less toxic and biodegradable source of energy. Surface tension plays significant roles in fuel atomization and diesel with high surface tension cannot easily form droplets of liquid fuel which ultimately affects the combustion of fuel in engines. Therefore, accurate estimation of surface tension of biodiesel is very essential. Despite the significance of surface tension, its experimental determination is time consuming and expensive which calls for various theoretical predictions and modellings. This work develops support vector regression (SVR)-based model with which surface tensions of eight different types of methyl esters were accurately estimated. SVR-based model was developed by training and testing using SVR algorithm with the best parameters obtained through test-set–cross validation technique. Surface tensions obtained using the developed SVR-based model was compared with the experimental values and the results of Parachor model as well as Goldhammer model. Mean absolute errors and root mean square errors for eight different classes of methyl esters biodiesel were also compared for each of the models. Outstanding performance of the developed SVR-based model over other compared models suggests its potential of being a useful tool in estimating surface tensions of methyl esters for diesel engines applications.

Keywords: Methyl esters biodiesel, support vector regression, SVR-based model, petrodiesel and surface tension.

1. Introduction

Methyl esters belong to chemical compounds known as oleochemicals [1][2]. They are synthesized by reacting fatty oils (from plants or animals) with methanol through a process called transesterification [3]. Methyl esters have been found to perform similar functions as petrodiesel in diesel engines and serve as potential alternatives to petrodiesel [4]. Efforts are being made to reduce the concentrations of greenhouse gases produced from the combustion of petrodiesel from diesel engines, thus there is a need for alternative to petrodiesel which is cleaner, renewable, less toxic, and biodegradable. With biodiesels of methyl esters, little or no modifications are needed to the standard diesel engines. Biodiesels may also be blended with petrodiesel in varying proportion such as B20 (20 % biodiesels, 80 % petrodiesel) and B5 (5 % biodiesels, 95 % petrodiesel), depending on engines. The effects of some of these blends on standard diesel engines have been observed elsewhere [5] and the environmental impacts of their emissions have also been reported [6]. One of the physical properties of methyl esters which make them good candidates for diesel engines is the surface tension. Surface tension is the property of a fluid which is attributed to the cohesive force between the molecules of the fluid. Surface tension controls the atomization of liquid fuel in diesel engines. Efficient diesel engine with excellent combustion and less pollutant emission is achieved with enhanced atomization and proper air-fuel mixing [7]. In order to ensure high combustion efficiency in diesel engines, high quality atomization efficiency is required which can be achieved by using diesel with a very low surface tension [8][9]. Accurate surface tension estimation technique is crucial for selecting certain biodiesels of methyl esters from different kinds of known biodiesels with the appropriate surface tensions. Moreover special biodiesel engines can be designed for any types of methyl esters that can be produced in large quantity with relatively low cost.

SVR is a machine learning tools that estimates desired targets through pattern acquisition. It performs excellently well in many fields of studies ranging from material science[13][14] to reservoir characterization[15]. SVR algorithm combines many unique properties such as accurate generalization and excellent predictive ability, sound mathematical foundation and non-convergence to local minima due to the adoption of convex optimization [15]. These unique properties enhance its generalization and predictive ability even in the presence of dataset with few descriptive features[16][13]. The excellent predictive and generalization ability of SVR in solving numerous problems coupled with the need to have less complex, effective and accurate model in estimating surface tensionS of methyl esters for enhancing atomization of biodiesel fuel, serve as motivations for carrying out this research work.

The results of our modeling and simulations indicate that the proposed model has excellent potential in estimating surface tensionS of methyl esters with high degree of accuracy. The outstanding performance of the developed SVR-based model is justified through persistence closeness of its

estimated surface tension with the experimental values at different temperatures. Low root mean square errors and mean absolute errors of the surface tensions obtained by the developed SVR-based model for different classes of methyl esters as compared with other model such as Parachor and Goldhammer model, further strengthen the excellent performance of the developed model.

The outline of the remaining part of this work is organized as follows: section 2 describes the proposed method. Section 3 contains empirical studies that include the description of the dataset, computational methodology and the optimization strategy. Section 4 presents and discuses results while section 5 states the conclusions and recommendation.

