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Application of modeling techniques for prediction and optimization of biodiesel production processes

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Abstract. Biodiesel has found a great deal of significance in recent years. Environmental challenges have been key factors to justify the necessity of a renewable clean fuel. On the other hand, the production and utilization of biodiesel in a proper state is of concern regarding the numerous plants and industries engaged with the biodiesel. Economical production of biodiesel requires uncovering the process and optimization of the parameters. New methodologies have emerged to satisfy this purpose. In this paper, several features related to the industrial production of biodiesel are discussed. However, modern trends to model the process together with their scope and range of application have been detailed.

Keywords: biodiesel, optimisation, modelling.

1. Introduction

Global air pollution is a serious threat which has been caused by excessive use of fossil fuels for transportation. At present, biodiesel is the most promising source of renewable energy with high potential to replace petroleum-derived diesel fuel, owing to similarity in physico-chemical properties between them [2]. Also due to the highly analogous properties of diesel and biodiesel, biodiesel can be utilized with minor modifications on diesel engines. [3]. Biodiesel, known as non toxic, environmental friendly (leading to lower CO_2, CO, NO_X emission levels compared to commercial diesel), has found to be advantageous of being potentially renewable source of energy which benefits from facilitated storing and transportation. However, it has the disadvantages of 1) high production cost, 2) reduced cold flow properties, 3) detergent characteristics in fuel tank, 4) high viscosity and 5) low volatility [4]. It can be seen that the fuel properties of biodiesel play a major role in the combustion process. Since the nature of fuel components determines fuel properties, the precise information on the structure of the fuel seems necessary [6]. This highlights the importance of developing suitable models in order to cover an exact view of the phenomena and sequences occurred when biodiesel is used as a blend. On the other hand, in various applications, optimization of relevant parameters in transestrification reaction and biodiesel fuel properties by laboratory tests are time-consuming and costly [1].

The main objective of this study is the investigation of various models for prediction and optimization of biodiesel production process as well as considering the pros and cons for each. Moreover, the integrated models and best to suggest ones are discussed.

2. Modeling techniques in the production of biodiesel

Modeling in biodiesel is generally carried out with two different approaches; first, modelling biodiesel production process, simulation of transestrification reaction under variable amount of raw materials and catalysts and also reaction conditions. The second approach includes modelling the biodiesel combustion reaction and simulation of the different compositions of fuels in order to predict the engine performance and

emissions. The later approach is of great concern since high costs of engine experiments and emissions tests would be eliminated [1, 4 and5].

2.1. Artificial Neural Networks

Artificial neural network (ANN) approach has been one of the well-known types of evolutionary computation methods in the last decades. Being as ongoing field of engineering research, ANNs are nonlinear computer algorithms which are extensively and successfully applied in different domains such as mathematics, engineering, medicine, meteorology, psychology, neurology and biology [5]. Recently, ANN is presented a suitable method to simulate complex issues as a technology. Various studies have proved that ANN is a powerful technique for process modeling of biofuels [7]. Several topologies of ANN are used for prediction and optimization of the engine performance and exhaust emissions (cetane number, density, volatility, oxygen and sulfur content), transestrification reaction and property of fuel [3]. Since varieties of vegetable oils have different fatty acids, fuel properties of biodiesel are influenced by different types of raw material. The results of ANN serve as a tool for better understanding of biodiesel chemical structure, fatty acid combination and particle matter emission. Furthermore, ANNs play an important role in modeling and prediction of performance of internal combustion engines [8]. Figs 1 and 2 show schematic view of neural network topology.

