CHARACTERISTICS PREDICTION OF HYBRID FEEDSTOCK BIODIESEL DERIVED FROM HIGH FFA OILS USING MACHINE LEARNING (ML) TECHNIQUE

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Introduction:

The challenges posed by fossil fuels such as price escalation, depletion of reserve, adverse environmental impact and associated climate change have spurred significant interest in alternative energy sources like biofuels. Biodiesel, in particular, is considered a cost- effective and environment friendly alternative to fossil fuels due to its biodegradability, lower emissions, and comparable performance to conventional diesel. However, a major hurdle in ensuring a sustainable biodiesel supply is the limited as well as seasonal availability of the feedstocks. Even though non edible oils are considered as promising feedstocks, their limited and seasonal availability along with the high free fatty acid content respectively disrupts the sustainable biodiesel availability and makes oil to biodiesel transmutation more complex. The issue can be addressed by performing direct transesterification using mixed oil feedstocks by controlling the free fatty acid value of the oil blend. The properties of the biodiesel produced by blending different feedstocks will be different from those obtained from the constituent feedstocks and depends on the fatty acid profile and proportion of each constituent in the oil blend. Thus, the information regarding the properties of the biodiesel derived from different proportions of mixed feedstock is limited and experimental determination of the same for various blends is cumbersome. This can be overcome by developing a model using machine learning techniques to predict the properties of biodiesel derived from mixed oil blends. The present study deals with the development of Adaptive Boosting based model to predict the properties of biodiesel derived from the binary blends of pig fat with jatropha oil and pongamia oil at various proportions.

Objectives:

- Development of model to predict the characteristics of hybrid feedstock biodiesel using machine learning technique.
- Determination of free fatty acid (FFA) of jatropha, pig fat, pongamia and binary combinations of jatropha and pongamia oils with pig fat.
- Characterization of fatty acid profile of the parent and binary feedstock combinations.
- Transesterification of binary combinations of jatropha and pongamia oils with pig fat.
- Determination of density, viscosity, flash point and calorific value of the biodiesel samples.
- Determination of the characteristics of binary feedstock biodiesel derived from jatropha and pongamia oils with pig fat using the developed model.
- Comparison of experimentally determined biodiesel characteristics with those predicted using machine techniques.
- To perform public biofuel awareness programme and demonstrate the prepared hybrid feedstock biodiesel in vehicles.

Methodology:

Collection of feedstocks and oil extraction from pongamia seeds.

The pig fat is collected from local pork venders and is heated to extract the triglyceride from it. The non-edible jatropha oil is purchased from “Jatropower Bio-Trading Pvt. Ltd”. Pongamia seeds is collected from nearby villages and dried before extracting oil using an oil extractor. The extracted oil is allowed to settle and is then stored in air tight bottles after filtration.

Preparation of binary oil blends by mixing pig fat with jatropha and pongamia oils at different proportions and determination of fatty acid profile and FFA of individual feedstocks and their binary blends.

Binary feedstocks blends are prepared by combining pig fat with nonedible oils, namely jatropha oil and pongamia oil at various proportions. Two binary blends of pig fat and jatropha oil, namely JP1 and JP2 are prepared by mixing the feedstocks in the ratios 70:30 and 80:20 respectively. Similarly, binary blend of pig fat and pongamia oil in the ratio 80:20 is represented as PP1. The free fatty acid (FFA) content of the blends is determined for the parent oil and binary feedstock blends prepared. The FFA analysis is performed through titration of the oil blends using 1N sodium hydroxide (NaOH) solution, with phenolphthalein serving as the indicator. The fatty acid composition of pig fat, jatropha oil, pongamia oil and the binary blends JP1, JP2 and PP1 are determined using GC analysis.

Fig. 1 Determination of free fatty acid

Transesterification of parent feedstocks as well as hybrid oil blends to prepare biodiesel and characterization of the biodiesel samples prepared.

