Deep learning and machine learning models in biofuels research: Systematic review

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Abstract. The importance of energy systems and its role in economics and politics is not hidden for anyone. This issue is not only important for the advanced industrialized countries, which are major energy consumers, but is also important for oil-rich countries. In addition to the nature of these fuels which contains polluting substances, the issue of their ending up has aggravated the growing concern. Biofuels can be used in different fields for energy production like electricity production, power production or for transportation. Various scenarios have been written about the estimated biofuels from different sources in the future energy system. The availability of biofuels for the electricity market, heating and liquid fuels is very important. Accordingly, the need for handling, modelling, decision making and future forecasting for biofuels can be one of the main challenges for scientists. Recently, machine learning and deep learning techniques have been popular in modeling, optimizing and handling the biodiesel production, consumption and its environmental impacts. The main aim of this study is to evaluate the ML and DL techniques developed for handling biofuels production, consumption and environmental impacts, both for modeling and optimization purposes. This will help for sustainable biofuel production for the future generations.

Keywords: Deep learning, Big data, Machine learning, Biofuels.

Nomenclatures

Artificial neural network	ANN	Random forest	RF
Extreme learning machine	ELM	Non-random two-liquid	NRTL
Machine learning	ML	Recurrent neural network	RNN
Support vector machine	SVM	Partial least squares	PLS
Wavelet neural networks	WNN	Discriminant analysis	DA
Deep learning	DL	Principal component analysis	PCA
Autoregressive integrated moving average	ARIMA	Linear discriminant analysis	LDA
Feed-forward neural networks	FFNN	Support vector regression	SVR
Multi layered perceptron	MLP	Least-squares	LS
Decision tree	DT	Sparse Bayesian	SB
Response surface methodology	RSM	Multi criteria decision making	MCDM
Back propagation neural network	BPNN	Genetic programming	GP
Centroid mean	CM	Multi linear regression	MLR
Adaptive neuro fuzzy inference system	ANFIS	Step-wise Weight Assessment Ratio Analysis	SWARA
Analytic network process	ANP	Multi Objective Optimization by Ratio Analysis	MOORA

1 Introduction

The global energy systems are highly dependent on fossil fuels [1, 2]. The importance of energy systems and its role in economics and politics is not hidden for anyone [3, 4]. This issue is not only important for the advanced industrialized countries, which are major energy consumers, but is also important for oil-rich countries [5]. Because countries have to understand the fact that fossil fuel resources are limited resources. In addition to the nature of these fuels which contains polluting substances, the issue of their ending up has aggravated the growing concern. Therefore owing to depleting non-renewable energy resources, pollution and environmental damage, the world is turning towards renewable energy resources [6]. The fossil fuels still remain as one of the major energy resources worldwide [7]. Heavy dependence on fossil fuels has caused an energy crisis. Using fossil fuel for economic activities leads to GHG emissions from almost all regions of the world [8]. Renewable resources like biofuels make an attractive contribution towards meeting the growing demand for energy supply [9-11]. Owing to environmental concerns and the rise and fluctuations in the fossil fuel resources, worldwide interests have moved towards biodiesel, a clean and renewable alternative for fossil fuels [12, 13]. Biofuels can be used in different fields for energy production like electricity production, power production or for transportation [14]. The economy of biofuels and related refineries will be shaped by policies that have shaped the economy of hydrocarbon and its refineries over the last century [15-18]. Due to the environmental benefits of biofuels, their contribution to the automotive fuel market is increasing sharply. Various scenarios have been written about the estimated biofuels from different sources in the future energy system. The availability of biofuels for the electricity market, heating and liquid fuels is very important. Therefore the need for handling, modelling, decision making and future forecasting for biofuels can be one of the main challenges for scientists [19-22]. Figure.1 shows the research trend in literature considering biofuels. Note that, since 2015 the research in this realm has been constant and start decreasing.