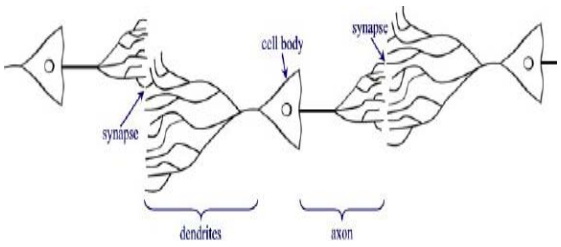

Fig 1. A biological depiction of neural system

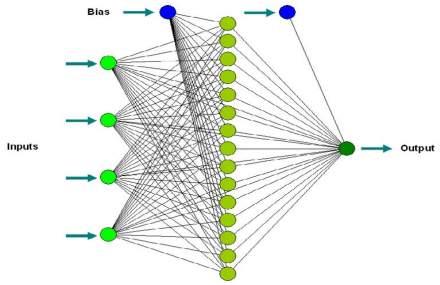

Fig 2. Neural networks: nodes, layers and architecture

2.2. Response Surface Methodology

RSM method has been known as a powerful tool containing general benefits. Using RSM in several fields such as chemical engineering, process control and chemical analysis among many other applications is extensively reported in the literature. Due to production of biodiesel from various raw materials, necessity of transestrification reaction with any feedstock is satisfied. The response surface methodology (RSM) was used to determine the optimum condition for the transestrification reaction [10].

2.3. Integrated models

Due to drawbacks of conventional models, there has been a massive tendency toward using combined methodologies to eliminate the disadvantages of single ones. Therefore, numerous integrated models have been developed. Some of the available schemes include expert systems, statistical method, fuzzy logic, wavelet transform and genetic algorithm (GA). Among these, GA solves the optimization problem by mimicking the principle of biological evolution, and it is also cost-effective and less time consuming technique [7]. Factorial design of experiments gives more information per experiment than unplanned approaches; it allows seeing interactions among experimental variables within the range studied, leading to better knowledge of the process and therefore reducing research time and costs [9].

3.

3.1. production of biodiesel: process approach

Accurate simulation of transestrification for production of biodiesel from waste olive oil was carried out by Antonio et al. (2006). They applied an ANN model to introduce a tool for decision in experimental process of the biodiesel production. The amount of catalyst (e.g. KOH), alcohol (e.g. methanol), reaction time and reaction temperature were claimed as the most crucial parameters involved in the optimization of the transestrification process. Results proved that ANN is a powerful alternative to experimentally testing needed to find optimal parameters to produce biodiesel from waste oil olive, as well as a capable tool to

produce process model [1]. In order to produce biodiesel, canola oil with methanol was analyzed from immobilized Candida rugosa lipase (CRL) on chitosan catalyzed [11]. ANN analysis showed desirable correspondence between experimental and predicted values. Ahmad *et al* (2009) optimized the process variables in transestrification reaction. To achieve maximum production of biodiesel yield, process variables including reaction temperature, methanol to oil ratio, weight of the catalyst and reaction time have been used simultaneously in RSM method. To determine the effects of process variables on biodiesel yield central composite design (CCD) was performed. Predicted values and actual values were in a desirable correlation (R^2=0.94). The main conclusion of this study was optimization of biodiesel production process in order to obtain optimal conditions to give maximum biodiesel yield. These results illustrated that the mesoporous can be an alternative catalyst for transestrification of raw materials. Also RSM based on CCD was suitable approach for simultaneous study of effects of process variables on the biodiesel production [12]. Kok. *et al* (2010) used RSM method to optimize the supercritical dimethyl carbonate (SCDMC) technology for producing biodiesel. In order to study the effect of variables on the production of biodiesel as a response, rotatable central composite design (RCCD) was applied. Coefficient of determination of R^2= 0.9904 was obtained. As a result, there was a good correlation between predicted and tested responses which introduced RSM as a powerful technique to model the biodiesel yield [2]. Jeong and Park (2009), using RSM method optimized the reaction factors of biodiesel from non-edible castor oil. They evaluated the effect of various parameters and their interaction using a five-level three-factor RSM design. Results of experimental analysis for the produced biodiesel under predicted conditions showed that the prediction of producing biodiesel process from castor oil was accurate [13]. In another study, Ferella et al (2010) carried out optimizing with RSM method for transestrification reaction of rapeseed oil. The objective of this study was to determine the best operating conditions for industrial transestrification process. Responses selected for testing of yield levels of transestrification were triglyceride (TC), diglyceride (DC) and monoglyceride (MC) concentration. The statistical model selected to predict the TC, DC and MC demonstrated a good agreement between experimental and calculated yields (R^2 =0.96) which suggests that regression analysis is a useful tool to optimize the process [14]. Selection of appropriate catalyst and its optimal values for transestrification process of sunflower oil (SFO) was accomplished by Vicente et al (1998). RSM and factorial design were set up in a way that temperature and catalyst concentration were selected as the factors and TG conversion to ME after 4 min was assigned to the response. The effects were measured to be significant. The obtained optimal conditions for producing the highest ME (Biodiesel) was the mild temperature (25-50%) and large concentration of catalyst (1.3%) [15]. Biodiesel, produced by transestrification of the oil extracted from the B. carinata seeds, displayed physical–chemical properties suitable for the use as diesel car fuel. Different variables affecting the alkaline ethanolysis of several vegetable oils, high oleic sunflower oil, high and low erucic B. carinata oils were evaluated. The optimum value of the variables affecting the process was determined by application of factorial design and response surface methodology [16]. ANN combined with genetic algorithms (GA) for predicting the optimum process parameters needed to reduce high free fatty acid of any vegetable oil for complete transestrification is also reported. Initial acid value of vegetable oils (IVA), methanol to oil ratio (M), catalyst concentration (C) and reaction time (T) were selected as the inputs for the ANN while final acid value (FAV) of oils was the output to be predicted .The experimental data were analyzed by RSM with the second polynomial equations. The performance of ANN (well trained and tested) was evaluated by the relative percent deviation (RPD) and mean square error (MSE) of 1.167% and 0.0024, respectively. There was a desirable matching between CCRD technique and developed ANN model for the final fatty acid content. It could be concluded from the results that the developed ANN–GA model is an effective tool for predicting optimized pretreatment process parameters for biodiesel production [7]. A GA-ANN model was developed to determine the best parameters of pretreatment process to reduce high FFA levels of vegetable oils. It was concluded that using GA with RSM method based on CCRD or other similar experimental techniques reduces time and cost of the production [17].