The feedstocks are converted to biodiesel through direct transesterification or by esterification followed by transesterification based on their free fatty acid content. If the free fatty acid content in the feedstock is less than 2%, direct transesterification is sufficient whereas if the value is grater that 2% acid esterification should be done prior to transesterification. In the esterification process, the feedstock (with FFA greater than 2%) mixed with predetermined amount of alcohol and sulphuric acid is heated to 65℃

for 1.5 hours in a three-neck flask with continuous stirring. The resultant mixture with FFA less than 2% obtained after esterification is subjected to transesterification. The binary hybrid oil blends are prepared by limiting the free fatty acid content below 2% to enable direct transesterification. In direct transesterification, one liter of feedstock is combined with a predetermined amount of alcohol and catalyst, and the mixture is heated to 65 °C for two hours in a three-neck flask with continuous stirring. During the reaction, triglycerides in the feedstock are converted into biodiesel and glycerol. After the reaction, the heating is stopped, and the mixture is left undisturbed for 12 hours to allow phase separation. The biodiesel is separated from glycerol and washed to remove the residual catalyst and alcohol. The washed biodiesel is heated above 100 ℃ to remove the moisture content. the jatropha oil and pongamia oil is converted to biodiesel with esterification whereas pig fat, JP1, JP2 and PP1 are transmuted to biodiesel using direct transesterification. Characterization tests are performed on biodiesel samples prepared from parent oil and the binary oil blends to determine the main properties such density, viscosity, flash point and calorific value of the biodiesel.

Fig. 2 Transesterification


(a)


(b)

Fig. 3 Biodiesel separation (a) pig fat- jatropha 70:30 (b) pig fat- pongamia 80:20

Prediction of characteristics of biodiesel samples using machine learning techniques.

A model is developed to predict the properties of biodiesel based on the fatty acid composition of the feedstock using Adaptive Boosting (AdaBoost) machine learning algorithm. AdaBoost is an iterative algorithm which can train different learning algorithm for the same training set. AdaBoost is a sequential ensemble meta-algorithm that combines multiple weak learners to build to build more accurate prediction models. The model is developed in Orange platform and is trained by adapting the fatty acid composition of soyabean, rapeseed, rice bran, jatropha, karanja, mahua indica, tamarind seed, waste cooking oil and chicken fat oil feedstocks available in the literature to enhance the prediction accuracy of corresponding biodiesel properties. The trained model predicted the biodiesel properties with an average deviation of 8.12%, 1.02% and 8.26%. Further, the fatty acid composition of parent feedstocks namely pig fat, jatropha and pongamia is fed to the model and the characteristics (density, viscosity, flash point and calorific value) of biodiesel derived from the binary blends of pig fat with jatropha (80:20 and 70:30) and pig fat with pongamia (80:20) is predicted. An average accuracy of 99.25%, 93.71%, 97.87% and 99% is obtained when the model predicted values are compared with corresponding experimental values. The flow sheet of the model developed in Orange platform is depicted in figure 4.

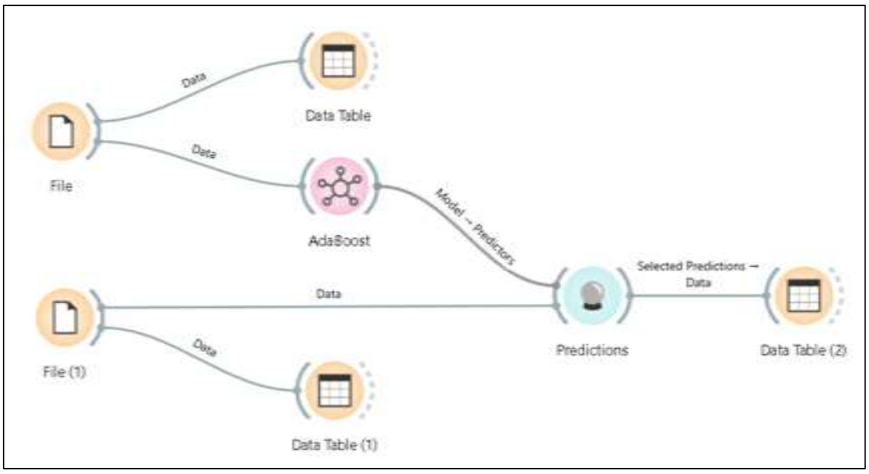

Fig. 4 Flow sheet of the model

Results and Conclusions:

The FFA values of parent oils and the binary combinations are given in table 1. It is found that free fatty acid value of pig fat is minimum and that of pongamia and jatropha as 5.56 and 4.72 respectively, which is well above the limiting value 2 for direct transesterification. Compared to the parent oils, binary blends of pig fat with jatropha in the ratios 80:20 and 70:30 as well as the blend of pig fat with pongamia in 80:20 ratio exhibited FFA values well below 2%, thereby suitable for direct transesterification.