2. Empirical study

2.1 Computational methodology

.Optimum parameters associated with SVR were obtained through test-set-cross validation technique. Procedures for the test-set-cross-validation method used in optimizing the parameters associated with SVR go thus: For every run of training and testing set, values for the generalization performance evaluation (Root-mean square , Correlation coefficient and mean absolute Error) were observed for a group of parameters Ɛ(epsilon) , C (bound on the Langrangian multiplier), kernel option (η) and λ (conditioning parameter for QP methods). The performance measures coupled with the corresponding generalization performance evaluation criteria were noted and recorded. The performance measures and the corresponding parameter values were noted and recorded. The experiment was then repeated using every available kernel function with an incremental step of the values of the parameters. The optimal values of the generalization performance evaluation parameters as well as the associated kernel function with the best performance measure were noted. The overall procedures are summarized as described below:

Step 1: Initial kernel function was selected from the available kernel functions.

Step 2: Selection of the best values for λ , C, $\mathcal{E}$ and kernel option was conducted using test-set-cross-validation method.

Step 3: Steps 1 and 2 were repeated using all the available kernel functions.

Step 4: Kernel functions and the values of the generalization performance evaluation parameters corresponding to the best performance measures were noted as the optimum parameters.

Step 5: Final SVR was trained with the obtained optimum parameters.

Step 6: The generalization performance evaluation criteria for both the training and testing sets as obtained from **Step 5** were recorded and presented in table 3**.**

Table 2: Optimum parameters for the proposed SVR-based model

C	94
Hyper-parameter(Lambda)	1E-7
Epsilon($\mathcal{E}$)	0.3
Kernel option	0.5
Kernel	Polynomial.

3. Results and discussion

3.1. Development of SVR-based model

Development of SVR-based model involves training and testing SVR using best parameters obtained through test-set-cross- validation technique. The developed SVR-based model estimates the surface tensions of methyl esters with high degree of accuracy as indicated from the correlation coefficients. Correlation coefficients of 98.22% and 98.30% were obtained during training and validation stages of the model respectively and presented in Fig. 1 and 2.