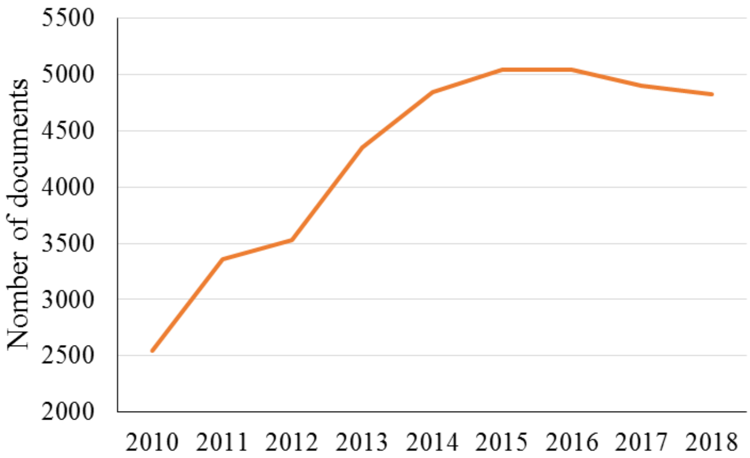

Fig. 1. The research trend in literature considering biofuels research (Web of Science)

Recently, machine learning and deep learning techniques have been popular in modeling, optimizing and handling the biodiesel production, consumption and its environmental impacts by considering the effect of parameters on biofuel production yield because production of a desired product needs an effective use of experimental model [23]. These methods provides an independent modeling approach to the nature of the process or its mathematical models and is able to model the process with a high accuracy [9, 11, 24, 25].

The main purpose of this study is to present a review in a specific field to find the strengths and weaknesses of the field and to provide a complete background. The main aim of this study is to evaluate the ML and DL techniques developed for handling biofuels production, consumption and environmental impacts, both for modeling and optimization purposes. The study initially explains and defines the different biofuels. Then provides a general survey about the characteristics and the basis of the developed studies. In the next stage, explains the state of art of the DL and ML techniques employed in the field. Finally, concludes the results and achievements and proposes the strengths and weakness of different DL and ML techniques.

2 ML and DL methods in biofuels research

Prediction of demand in building energy sector is essential for planning and managing energy systems.

The most popular ML and DL methods are identified and reviewed in this section. During the past decade the application of these intelligent algorithms have been dramatically increases in biofuels research. Figure. 2 represents the increasing demand and popularity of using DL and ML in handling biofuels. It is apparent that since 2010 the use of DL and ML has been increasing till the year 2017. Since then, it starts to decline. The reason can be found in the overall decrease in the number of literature in biofuels research. We made three classification of the methods, i.e., neural networks-based methods, single ML methods, and a separate group for deep learning, ensembles, and hybrid models.

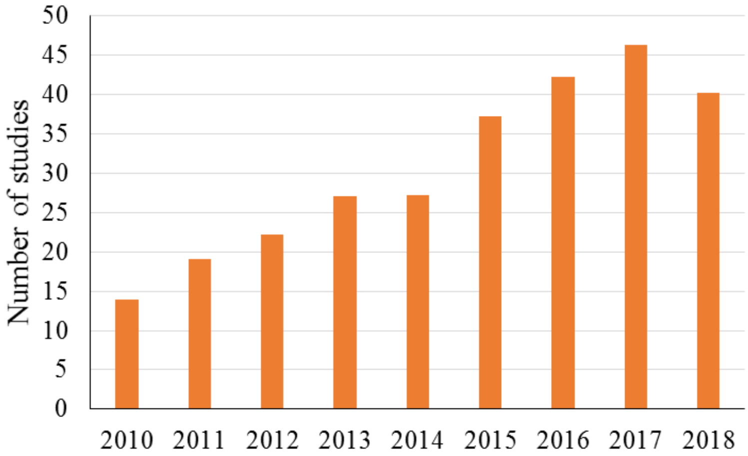

Fig. 2. Demand and popularity of using DL and ML in biofuels research (Web of Science)

2.1 Neural networks-based ML models for biofuels research

This section includes the application of artificial neural networks (ANNs), Multi-layer perceptron (MLP), Extreme learning machines (ELM), feedforward neural networks (FFNNs) and Backpropagation ANNs in biofuels research.