Table 1 Free fatty acid values

Sl no	Feedstock	FFA
1	Pig fat	0.175
2	Jatropha	4.72
3	Pongamia	5.56
4	Pig fat and jatropha (80:20)	1.309
5	Pig fat and jatropha (70:30)	1.72
6	Pig fat and pongamia (80:20)	1.529

The fatty acid profile of pongamia oil, jatropha oil, pig fat and binary combinations of pig fat with jatropha and pongamia oils are obtained through GCMS (Gas

Chromatography-Mass Spectrometry) technique to identify the feedstock constituents. The fatty acid composition of the pig fat, jatropha, pongamia as well as binary combinations of pig fat with jatropha (80:20 and 70:30) and pig fat with pongamia (80:20) are given in the tables 2, 3, 4, 5, 6 and 7. The fatty acid profile of the parent oils are used as input in the machine learning model to predict the properties of biofuel derived from binary feedstock combinations.

Table 2 Free fatty acid profile of pig fat

Sl no	Acid name	Percentage (%)
1	9-Octadecenoic acid, methyl ester, (E)-	44.65
2	Hexadecanoic acid, methyl ester	18.19
3	9,12-Octadecenoic acid (Z, Z)-, methyl ester	14.44
4	Methyl stearate	13.79
5	(6Z,9Z,12Z)-1,3-Dimethoxypropan-2yl octadeca-6,9,12-trienoate	2.92
6	Methyl tetradecanoate	2.30
7	3-(2-Methoxyethoxy) propanoic acid, trimethylsilyl ester	1.92
8	9-Hexadecenoic acid, methyl ester, (Z)-	1.80
	Total	**100**

Table 3 Free fatty acid profile of jatropha

Sl no	Acid name	Percentage (%)
1	9-Octadecenoic acid, methyl ester, (E)-	38.44
2	9,12-Octadecenoic acid (Z, Z)-, methyl ester	34.83
3	Hexadecanoic acid, methyl ester	16.73
4	Methyl stearate	8.60
5	9-Hexadecenoic acid, methyl ester, (Z)-	0.92
6	9,12,15-Octadecatrienoic acid, methyl ester, (Z, Z, Z)-	0.30
7	Methyl tetradecanoate	0.17
	Total	**100**

Table 4 Free fatty acid profile of pongamia

Sl no	Acid name	Percentage (%)
1	Oleic Acid	39.97
2	9,12-Octadecadienoic acid (Z, Z)-	25.53
3	9-Octadecenoic acid, methyl ester, (E)-	11.66
4	Octadecanoic acid	7.51
5	9,12-Octadecadienoic acid (Z, Z)-, methyl ester	4.84
6	Methyl 20-methyl-heneicosanoate	3.79
7	Hexadecanoic acid, methyl ester	2.96
8	Methyl stearate	2.04
9	9,12,15-Octadecatrienoic acid, methyl ester, (Z, Z, Z)-	0.76
10	Eicosanoic acid, methyl ester	0.52
11	11-Eicosenoic acid, methyl ester	0.43
	Total	**100**

Table 5 Free fatty acid profile of pig fat-jatropha (80:20)

Sl no	Acid name	Percentage (%)
1	9-Octadecenoic acid, methyl ester, (E)-	38.17
2	9,12-Octadecadienoic acid (Z, Z)-, methyl ester	29.44
3	Hexadecanoic acid, methyl ester	18.77
4	Methyl stearate	8.57
5	9-Hexadecenoic acid, methyl ester, (Z)-	1.93
6	Methyl tetradecanoate	1.62
7	cis-Methyl 11-eicosenoat	0.44
8	cis-11,14-Eicosadienoic acid, methyl ester	0.43
9	Dodecanoic acid, methyl ester	0.35
10	9,12,15-Octadecatrienoic acid, methyl ester, (Z, Z, Z)-	0.29
	Total	**100**