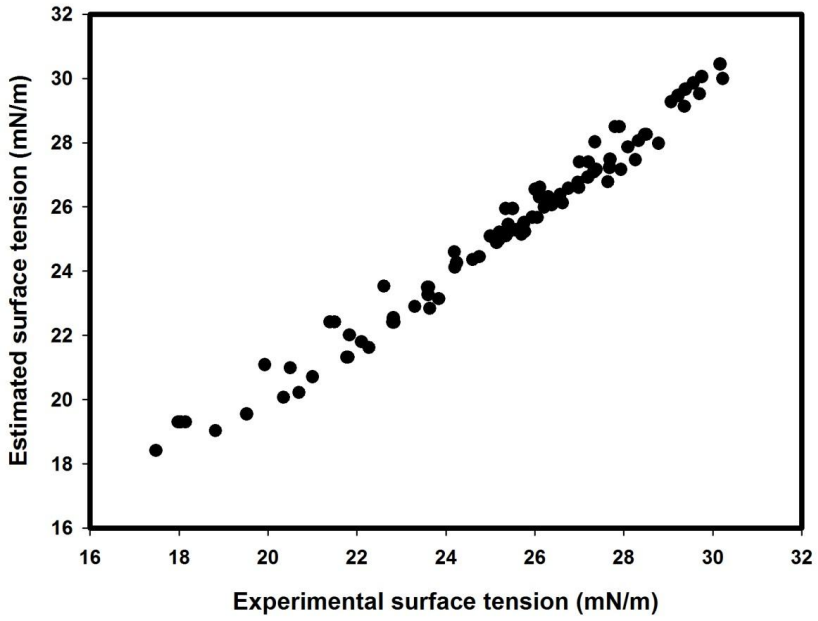

Fig 1: Correlation between experimental and estimated surface tension of esters

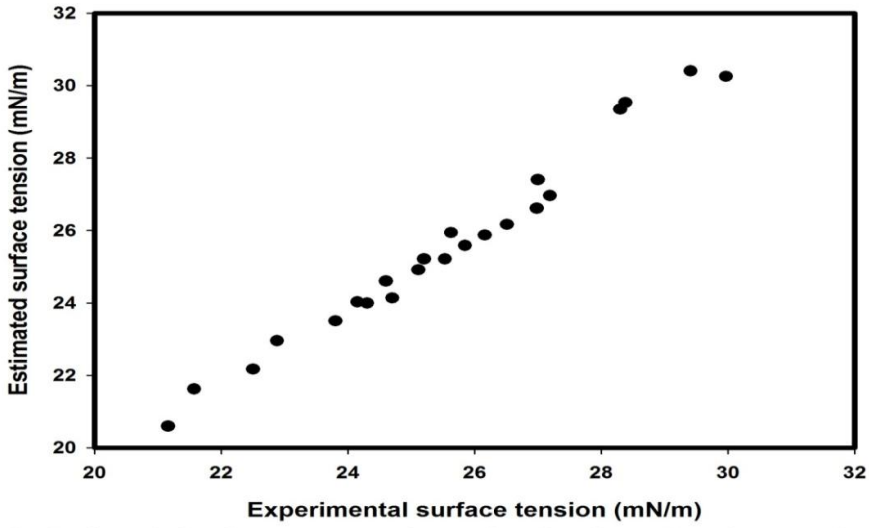

Fig 2 : Correlation between experimental and estimated surface tension of esters

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The RMSE and MAE obtained during the training and testing phase of the developed SVR-based model are presented in table 4. The developed model is characterized with low RMSE and MAE.

Table 3: Determinants of the quality of performance of the developed SVR-based model

	Training	Testing
CC	98.66%	98.90%
RMSE	0.505	0.480
MAE	0.412	0.370

3.2. Comparison of the estimated surface tension with the experimental results and the results of Parachor model and Goldhammer model

We compared the surface tension estimated by the developed SVR-based model at different temperatures with the experimental results and the results of Parachor model illustrated in [17], implemented using the data published in [18]. The results of the developed model were also compared with the surface tensions obtained from Goldhammer model outlined in [17] using the available published data in [26]- [27]. Comparison of surface tensions of methyl heptanoate with the experimental results and the results of Parachor model is presented in Fig 3. The results of Parachor model deviate from the experimental results at low temperatures while the results of the developed SVR-based model agree excellently with the experimental data. Similarly, surface tensions of methyl pentanoate obtained from Parachor model presented in fig.4 deviate from the experimental values at low and high temperatures. The results of the developed model match well with the experimental values.

Fig.5 depicts the comparison of surface tensions of methyl hexanoate obtained from the developed SVR-based model with the results of Parachor model and experimental values. The results of Parachor model agree well with the experimental results at lower temperature and show deviations as temperature increases. The results of the developed SVR-based model show excellent agreement with the experimental data at all temperatures. For Surface tensions of methyl butyrate presented in fig.6, the results of Parachor model deviate in the same manner. The estimated surface tensions of short chain methyl esters could not be compared with the results of Goldhammer model due to unavailability of published data needed for its implementation [26]- [27].

The results of the developed SVR-based model were compared with the surface tensions obtained from Goldhammer model in addition to Parachor model for long chain methyl esters. The comparisons are presented in Fig.7,Fig.8, Fig.9 and Fig.10 for methyl caprylate, methyl caprate, methyl laurate and methyl myristate biodiesel respectively. The results of the developed SVR-based model are closer to the experimental values than the results of the other compared models. This excellent predictive and generalization ability demonstrated by the developed SVR-based model can be generalized to other methyl esters biodiesel in order to select methyl ester biodiesel of appropriate surface tension for particular diesel engine applications.