Table 1. top studies developed by ANN based methods in biofuel

Reference	**Contribution**	**method**	**Application domains**
[26]	To optimize the prediction of liquid-liquid equilibria which is employed in the simulation of biofuel process by the use of a novel non-random two-liquid-ANN method.	NRTL-ANN	-NRTL -Biofuels

[9]	To develop different types of MLP networks for the estimation of enzyme function.	MLP	-Enzyme function -machine learning
[27]	To develop ANN method for the prediction of un-measurable variables during hydrogen and methane production through anaerobic digestion process.	RNN	-Biofuels -RNN
[28]	To develop a comprehensive survey about the use of ANN in the optimization and estimation of variables in biofuels production process	ANN	-ANN -Biofuel production
[25]	To employ ANN methods for the prediction of cetane number of biofuel samples in the presence of furanic additives	ANN	-Machine learning -Biofuels

Reynel-Ávila et al. [26] developed an innovative hybrid non-random two-liquid-ANN method in order to increase the estimation performance of the liquid-liquid equilibria which is used to simulate the biofuel process. Non-random two-liquid method is considered as a thermodynamic method to be used in a multi component system therefore hybridization of this method with ANN method can improve the system accuracy for the regression and fitting proposes. Evaluation of the proposed method has been performed using RMSD factor for measuring the agreement between target and estimated values. This method as a flexible method could successfully cope with the estimation task as well as increasing the accuracy of estimation.

Concu et al. [9] developed a study in order to employ different machine learning techniques for the estimation of protein function through a conversion process as a type of enzyme for considering in bioethanol production. The developed machine learning techniques included the single method containing different architectures of MLP methodology. Results have been evaluated using accuracy, sensitivity and specificity. Methods have different number of neurons in hidden layer. The accuracy of the proposed MLP method was acceptable as well as its higher sustainability. Camberos et al. [27] developed recurrent neural network method in order to estimate un-measurable variables during hydrogen and methane production through anaerobic digestion process. The reason was the ability of recurrent NN method in the predicting the behaviour of unknown and complex systems. The method was a single method which benefited the external disturbances as well as the parameter uncertainties. Results have been evaluated using mean square error. Based on results, the proposed RNN method could successfully provide a high performance in confrontation with the complex system. Also, the method provided a high sustainability by a high stability in the presence of the external distributions.

Sewsynker-Sukai [28] did a comprehensive survey about the application of ANN, as one of the most popular and applied machine learning methods, in the field of biofuels for the optimization and estimation purposes. This study also presents a brief explanation about the comparison of the performance of ANN with another methods and discussing about the architectures of the developed ANN methods. Comparisons were performed using coefficient of determination as the performance factor. Based on results, developing ANN methods in this field provides a high production performance as well as reducing the time and the cost consuming. Reduction of the time and cost in the biofuels production and consuming processes also increases the sustainability and reliability of the system. Therefore, ANN can be an effective tool for handling biofuels and for managing the production and consuming processes for policy makers in the future researches. Kessler et al. [25] presented a study to estimate the cetane number of biofuel samples in the presence of furanic additives. Results have been evaluated using RMSE values. ANN as a predictive method, could be successfully applied for the prediction of cetane number with a low error.

Different applications of ANN tools in different fields of biofuels have been already discussed. But there is a need for metrics and different criteria for the evaluation of the performance of each methods. Table 2 present a brief comparison about the accuracy, reliability and sustainability of methods developed for handling biofuels using different types of ANN methods. These factors have been prepared and presented based on different aspects which have been concluded by the reviewed studies.