Sl no	Acid name	Percentage (%)
1	9-Octadecenoic acid, methyl ester, (E)-	37.87
2	9,12-Octadecadienoic acid (Z, Z)-, methyl ester	31.34

3	Hexadecanoic acid, methyl ester	17.36
4	Methyl stearate	8.24
5	9-Hexadecenoic acid, methyl ester, (Z)-	1.60
6	Methyl tetradecanoate	1.25
7	-	0.44
8	11-Eicosenoic acid, methyl ester	0.34
9	cis-11,14-Eicosadienoic acid, methyl ester	0.33
10	Methyl hexadec-9-enoate	0.31
11	9,12,15-Octadecatrienoic acid, methyl ester, (Z, Z, Z)-	0.27
12	Dodecanoic acid, methyl ester	0.25
13	Eicosanoic acid, methyl ester	0.20
14	5,8,11,14-Eicosatetraenoic acid, methyl ester, (all-Z)-	0.20
	Total	**100**

Table 6 Free fatty acid profile of pig fat-jatropha (70:30)

Table 7 Free fatty acid profile of pig fat-pongamia (80:20)

Sl no	Acid name	Percentage (%)
1	9-Octadecenoic acid, methyl ester, (E)-	47.88
2	9,12-Octadecadienoic acid (Z, Z)-, methyl ester	20.74
3	Hexadecanoic acid, methyl ester	14.30
4	Methyl stearate	8.14
5	Docosanoic acid, methyl ester	3.02
6	9,12,15-Octadecatrienoic acid, methyl ester, (Z, Z, Z)-	2.35
7	9-Hexadecenoic acid, methyl ester, (Z)-	1.01
8	Methyl 18-methylnonadecanoate	0.95
9	cis-Methyl 11-eicosenoate	0.84
10	Methyl tetradecanoate	0.78
	Total	**100**

The density, viscosity, flash point and calorific value of biodiesel derived from parent feedstocks and the binary combination are represented in table 8. Among the biodiesel derived from binary feedstock combinations, pig fat and jatropha in 80:20 and 70:30

ratios are found to have lower viscosity value of nearly 5.20 cSt compared to pig fat and pongamia combination. The 80:20 pig fat-jatropha combination exhibited 6.4% more biodiesel yield compared to 70:30 pig fat-jatropha combination.

Table 8 Characteristics and yield of various biodiesel samples

Sl no	Biodiesel samples	Yield (%)	Density (kg/m³)	Viscosity (cSt)	Flash point (°C)	Calorific value (kJ/kg)
1	Pig fat	75.52	812	5.01	188.5	39070
2	Jatropha	69.9	806	4.98	175.5	38990
3	Pongamia	63.5	802	5.58	182.5	38377
4	Pig fat and jatropha (80:20)	75.84	806	5.21	185.5	39045
5	Pig fat and jatropha (70:30)	71.28	802	5.20	192.5	39266
6	Pig fat and pongamia (80:20)	77.5	804	5.57	202	38114

The developed machine learning model using AdaBoost algorithm in Orange 3.38.0 platform is used to predict density, viscosity, flash point and calorific values of binary feedstock biodiesel samples. An average percentage deviation of 0.75, 6.29, 2.13 and 1.00 is respectively obtained when the model predicted values of viscosity, flash point, calorific value and density are compared with the corresponding experiment values.