3.2. Fuel Properties

The fuel properties of biodiesel such as cetane number, oxidative stability, cloud point, pour point, viscosity, density, and heating value are directly related to the fatty acid (FA) profile of the original source material [18]. Attempts have been made by various researchers to determine the best composition of

biodiesel that would enhance the combustion process. Cetane Number (CN) is a commonly used indicator for the determination of diesel fuel quality, especially the ignition quality. It measures the readiness of the fuel to auto-ignite when injected into the engine. Ignition quality is one of the properties of biodiesel that is determined by the structure of the FAME component. It is established that the FAME composition of the methyl esters used has a predominant effect on the cetane number (CN) of the biodiesel. From the results obtained, it is evident that CN is affected by the % composition of the FAME in the fuel. An equation was developed to predict the CN based on the FAME composition and it was able to predict with 88% accuracy. The developed equation can effectively predict the CN of the biodiesel based on its FAME composition [6]. Ramadhas et al (2006) implemented four types of ANN models to predict the cetane number of biodiesel. Network models used were multi-layer feed forward (MLFFN), radial base function (RBFN), generalized regression (GRNN), and recurrent network (RNN). The fatty acid composition in percentage of various esters in pure form as well as mixtures of esters (biodiesel) and their experimental CN were taken into account for developing the present model. The least error was obtained for MLFF network and recurrent network [5]. Kumar et al. (2007) selected the best ANN for estimating properties of diesel-biodiesel blends. In order to predict properties of diesel-biodiesel blends, they used seven neural network architectures with tree training algorithms within ten different types of weight and biases. In their study, the mentioned model gave the best estimation of properties of diesel-biodiesel blends [4]. Application of factorial design and RSM for optimizing and expanding production of biodiesel from combination of bioethanol and Brassica carinata oil is reported. One of the main problems in storing biodiesel is deterioration of the qualitative properties during storage period. Resistance to oxidative damage during storage is very important for successful development and viability of alternative fuels. These models were claimed to be useful and cost effective to determine the optimal operations conditions in industrial process with a minimum number of tests. According to the results of this work, a non-linear model developing would be an alternative to overcome the available problems in the long term storage of biodiesel [9].

