Modelling of nicotiana tabacum l. oil biodiesel production: comparison of ann and...

[Health & Medicine]

Introduction

Notable properties associated with methyl and ethyl esters of oils such as renewability, environmental friendliness, and others, have propelled researchers and scientific communities to substitute such renewable fuels for diesel fuel in diesel and automotive engines (cars, trucks, farm machinery, marine vessels, and even aircraft) (Enweremadu and Mbarawa, 2009 ; Huang et al., 2012 ; Huang et al., 2019 ; Jayaprabakar et al., 2019 ; Shrivastava and Verma, 2019). In time past, clean and sparkling oily feedstock has been a preferred option for investigation by researchers in terms of biodiesel production since the oils possess the shortest reaction time and do not need pre-treatment prior to the base transesterification (Giwa et al., 2010). However, non-edible seed oils from castor, rubber, jatropha, tobacco seed, and others have been considered for biodiesel production globally. This consideration is associated with non-edible oils as they can lessen the cost of biodiesel production. Among non-edible oils, tobacco seed oil (TSO) seemed appealing for biofuel production which is often observed to possess close basic properties with diesel fuel (Andrianov et al., 2010). In addition, the literature (Giannelos et al., 2002 ; Moser, 2009) remarked on the viability of biodiesel production from TSO.

The tobacco plant is readily available as it is abundant in over 118 nations globally (Usta, 2005). There is a remarkable growth in tobacco cultivation. The African tobacco plantation grew from 440, 000 tons in 2003 to 650, 000 tons in 2012. Also, the 20 top-ranked countries (global) in the production of tobacco in 2012 consisted of Malawi (sixth), Tanzania (eight), Zimbabwe (ninth), Zambia (sixteenth), and Mozambique (seventeenth) position (Hu and Lee, 2015). Figure 1 depicts the tobacco production capacity of some countries in 2018 (Statista, 2020), and that of Nigeria in 2017 (FAO statistics, 2008). As observed, China was the largest producer in 2018 while the tobacco plantation in Nigeria was higher compared to those of other countries. There is a need to revamp tobacco farming to meet the feasible production for a biorefinery in the nearest future.

FIGURE 1

Tobacco production capacity for ten countries.

The leaf from the tobacco plant and its seed possess commercial values. For example, the tobacco industry adopts leaves for cigarette production, but alternate use of tobacco by-product is at the top gear (Grisan et al., 2016). The authors further remarked that researchers are projecting alternate application of tobacco such as biofuel. Such reports might be attributed to people's awareness of the dangerous implication of cigarette smoking (Usta et al., 2011). However, the by-product, which is tobacco seeds contains no nicotine which can be employed for tobacco-based biodiesel production. This will reduce undesirable implications on the health and well-fare of the populace and promote the socio-economic balance in Africa and the world at large (Hu and Lee, 2015).

Refs. (Uzun et al., 2012 ; Samuel et al., 2020a ; 2020b) hinted that optimization is a prerequisite to boost yield and biofuel production in a biorefinery plant. Among high-level optimization techniques, a breed of

Artificial Neural Network (ANN) and the Fuzzy Logic (FL), which gives the hybrid algorithm, Adaptive Neuro-Fuzzy Inference System (ANFIS), has been the preferred option in terms of problem-solving, the combination has numerical advantages discussed elsewhere (Okwu and Adetunji, 2018). The ANFIS is a controlling data-driven and adaptive computational tool having the capability of mapping non-linear and complex data (Gupta and Sharma, 2014). On the contrary, the limitation of ANN is its black box which fails to link input parameters with the response. Jang and Sun (1995) linked the failure of the black box technique of the ANN model to the inability of the model to accommodate linguistically information unswervingly. On the other hand, Yaghoobi et al. (2016) attributed the superiority of the ANFIS model to its capacity to handle lapses in the ANN model.

Relevant studies on the TSO biodiesel have been reported by researchers. For instance, Veljkovic et al. (2016) indicated the feasibility of a two-way process on biodiesel production from TSO having high FFA. Usta et al. (2011) indicated suitable for the antioxidant for TSOME. Sharma et al. (2020) explored RSM for modelling the diesel engine performance parameters of IC engines fuelled with TSOME and diesel blends. However, published literature on ANN-ANFIS based modelling of biodiesels from non-edible oils is scarce. A hybrid of ANN and ANFIS was adopted to optimize biodiesels from sorrel oil (Ishola et al., 2019), palm kernel oil (Betiku et al., 2018), Vitis vinifera seed oil (Hariram et al., 2019), and waste cooking oil, aided with a prepared heterogeneous catalyst (Betiku and Ishola, 2020).