Property	Biodiesel samples	Experiment value	Model value	Percentage (%) deviation
Density	Pig fat-Jatropha (80:20)	806	812	0.75
	Pig fat-Jatropha (70:30)	802	812	1.25
	Pig fat-Pangomia (80:20)	804	806	0.25
	Average % deviation			0.75
Viscosity	Pig fat-Jatropha (80:20)	5.21	4.98	4.41
	Pig fat-Jatropha (70:30)	5.20	4.97	4.42
	Pig fat-Pangomia (80:20)	5.57	5.01	10.05
	Average % deviation			6.29
	Pig fat-Jatropha (80:20)	185.5	188.5	1.62

Flash Point	Pig fat-Jatropha (70:30)	192.5	190.0	1.30
	Pig fat-Pangomia (80:20)	202.0	195.0	3.47
	Average % deviation			2.13
Calorific Value	Pig fat-Jatropha (80:20)	39045	39050	0.01
	Pig fat-Jatropha (70:30)	39266	39070	0.50
	Pig fat-Pangomia (80:20)	38114	39055	2.47
	Average % deviation			1.00

Table 9 Comparison of model predicted characteristics with experimental value

In addition to this, the commitment towards society is expressed by performing biofuel awareness programme to the people of Bevinahalli village of Mandya district and demonstration of prepared biodiesel in a tractor. A total of 43 members attended the awareness programme in which the project group members provided awareness on production, utilization and benefits of biodiesel. The photographs of the programme is included in figures 5 and 6.

Fig. 5 Biofuel awareness programme

Fig. 6 Demonstration of biodiesel in vehicle

In conclusion, a model is created to predict the characteristics of hybrid feedstock biodiesel derived from high FFA oil using machine learning algorithm (Adaptive boosting). The characteristics (density, viscosity, flash point and calorific value) of biodiesel derived from the binary blends of pig fat with jatropha (80:20 and 70:30) and pig fat with pongamia (80:20) is predicted with an average accuracy of 99.25%, 93.71%, 97.87% and 99% when model predicted values are compared with corresponding experimental values.

Project Outcome & Industry Relevance:

- A model using machine learning technique to predict the characteristics of hybrid feedstock biodiesel from their fatty acid composition.
- Fatty acid composition of pig fat, pongamia oil and jatropha oil. Also, the change in fatty acid composition in the binary blend of pig fat, with pongamia oil and jatropha oil at various blending ratio.
- Important characteristics of hybrid feedstock biodiesel such as density, viscosity, flash point and calorific value.
- Awareness on biofuel to public and demonstration of produced biodiesel in vehicles.

The proposed project is directly relevant to the society, environment and biodiesel industries. Utilization of mixed feedstock strategy mitigates the issue of limited feedstock availability faced by biodiesel industries for seamless biofuel supply. Also, production of biodiesel from hybrid feedstocks, involving high FFA constituent oils through direct transesterification, reduces the process complexities, cost and time consumed for biodiesel production. Furthermore, development of machine learning enabled model to predict the properties of hybrid biodiesel helps to reduce the effort, cost and time consumed in the experimental characterization.

Working Model vs. Simulation/Study:

The present work is the simulation performed in Orange 3.38.0 platform to predict characteristics of biodiesel obtained from binary feedstock blends from there fatty acid profile. The model is validated by comparing the model predicted characteristics with those obtained through experiments.

Project Outcomes and Learnings:

- A model using machine learning technique to predict the characteristics of hybrid feedstock biodiesel from their fatty acid composition.
- Fatty acid composition of pig fat, pongamia oil and jatropha oil. Also, the change in fatty acid composition in the binary blend of pig fat, with pongamia oil and jatropha oil at various blending ratio.
- Important characteristics of hybrid feedstock biodiesel such as density, viscosity, flash point and calorific value.
- Awareness on biofuel to public and demonstration of produced biodiesel in vehicles.
- From the work it is established that the properties of the biodiesel can be predicted by knowing the fatty acid composition of the feedstock or feedstock blends. It is also learned that high FFA oil can be directly converted to biodiesel by blending it with the low FFA feedstocks, thereby reducing the cost, time and multi-step procedure required for direct conversion.

Future Scope:

The future scope of this project includes:

1. A feedstock having high FFA value can be blend with even two feedstocks known as trinary blend in such a way that its FFA value fall below 2 and suitable for direct transesterification.

2. The transesterification process can also be carried out with different catalyst other than NaOH which gives a better result.
3. The transesterification process can also be carried out with different alcohol other than methanol which gives a better result.