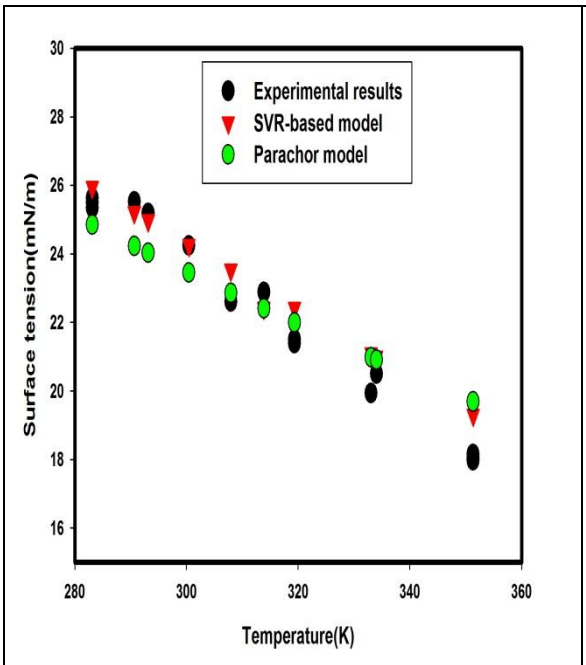

Fig 3 : Comparison between surface tension of methyl butyrate obtained using SVR-based model with experiemental results and the results of parachor model at different temperature (molecular weight of 102.1317 g/mol)

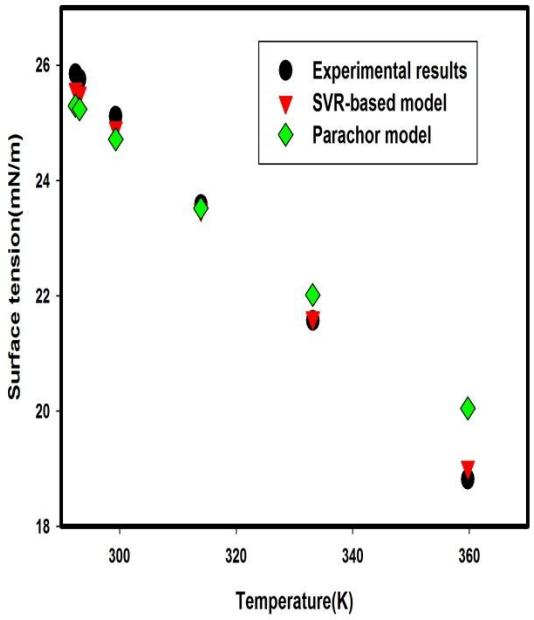

Fig 4 : Comparison between surface tension of methyl pentanoate obtained using SVR-based model with experiemental results and the results of parachor model at different temperature (molecular weight of 116.1583 g/mol)

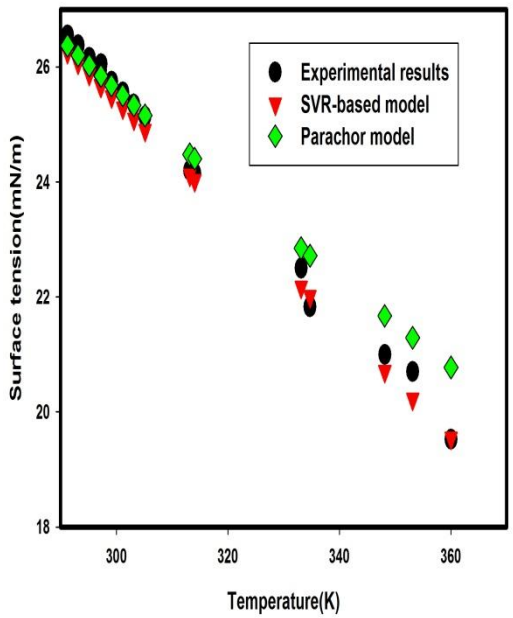

Fig 5 : Comparison between surface tension of methyl hexanoate obtained using SVR-based model with experiemental results and the results of parachor model at different temperature (molecular weight of 130.1849g/mol)