To the best of the authors' knowledge, a hybrid tool such as ANN integrated with the ANFIS has not been explored to model transesterification parameters of biodiesel production from TSO. On the contrary, the hybrid tool has been employed in other engineering applications. For instance, a handful of exploration of ANN and ANFIS in the distributed system (Okwu and Adetunji, 2018), mechanical properties of concrete (Boğa et al., 2013), wind speed sensor (Rahman and Rahim, 2016), grade estimation (Tahmasebi and Hezarkhani, 2012 ; Amirkhani et al., 2015), and under convective hot air dryer (Kaveh et al., 2018), sheet hydroforming process (Yaghoobi et al., 2016), etc., have appeared in the literature. Also, the adoption of ANN and ANFIS models are relevant since it strengthens the performance of the model and enables robust modeling for effective productivity and sustainability. Unfortunately, the perusal of the survey showed that there are (1) no established ANN model for TSOME production and (2) comparison capacity of hybrid models such as RSM and ANN models for TSOME's parameters in the literature are scarce. Hence, there is a need to truncate the lapses in the knowledge of such reports and establish robust models models capable of promoting sustainable production of biodiesel alongside tobacco production in developing countries.

Materials and Method

Data Preparation and Modelling Technique

Creative and intelligent techniques should be adopted for modeling and optimizing limited nonlinear as well as ill-defined engineering problems such as the methylic process. To end this, the ANN and ANFIS were employed herein to model the methylic biodiesel production from TSO on a lab scale.

Figure 2 portrays tobacco seeds (TS) as a by-product from leaves of tobacco, and the TS are small but compact together (Giannelos et al., 2002). TSO comprises linoleic acid (C18: 2; 73. 19 wt %), oleic acid (C18: 1; 7. 97 wt %), and palmitic acid (C16: 0; 11. 73 wt %) (Figure 3). As detected in Figures 3 and 4 , the overall saturated and unsaturated fatty acids contained in TSO were 73. 43 and 26. 57 wt %, respectively. TSO having high saturated fatty acid content has a tendency to improve the cetane number of the fuel (Samuel et al., 2020a).

The efficacy of ANN and ANFIS models are indicated in biodiesel productions from palm kernel oil (Betiku et al., 2018), Vitis vinifera seed oil (Hariram et al., 2019), waste cooking oil (Najafi et al., 2018). The theory associated with the models can be found elsewhere (Ighose et al., 2017). Table 1 highlights the databases utilized for the development of ANN and ANFIS models (Waheed et al., 2015).

FIGURE 2

Tobacco seeds.

FIGURE 3

Fatty acid composition of TSO.

FIGURE 4

Tobacco seed oil’s GC chromatogram.

TABLE 1

Dataset for TSOME (Waheed et al., 2015).

The comprehensive information on the employed materials, biodiesel development methodology, and analytical techniques could also be found elsewhere (Waheed et al., 2015). Reaction time, A (40, 60, and 80°C), methanol/oil molar ratio, B (4: 1, 6: 1, and 8: 1), and catalyst amount, C (0. 5, 1. 0, and 1. 5 wt %) were adopted as input variables to the hybrid models. The biodiesel yield/TSOME's yield was separately adopted as the response of the models. To implement the predictive models, MATLAB ® R2019a was employed. The established models for the prediction were the ANN technique based on a multilayer perceptron (MLP) algorithm integrated with the ANFIS.

ANN and ANFIS Modelling

ANN Modelling

The ANN modelling was systematically conducted by using the dataset presented in Table 1 . The steps involved in the ANN modelling for TSOME production are presented in the Supplementary Figure S1 . The optimum model implemented based on the ANN technique focused on three key steps: (1) optimum neuron value, (2) selection of the appropriate training algorithm, and (3) model testing and validation. Twenty samples of the dataset were considered for the experiment, with 70% allocated for sample training, 15% samples used for validation, and 15% of samples engaged for testing. Utilizing the presented experimental data, the Levenberg–Marquardt (LM) ANN fitting tool and Logistic Sigmoid Activation Transfer Function 3–10–

1 (number of the input layer, neurons in the hidden layer, and output layer nodes) model were applied as portrayed in the Supplementary Figure S2 . The LM back propagation highlights the process of data training, network inputs, and target/response standardized with a fitted maximum and minimum level. The literature provides details on the adoption of the standardization limits (Aghbashlo et al., 2016 ; Okpalaeke et al., 2020 ; Okwu et al., 2020).