3.3. Engine Performance and emissions using fuel blends

Empirical study on the performance and emissions of a diesel engine are very complex, time consuming and expensive, especially when studies are done on different blends. Monitoring performance and emissions of an engine is also a matter of challenge. On the other hand, mathematical models are not always effective due to their intrinsic drawbacks and limitations. ANN has been proved to be an option in detecting the complex nonlinear processes **[**3**]**. Some researchers studied this method to predict internal combustion engine characteristics. used ANNs to predict specific fuel consumption and exhaust temperature for a Diesel engine. have investigated combustion analysis of IC engines performance using biofuels with an artificial neural network. analyzed the effect of cetane number on exhaust emissions from engine. The effects of valve-timing in a spark ignition engine on the engine performance and fuel economy was investigated by Golcu et al. Investigated the Performance and exhaust emissions of a gasoline engine using ANN. reviewed Artificial intelligence for the modeling and control of combustion processes [18]. In the existing literatures, it was shown that the use of ANN is a powerful modeling tool that has the ability to identify complex relationships from input–output data. Therefore, Kiani Deh Kiani et al.(2009) developed a neural network model for predicting the brake power, torque and the emissions of CO, CO2, HC and NOx of the engine in relation to input variables including engine speed, engine load and fuel blends. This model is of a great significance due to its ability to predict engine performance under varying conditions. Results showed that the ANN provided the best accuracy in modeling the emission indices with correlation coefficient equal to 0.98, 0.96, 0.90 and 0.71 for CO, CO2, HC and NOx, and 0.99 and 0.96 for torque and brake power respectively [18]. In the recent years, some researchers have used ANNs for prediction of performance of engine and exhaust emissions using fuel properties such as cetane number, density, volatility and sulfur content, etc. In a study, Ghobadian et al (2009) used an ANN model to predict engine parameters such as exhaust emission; fuel consummation and torque related to input variables like engine speed and blend biofuels. The network with two variables, engine speed (rpm) and content of biodiesel in diesel (%) as inputs, predicted four variables of engine performance such as torque (N.m), specific fuel consumption (l/kwh) and exhaust emissions like HC and CO (ppm) with the correlation coefficients of 0.9487, 0.999, 0.929 and 0.999, respectively. The authors concluded that BP training algorithm is appropriate to predict performance and exhaust emissions of engine

for different speeds and different fuel blendes [18]. Canakci et al (2006) examined the application of ANN to determine efficiency and emission of a diesel engine fueled with biodiesel blend of 1%, 2%, 5%, 15% and 20%. The developed network yielded R^2 values of 0.99. According to the results of study, ANN was proposed to predict engine performance and emission of a diesel engine [3].

4. Conclusions

Results proved that ANN is a powerful alternative to find optimal parameters to produce biodiesel from different feedstock, as well as a capable tool to provide a process model. Biodiesel conversion was increased markedly by neural network analysis. It could be concluded from the results that the developed ANN-GA model is an effective tool for predicting optimized pretreatment process parameters for biodiesel production. According to the results, a non-linear model developing would be an alternative to overcome the available problems in the long term storage of biodiesel. On the other hand, mathematical models are not always effective due to their intrinsic drawbacks and limitations. ANN has been proved to be an option in detecting the complex nonlinear processes. This model is of a great significance due to its ability to predict engine performance and fuel properties under varying conditions. RSM method has been used for optimization of biodiesel production process in order to give maximum biodiesel yield. Also, RSM based on CCD was suitable approach for simultaneous study of effects of process variables on the biodiesel production. There was a good correlation between predicted and tested responses which introduced RSM as a powerful technique to model the biodiesel yield. Moreover, the optimum value of the variables affecting the process was determined by application of factorial design and response surface methodology. In general, using integrated models including GA, RSM and ANN offers a promising outlook in the estimation of the optimum variables for biodiesel production resulting in saving energy, costs and time.

5. References

[1] Antonio J. Yuste, and M. Pilar Dorado. A Neural Network Approach to Simulate Biodiesel Production from Waste Olive Oil. Energy & Fuels. 2006, 20. 399-402.