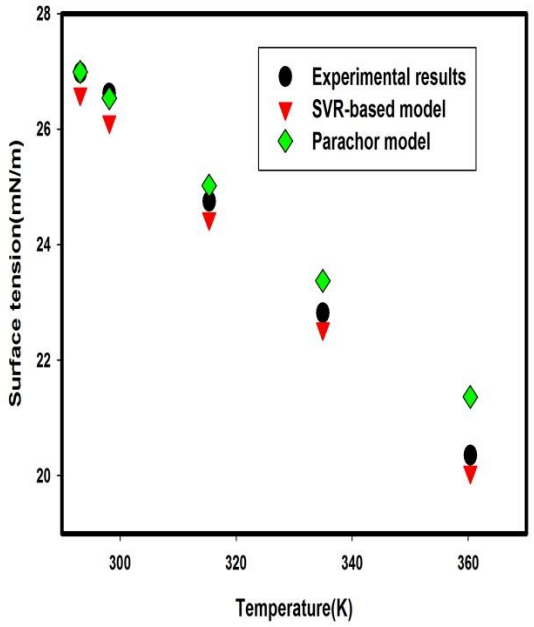

Fig 6: Comparison between surface tension of methyl heptanoate obtained using SVR-based model with experiemental results and the results of parachor model at different temperature (molecular weight of 144.2114g/mol)

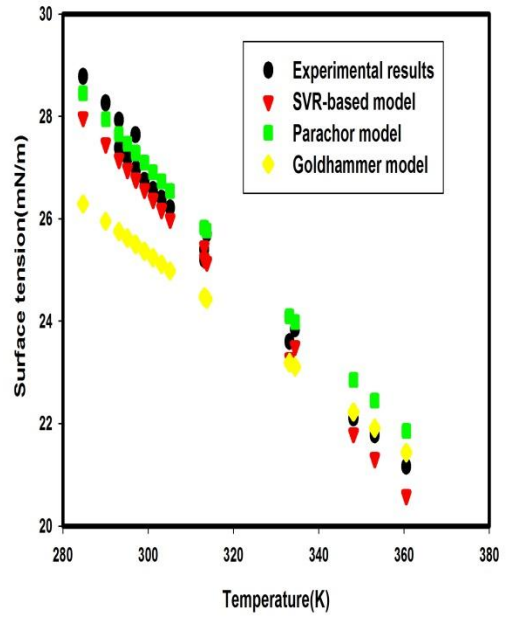

Fig 7: Comparison between surface tension of methyl caprylate obtained using SVR-based model with experiemental results,results of parachor model and Goldhammer model at different temperature (molecular weight of 158.2380g/mol)

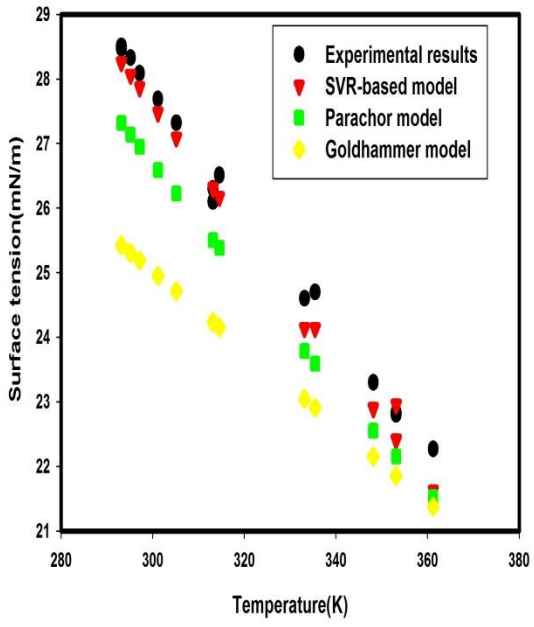

Fig 8: Comparison between surface tension of methyl caprate obtained using SVR-based model with experiemental results,results of parachor model and Goldhammer model at different temperature (molecular weight of 186.2912g/mol)