ANFIS Modelling

The ANFIS is a high-level creative algorithm obtained by combining the quantitative strength of ANN and the qualitative strength of Fuzzy Logic. The architecture of the ANFIS showing the input variables is presented in the Supplementary Figure S3 . The step presented in the fuzzification was such that the crisp value of inputs and output variables was transformed into linguistic terminologies leading to the sectioning of the membership function plot for easy and accurate analysis. The triangular membership function is selected for the input parameters as portrayed in Figure 5 . It can be observed that the reaction time (40–80 min), methanol/oil molar ratio (4–8), and catalyst amount (0. 5–1. 5 wt %) are presented in Figures 5A–C , respectively. The trapezoidal membership function was preferred for the yield of TSOME (Figure 5).

FIGURE 5

Membership function of(A)reaction time,(B)methanol/oil molar ratio and(C)catalyst amount.

The characteristics fuzzy instruction indicated by Ighose et al. (2017) have been accosted for this study. Table 2 presents the number of membership functions and their ranges. From this, fuzzy rules were formulated as given in Table 3 using the input output-data pair specified in Table 1 . Thereafter, the defuzzification the yield was completed and presented in Figure 6 . To predict the yield of TSOME, a Mamdani-type fuzzy inference system IF-THEN rules were implemented.

TABLE 2

Parameters for membership for input and output for TSOME.

TABLE 3

Rule base of fuzzy inference system.

FIGURE 6

Membership function plot of TSOME.

The mathematical expression that forecasts the behavior of the dependent parameters was expressed with the aid of Eq. 1 (Quesada et al., 2019).

y e = ∫ l = l mr a 1 * [∏ l = l nr μ Fi* (x i , θ i l) l] ∫ l = l mr [∏ l = l nr μ Fi* (x i , θ i l) l] (1) where mr, nr is the number of rules and number of independent parameters while a 1 and y e are the constant model and appraised values of the studied characteristics, respectively.

Assessment of the Development Models

The precision of both ANN and ANFIS models were investigated with the aid of Eqs. 2 – 6 as applied by Samuel et al. (2020b) .

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (E_{i,p} - P_{1,e})^2}{\sum_{i=1}^{n} (E_{i,p} - P_{e,ave})^2} \quad (2)$$

$$MSE = \frac{\sum_{i=1}^{n} (E_{i,e} - P_{i,p})^2}{n} \quad (3)$$

$$MAE = \frac{\sum_{i=1}^{n} [E_{i,e} - P_{i,p}]}{n} \quad (4)$$

$$SEP = \frac{RMSE}{T_{e,ave}} \quad (5)$$

$$AD = \frac{100}{n} \sum_{i=1}^{n} \frac{[E_{i,e} - P_{i,p}]}{(Y_{i,e})} \quad (6)$$

where $E_{i,e}$, $P_{i,p}$, and n are the experimental value, predicted value, and several data, respectively. MSE is the mean standard error, MAE is the mean average error, RMSE is the root mean square error, AD is an average deviation, and SEP is the standard error of prediction.

Results and Discussion

ANN Modelling

Employing MATLAB® R2019a, the prediction of TSOME's yield using ANN has been effectively implemented in this study. Table 2 highlights the grouped available dataset. As obtained, the first sample collection includes 70% dataset for training, 15% for testing, and another 15% for validation. The iteration provided an unsatisfactory result for the first iteration since the MSE value for the training was high. If R-value is close to unity with low MSE values, it becomes appropriate and good for prediction. The iteration performance value was observed until the best values of R and MSE were obtained as shown in Table 4 , with the best training value of 0. 9909. To achieve the best value as presented in Table 2 , the iteration was conducted repeatedly. The best solution was observed for training, testing, and validation at the twenty-fifth iteration with the lowest MSE value and the highest R values.

TABLE 4

ANN training dataset.

Figure 7 presents the relationship between the output and target data. As observed, the straight lines correlate the data. Also, the real and expected correlation coefficients (R) are 0. 9909 (training), 0. 9181 (testing) and 0. 9267 (validation). Therefore, in terms of correlation, the prediction of ANN is significant with an overall value of 0. 8941, as presented in Figure 8 . Figure 9 depicts the best validation performance drawn from the curve of a different epoch. As shown, the best validation performance is 286. 02 at the epoch of 1. Error histogram is another tool used to obtain more information about the neural network Figure 10 portrays the error histogram attained for the regression curves for the chosen network. As seen, a good signal of the values of outliers is obtained.