[2] K. T. Tan, K. T. Lee, A. R. Mohamed . Optimizations of supercritical dimethyl carbonate technology for the production of biodiesel and value-added glycerol carbonate. Fuel. 2010, 89, 3833-3839.

[3] M. Canakci, A. Erdil, E. Arcaklioglu. Performance and exhaust emissions of a biodiesel engine. Applied Energy. 2006, 83.594-605.

[4] J. Kumar, A. Bansal. Selection of Best Neural Network for Estimating Properties of Diesel-Biodiesel Blends. Greece, February. 2007,16-19

[5] Sulaiman, A., Nikbakht, A.M., Khatamifar, M., Tabatabaei, M. and Ali Hassan, M, (2010). Modeling anaerobic process for wastewater treatment: new trends and methodologies. International Conference on Biology, Environment and Chemistry: ICBEC. Hong Kong, 28-30, December. Indexed in ISI and IEEE Xplore.

[6] A.I. Bamgboye1 and A.C. Hansen. Prediction of cetane number of biodiesel fuel from the fatty acid methyl ester (FAME) composition: Int. Agrophysics.2008, 22. 21-29.

[7] M.Rajendra, P. C. Jena, H. Raheman. Prediction of optimized pretreatment process parameters for biodiesel production using ANN and GA. Fuel 88 .2009,868–875.

[8] A. Dura´n, M. Lapuerta, J. Rodrı´guez-Ferna´ndez .Neural networks estimation of diesel particulate matter composition from transesterified waste oils blends. Fuel 84.2005, 2080–2085.

[9] A. Bouaid, M. Martinez, J.Aracil. Production of biodiesel from bioethanol and Brassica carinata oil: Oxidation stability study: Bioresource Technology 100 .2009, 2234–2239.

[10] S. Pinzi, F.J. L-Gimenez, J.J. Ruiz, M.P. Dorado. Response surface modeling to predict biodiesel yield in a multi-feedstock biodiesel production plant. Bioresource Technology.2010, 101. 9587–9593.

[11] Y. Ying, P. Shao, S. Jiang, and P. Sun. Artificial neural network analysis of immobilized lipase catalyzed synthesis of biodiesel from rapeseed soapstock. Boston: Springer.2009, pp. 1239–1249.

[12] A.Z. Abdullah, N. Razali, K. T. Lee. Optimization of mesoporous K/SBA-15 catalyzed transestrification of palm oil using response surface methodology. Fuel Processing Technology.2009, 90. 958–964.

[13] G-T. Jeong, and D-H.Park ,Optimization of Biodiesel Production from Castor Oil Using Response Surface Methodology. Appl Biochem Biotechnol .2009,156:431–441.

[14] F. Ferella, G. Mazziotti Di Celso, I. De Michelis, V. Stanisci, F. Vegli. Optimization of the transestrification reaction in biodiesel production. Fuel .2010, 89. 36–42.

[15] G. Vicente, A. Coteron, M. Martinez, J. Aracil. Application of the factorial design of experiments and response surface methodology to optimize biodiesel production. Industrial Crops and Products .1998, 8. 29–35.

[16] A. Bouaid, M.Martinez, J. Aracil. A comparative study of the production of ethyl esters from vegetable oils as a biodiesel fuel optimization by factorial design.Chemical Engineering Journal. 2007, 134. 93–99.

[17] P. C.Jena, H. Raheman, G. V. P. Kumar, M .Rajendra. Biodiesel production from mixture of mahua and simarouba oils with high free fatty acids. Biomass and bioenergy. 2010, 34. 1108 – 1116.

[18] M. Kiani Deh Kiani, B. Ghobadian, T. Tavakoli, A.M. Nikbakht, G. Najafi. Application of artificial neural networks for the prediction of performance and exhaust emissions in SI engine using ethanol- gasoline blends. Energy .2009, 1–5.

[19] B. Ghobadian,H. Rahimi,A.M. Nikbakht,G. Najafi,T. Yusaf. Diesel engine performance and exhaust emission analysis using waste cooking biodiesel fuel with an artificial neural network. Renewable Energy. 2009, 34(4):976–82.