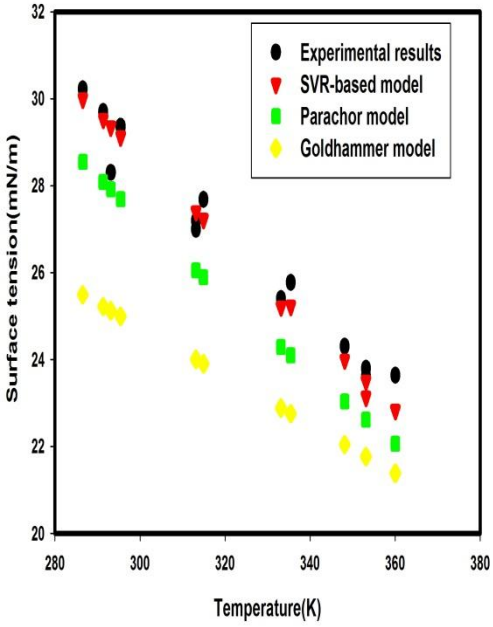

Fig 9: Comparison between surface tension of methyl laurate obtained using SVR-based model with experiemental results,results of parachor model and Goldhammer model at different temperature (molecular weight of 214.3443g/mol)

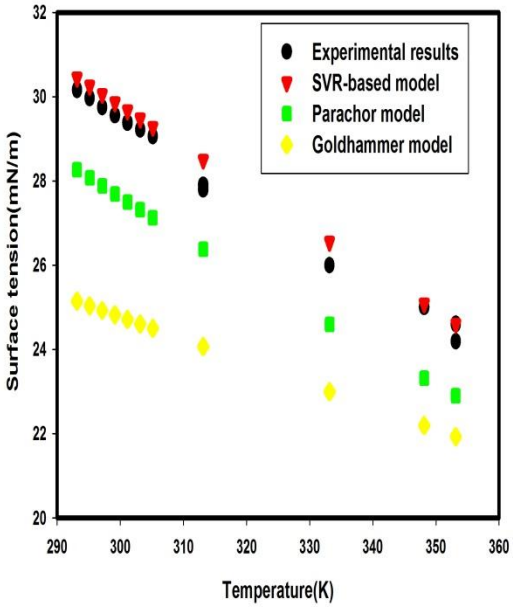

Fig 10: Comparison between surface tension of methyl myristate obtained using SVR-based model with experiemental results,results of parachor model and Goldhammer model at different temperature (molecular weight of 242.3975g/mol)

3.3. Comparison of the root mean square error and mean absolute error of the results of the developed SVR-based model with Parachor and Goldhammer model

We further justify the outstanding performance of the developed SVR-based model by comparing the root mean error and mean absolute error of the results of the model with that of Parachor and Goldhammer model for different classes of methyl esters.