FIGURE 7

Fuzzy logic rule viewer.

FIGURE 8

Regression plots for the selected network.

FIGURE 9

Performance-plot of the selected network.

FIGURE 10

Error histogram of the selected network.

ANFIS Modelling

Figure 11 depicts the architecture of the developed ANFIS model of the membership functions for three inputs (reaction time, methanol/oil molar ratio, and catalyst amount). Figure 12 displays the actual yield and those of ANN and ANFIS models. As seen, the yield predicted by the ANFIS model is closer to the actual TSOME yield compared to the ANN model. Also, the effectiveness of the models was further substantiated through the plots of experimental values against model predicted values (Figure 13). As seen in Figures 13A, B , the linear equations such as (0. 9104x + 9. 1009) and (1. 0401x − 2. 6601) are detected to be appropriate for the variations of ANN predicted and actual TSOME yields and ANFIS predicted and actual TSOME yields. The high regression coefficients (R^2) of 0. 9048 in the ANN model and 0. 9496 in the ANFIS model imply that over 90. 5 and 95% of the data fit into the respective models. Hence, the ANFIS model could predict the yield better than the ANN model with high accuracy. Similar reports were reported by researchers elsewhere (Betiku and Ishola, 2020 ; Giwa et al., 2020).

FIGURE 11

Architectures for model.

FIGURE 12

Runs vs. Experimental, ANN, and ANFIS predicted yields.

FIGURE 13

Comparison of actual and predicted ANN and ANFIS yield:(A)Actual and ANN predicted yields and(B)actual and ANFIS predicted yields.

Figures 14A–F present the response surface plot of transesterification parameters on the ANFIS predicted TSOME yield in comparison with RSM predicted yield. As observed in Figures 14A, D , TSOME yield remarkably increased from a methanol/oil molar ratio of 4–6 and reaction time of 40–60 min. The yield decreased outside these ranges. Similar observations were documented in the literature by other researchers (Encinar et al., 2010 ; Betiku et al., 2018). The reduction in TSOME's yield can be related to the interference of the separation between the esters and glycerol (Samuel et al., 2019). Tabatabaei et al. (2015) and Dhar and Kirtania (2009) hinted that suitable methanol needs to be employed in the transesterification process to minimize the cost of production. Pugazhendhi et al. (2020) attributed the enhanced yield at the range of reaction temperature to maximum activation energy attained during this period. The researchers further stressed that the reduction in TSOME yield at the high temperature is due to the reversal effect of the transesterification reaction. Figures 14 B, E demonstrate the yield of TSOME as a function of catalyst amount and reaction duration (RT). As noticed, TSOME yield remarkably increased from a catalyst amount of 0. 5–1. 0 wt % and reaction time (RT) of 40–60 min. The yield decreased outside these ranges. A similar observation was reported by researchers elsewhere (Rodrigues et al., 2009 ; Waheed et al., 2015). This reduction in the TSOME's yield is ascribed to the triglyceride in the TSO contributing to the soap formation rather than yield enhancement. Figures 14 C, F depict the yield of TSOME as a function of methanol/oil molar ratio (MR) and catalyst amount. As seen, TSOME yield remarkably increased from a catalyst amount of 0. 5–1. 1 wt % and MR of 4–6. Beyond these ranges, the yield decreased. This observation is further corroborated by Musa (2016) and Dhingra et al. (2016) emphasized that high catalyst amount reduced the yield of TSOME.

FIGURE 14

3D plots by(A–C)ANFIS and(D–F)RSM.

Comparative Evaluation of ANN and ANFIS Models

Figure 15 depicts the statistical indices of ANN and ANFIS models. As noticed, the higher R^2 (0. 978613), lower values of RMSE (3. 0635), SEP (4. 1370), MAE (1. 5311), and AAD (1. 9124) for the ANFIS model compared to those of R^2 (0. 8979), RMSE (7. 1026), SEP (9. 5916), MAE (4. 3446) and AAD

(6. 0529) for ANN model, establish the superiority of the ANFIS model over the ANN model.

FIGURE 15

Comparative of statistical indices of ANN and ANFIS.