Table 2. the comparison results of ANN based methods for biofuels handling

Method	*Application*	*Accuracy*	*Reliability*	*Sustainability*	*Reference*
Hybrid NRTL-ANN	Estimation	++	++	++	[26]
MLP	Estimation	++	+	+	[9]
RNN	Estimation	+++	+++	+++	[27]
ANN	Estimation	++	+	+	[28]
ANN	Optimization	++	++	+	[28]
ANN	estimation	++	+	+	[25]

2.2 Further single ML methods for biofuels research

This section includes support vector machines (SVM), decision trees (DTs) regression tree (RTs), bayesian, k-means and k-nearest neighbours.

Table 3. top studies developed by SVM based methods in biofuel

Reference	**Contribution**	**Method**	**Application domains**
[29]	To develop PLS-DA, SVM and PCA-LDA methods for the classification of biofuels	PLS-DA, SVM and PCA-LDA	-Classification -SVM
[30]	To develop prediction models for the estimation of biofuels pellet quality using LSSVM and PLSR methods as non-destructive methods	LSSVM and PLSR	-LSSVM -PLSR
[31]	To develop a fuzzy method for the prediction of cetane number of biodiesel fuel samples	Fuzzy	-Fuzzy -Cetane number
[32]	To develop a hybrid modeling method for the estimation of the engine performance fuelled by biofuel	SBELM	-Hybrid SBELM -Engine performance

[33]	To employ hybrid machine learning techniques for the estimation of biofuel production yield and optimization production process	ELM-RSM and SVM-RSM	-Biofuel production -Hybrid machine learning

Mancini et al. [29] developed three methods including partial least squares discriminant analysis, SVM and principal component analysis linear discriminant analysis for the classification of biofuels. Based on results, all the methods could successfully cop with the classification task but SVM has the best classification performance. Feng et al. [30] developed non-destructive prediction methods for the estimation of the quality of the biofuel pellet using partial least-squares regression and a least-squares support vector machine as non-destructive diagnosis methods to be compound with successive projections algorithm. The performance of the methods have been compared using determination coefficient and root mean square error values. Based on results, the best method was identified to be SPA-LSSVM method as a hybrid diagnosis method. This method employs the advantages of both LSSVM and SPA methods, consequently.

Faizollahzadeh et al. [31] developed a sugeno based fuzzy method for the prediction of biodiesel fuel cetane number in the presence of Carbon number, Double bond, Saponification number, and Iodine value. The performance of the developed model has been calculated using determination coefficient and root mean square error. The developed model has a high accuracy in both training and testing steps, but one of the most important factors for this method was its lower processing time and its user friendly application. These factors increase the method sustainability factor to be employed in the future researches. Wong et al. [32] developed a novel hybrid sparse Bayesian based extreme learning machine technique for the estimation of the engine performance fuelled by biofuel as well as the calibration of the ECU. The proposed method have been also compared with the performance of ELM, Bayesian ELM and back propagation neural network in terms of mean absolute percentage error and standard deviation. The proposed hybrid method have an acceptable accuracy in both training and testing steps compared with that for the ELM, BPNN and BELM methods. The proposed method also have a higher performance in the estimation of engine emissions.

Faizollahzadeh et al. [33] developed an innovative hybrid ELM-RSM and EVM RSM methods for the prediction of biofuel production yield and optimization of the production process for accessing a higher production yield. The developed methods have been compared with SVM, ANN and ANFIS methods in term of performance factors for the prediction phase. Based on results, hybrid ELM-RSM methods could provide a higher performance by increasing the production yield compared with that of the other methods. This study also indicates the importance and strength of the hybrid method over single methods. In fact, this method benefits the highest prediction capability of ELM method in parallel with the optimization capability of the RSM. Therefore this study highlights the highest performance of hybrid techniques in comparison with single ones. Table 4 presents the comparison results of SVM based methods for biofuels handling.