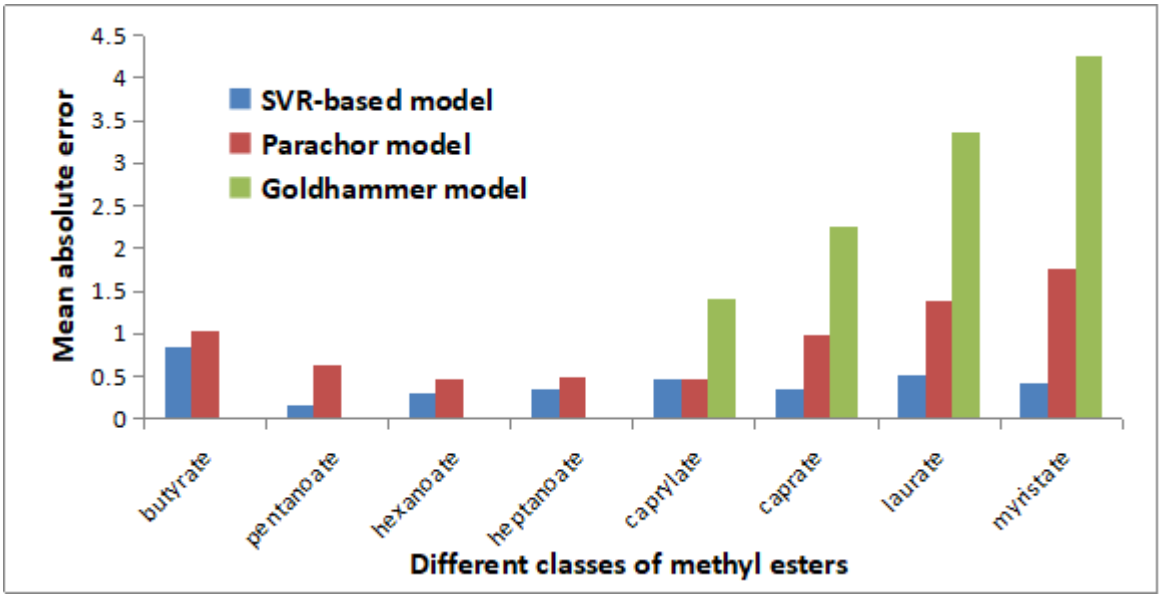

Fig.11. Mean absolute error of the results of the developed SVR-based model, Parachor model and Goldhammer model for different classes of methyl esters

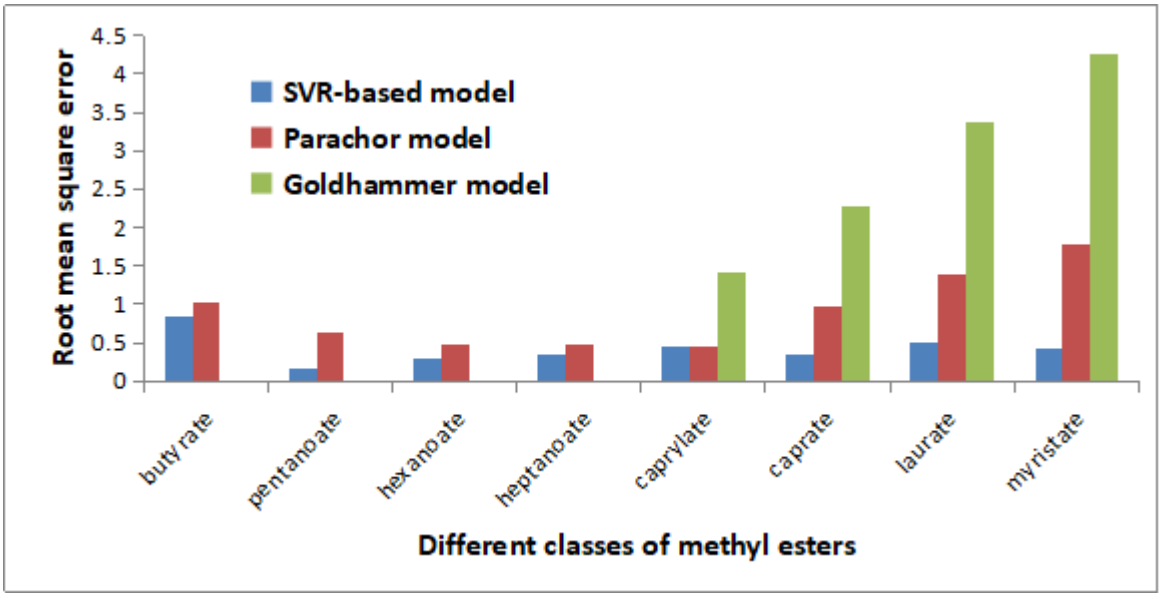

Fig.12. Root mean square error of the results of the developed SVR-based model, Parachor model and Goldhammer model for different classes of methyl esters

Fig.11 compares the mean absolute error of the results of the developed SVR-based model with that of Parachor and Goldhammer model for different classes of methyl esters. The mean absolute errors of the results of the developed SVR-based model are the lowest in all compared classes of methyl esters except in methyl caprylate in which the mean absolute error of the results of Parachor model almost equate that of the SVR-based model. Similarly, SVR-based model shows lowest root mean square error in all the classes of methyl esters except methyl caprylate.

4. Conclusion and recommendation

We developed SVR-based model by training and testing SVR with best parameters obtained through test-set-cross validation method. Surface tensions obtained from the developed SVR-based model show consistent closeness with the experimental values than the results of both Parachor and Goldhammer model. The developed SVR-based model is also characterized with low RMSE and MAE for different classes of methyl esters than other compared models. The excellent predictive and generalization ability of the developed SVR-based model suggests its potential in ensuring efficient atomization (which controls the combustion of fuel in engines) through accurate surface tension estimation of any desired methyl esters as potential alternative to petrodiesel.

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