Validation of Optimized Condition for TSOME

Table 5 summarizes the optimal conditions for TSOME. As seen, the yield of TSOME (90. 11%) was optimum at the methanol/oil molar ratio of 5. 99/1, catalyst dosage of 1. 10 wt %, and reaction time of 77. 6 min (Waheed et al., 2016). The justification test using the optimized experimental factors produced a predicted for the hybrid yield (90. 15%). The average error between the RSM based predicted and that of hybrid model were 0. 066 and 0. 004%. The validation results showed that the hybrid model developed was precise since the percentages of error in prediction were in a good pact.

TABLE 5

Hybrid model of TSOME.

TABLE 6

An overview on R^2 for ANN and ANFIS on TSOME with literature.

Hybrid Models for TSOME and its Comparison with Literature

Table 5 summarizes the ANN-ANFIS models of TSOME yield. As observed, the models of TSOME are comparable with those in the literature (Betiku et al., 2018 ; Najafi et al., 2018 ; Hariram et al., 2019). The variation in the hybrid models of the present study with those in literature might be ascribed to transesterification conditions and topologies associated with the ANN model.

Table 6 highlights the overview of R^2 of ANN and ANFIS models in the literature and TSOME. As observed, the R^2 value of ANN and ANFIS models for TSOME are comparable to those of literature but those of ANN model are lesser than ANFIS (Betiku et al., 2018 ; Hariram et al., 2019 ; Betiku and Ishola, 2020).

Fuel Properties of TSOME Produced

Supplementary Table S2 recapitulates the basic properties of TSOME formed. As detected, the density of TSOME (891. 1 kg/m^3) concurred with the EN 41214 (850–900 kg/m^3) standard, though somewhat higher than B0 (850 kg/m^3). TSOME having higher density compared to B0 will not significantly influence brake fuel consumption when injected (Niculescu et al., 2019).

The KVs of TSOME (3. 87 mm/s^2) agreed with the ranges of ASTM D6751 (1. 9–6. 0 mm^2/s) and EN14214 (3. 5–5. 0 mm^2/s), however, it was higher than that of fossil diesel (3. 61 mm^2/s). Fuels with modest values of KVs will safeguard complete combustion requiring to enhance engine power and reduction in the exhaust emission profile (Samuel and Gulum, 2019). Flash point (FLAP) of TSOME (126°C) is higher than that of diesel fuel (75°C), and it certified the safety requirements for both international standards. A higher value of FLAP diminishes the risk of fire and this property is a benefit of biodiesel over fossil diesel.

The lower calorific value (LCV) of TSOME (42. 53 MJ/kg) was lower than that of B0 (43. 78 MJ/kg). HSOME possessing LCV can lead to an upsurge in the brake-specific consumption (Xue et al., 2011 ; Adaileh and AlQdah, 2012 ; Samuel et al., 2020b).

Conclusion

The study established the application of the ANN model in comparison with the hybrid ANFIS in the modelling of transesterification parameters of biodiesel production from TSO. The suitability of TSOME produced was also verified for its appropriateness in internal combustion engines. The efficacy of the ANN and ANFIS models was assessed based on the statistical indices such as R^2 , MAE, and AD. The R^2 of 0. 8979, MAE of 4. 3446, and AD of 6. 0529 for the ANN model compared to those of the R^2 of 0. 9786, MAE of 1. 5311, and AD of 1. 9124 for the ANFIS model. The ANFIS model appears to be more reliable than the ANN model in predicting TSOME production for the tropics. The analysis of basic properties indicated that the produced TSOME is comparable to that of fossil diesel. To get a robust study in the nearest future, (i) other transesterification variables namely stirring speed and reaction time and (ii) the second law of thermodynamics can be explored on the TSOME production can be further investigated.

Data Availability Statement

The original contributions presented in the study are included in the article/ Supplementary Material , further inquiries can be directed to the corresponding author.

Author Contributions

OS provided the dataset and wrote the part of the first draft of the manuscript. MO and LT modelled the dataset and wrote part of the first draft of the manuscript. SG and ZO wrote the final draft of the manuscript, which was proofread, improved, and edited by MS. The concept of the study was envisioned by SG and SO.

Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Acknowledgments

The authors are grateful to Pastor Akinola Omotayo and Tayo of Food Science and Technology, Federal University of Agriculture, Abeokuta, Nigeria, for their assistance during the research work.

Supplementary Material

The Supplementary Material for this article can be found online at: https://www. frontiersin. org/articles/10. 3389/fenrg. 2020. 612165/full#supplementary-material .

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