Table 4. the comparison results of SVM based methods for biofuels handling

Method	*Application*	*Accuracy*	*Reliability*	*Sustainability*	*Reference*
SVM	classification	++	++	++	[29]
PCA-LDA	classification	++	+	+	[29]
PLS-DA	classification	+	+	+	[29]
SPA-LSSVM	classification	+++	+++	++	[30]
Fuzzy	Estimation	+++	+++	++	[31]
SBELM	Estimation	+++	+++	+++	[32]
ELM	Estimation	+	+	+	[32]
BELM	Estimation	++	+	+	[32]
ELM-RSM	Optimization	+++	+++	+++	[33]
SVM-RSM	Optimization	+++	++	++	[33]

2.3 Deep learning, machine learning, ensembles, and hybrid models for biofuels research

In this section the more sophisticated ML methods in addition to DL are presented. Here may include neuro-fuzzy models, various DL models and ensemble MLs.

Table 5. top studies developed by machine and deep learning based methods in biofuel

Reference	Contribution	Method	Research domain
[34]	To develop a novel Multi-criteria decision making for improving energy management system and increasing the energy efficiency	MCDM	-Decision making -Energy management
[35]	To develop different methods including hybrid and single methods for the prediction of short term energy parameters	ANFIS-CM, Genetic programming, M5Tree, RF and MLR	-Hybrid machine learning -Energy systems
[22]	To develop a comprehensive survey about the application of machine learning and deep learning methods in energy systems	Machine learning and Deep learning methods	-Hybrid machine learning -Single machine learning -Energy systems -Deep learning

Erdogan et al. [34] developed a novel multi criteria decision making system for choosing the best biodiesel fuel for a compression ignition engine in terms of the engine performance and combustion characteristics. Based on results, the hybrid Step-wise Weight Assessment Ratio Analysis- Multi Objective Optimization by Ratio Analysis method and hybrid Analytic network process- Multi Objective Optimization by Ratio Analysis provided the best performance for choosing the best fuel sample.

Deo et al. [35] developed different hybrid and single machine learning techniques for the prediction of sub-tropical photo-synthetically active radiation. The developed methods included ANFIS integrated with centroid mean, random forest, genetic programming, M5Tree and multiple linear regression. Methods have been compared in terms of mean absolute error and root mean square error. Results indicated that, the hybrid ANFIS-CM followed by GP methods could provide lowest error as well as a highest sustainability.

Mosavi et al. [22] developed a comprehensive survey about the application of machine learning methods including single and hybrid methods in the energy systems. The study have been developed in order to present a comprehensive state of the art of machine learning and to discuss their advantage and disadvantages, in detail. Methods have been compared in terms of root mean square error, determination coefficient, correlation coefficient and mean absolute percentage error. Based on results, hybrid machine learning have the best performance for prediction and optimization which can help policy makers for developing an accurate energy management systems.

Table 6. the comparison results of DL and ML based methods for biofuels handling

Method	*Application*	*Accuracy*	*Reliability*	*Sustainability*	*Reference*
SWARA-MOORA	Decision making	+++	+++	+++	[34]
ANP-MOORA	Decision making	+++	+++	+++	[34]
ANFIS-CM	classification	+++	+++	+++	[35]
GP	classification	+++	++	++	[35]
Hybrid ML	Estimation	+++	+++	+++	[22]
Single ML	Estimation	+++	++	++	[22]
Hybrid ML	Optimization	+++	+++	+++	[22]
Single ML	Optimization	+++	+++	++	[22]

3 Conclusion

This paper studies the applications and progress of ML and DL methods biofuels research. This study also presents a deep survey and analysis of the ‘hybrid model’ and ensemble models that integrates two or more techniques. Survey shows that, the single ML methods except ANNs have not been popular. However, the ensemble and hybrid models have emerged and continue to advance for higher accuracy and better performance. DL techniques also will bring tremendous amount of intelligence for better prediction models. In general, modelling, forecasting and decision making about the future of biofuels helps for developing sustainable energy resources which are low cost resources with a low environmental impacts. ML and DL techniques have been successfully employed in all fields of sciences and have improved the process. The various combinations of the hybrid and ensemble methods are found to be the most effective in handling biofuels.

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