JOTCS B
Journal of the Turkish Chemical Society
Section: B
Chemical Engineering
TURKISH CHEMICAL SOCIETY

Investigation of the Chemical Exergy of Torrefied Lignocellulosic Fuels using Artificial Neural Networks

This article was produced from a poster or oral contribution to the ICAIE Congress, 2017.

Ugur Özveren[1,*], Omer Faruk Dilmac[2], Mehmet Selcuk Mert[3], Fatma Karaca Albayrak[1]

[1]Marmara University, Engineering Faculty, Chemical Engineering Department, Kadikoy, Istanbul, 34722, Turkey
[2]Cankiri Karatekin University, Engineering Faculty, Chemical Engineering Department, Fatih, Cankiri, 18200, Turkey
[3]Yalova University, Engineering Faculty, Energy Systems Engineering Department, Merkez, Yalova, 77200, Turkey

Abstract: Torrefaction is a type of thermo-chemical pretreatment process to enhance energy density of lignocellulosic fuels. For a torrefaction process, a key challenge is to develop efficient thermal conversion technologies for torrefied fuels which can compete with fossil fuels. The calculation of chemical exergy is an essential step for designing efficient thermal conversion systems. However, there is a few correlations to predict the chemical exergy of solid fuels has been published so far. This study deals with a new method to characterize the chemical exergy of different kinds of torrefied lignocellulosic fuels by using Bayesian trained artificial neural network (ANN). The proposed model based on proximate analysis and higher heating values of torrefied fuels. Use of the artificial neural network method is encouraged to reduce variance in model results. The results indicate that the proposed model offers a high degree of correlation (R^2=0,9999) and its robustness and capability to compute the chemical exergy of any torrefied lignocellulosic fuels from its proximate analysis and heating value.

Keywords: Lignocellulosic fuels; Chemical exergy; Proximate analysis; Neural networks.

Submitted: October 05, 2017. **Accepted:** October 20, 2017.

Cite this: Özveren U, Dilmaç OF, Mert MS, Karaca Albayrak F. Investigation of the Chemical Exergy of Torrefied Lignocellulosic Fuels using Artificial Neural Networks. Journal of the Turkish Chemical Society, Section B: Chemical Engineering. 1(sp. is. 1):69–76.

***Corresponding author. E-mail:** ugur.ozveren@marmara.edu.tr

INTRODUCTION

Environmental and economic concerns of fuel supply have been motivating the torrefied fuel for thermal conversion systems. Torrefaction is a thermochemical process in which raw biomass is heated under atmospheric pressure, at a temperature range of 200–300 °C, in the absence of oxygen or under low oxygen concentrations (1). An efficient technology for torrefaction process which can produce torrefied fuel to substitute fossil fuels is a key challenge. Exergy analysis is commonly accepted as the most natural way to evaluate the performance of different processes and calculation of chemical exergy is the first step of exergy evolution (2). However, there is a few correlations to predict the chemical exergy of solid fuels have been published so far. These correlations are based on ultimate analysis of fuels. However, the ultimate analysis requires very expensive equipment and highly trained analysts. The proximate analysis on the other hand only requires standard laboratory equipment and can be run by any competent scientist or engineer (3).

Artificial neural network is an effective alternative of linear and nonlinear correlations in that they can represent highly complex and nonlinear processes. Furthermore, they are quite flexible and robust against input noise and, once developed and their coefficients determined, they can provide a rapid response for a new input (4).

In this study, a new artificial neural network model was developed to evaluate the chemical exergy of torrefied biomass fuel, which is based on higher heating value and torrefied fuel content obtained by proximate analysis.

MATERIAL AND METHODS

Samples

The data of 116 torrefied biomass samples with their proximate and ultimate analysis were taken from the study of Daya Ram Nhuchhen (5), who acquired the data from previous studies in this field (6 - 16). In order to develop a predictive model, the dataset used in this study was divided into two parts: the first part for training the model and the second for assessing the estimation capability of the obtained neural network architecture (called the "testing set"). All 116 torrefied biomass samples as well as a split of the samples into a training set with 97 samples and a testing set with 19 samples were randomly selected

by using the MATLAB software. Description of torrefied biomass samples was given Table 1.

Table 1. Torrefied Biomass Samples (5).

	Minimum (%)	Maximum (%)
Oxygen (% DAF*)	7,23	44,35
Nitrogen (%DAF)	0,00	2,65
Hydrogen (%DAF)	3,24	7,50
Carbon (%DAF)	49,25	88,50
Total sulfur (%DAF)	0,00	0,26
VM (%DAF)	15,71	87,37
FC (%DAF)	12,67	84,29
HHV (MJ/kg)	16,63	33,30

*DAF = Dry Ash free VM: Volatile Matter HHV: Higher Heating Value

In order to validate the artificial neural network model, un-torrefied biomass samples from the study of Chun-Yang Yin (17) also were tested to measure the extensity of the proposed exergy model in this study. Description of biomass samples used in this study for 23 samples was given Table 2.

Table 2. Biomass Samples (17).

	Minimum (%)	Maximum (%)
Oxygen (% DAF*)	33,02	48,99
Nitrogen (%DAF)	0,30	5,49
Hydrogen (%DAF)	4,49	7,34
Carbon (%DAF)	42,26	56,73
Total sulfur (%DAF)	0,02	0,85
VM (%DAF)	71,38	87,16
FC (%DAF)	12,84	28,57
HHV (MJ/kg)	15,09	21,95

*DAF = Dry Ash free VM: Volatile Matter HHV: Higher Heating Value

Artificial Neural Networks

An ANN is a massively parallel-distributed information processing system that simulates the functions of neurons using artificial neurons inspired from the studies of the brain and the nervous system (18). An artificial neuron is the fundamental processing element of ANN and can be implemented in many different ways. The general architecture of an artificial neuron is shown in Figure 1 (18,19).

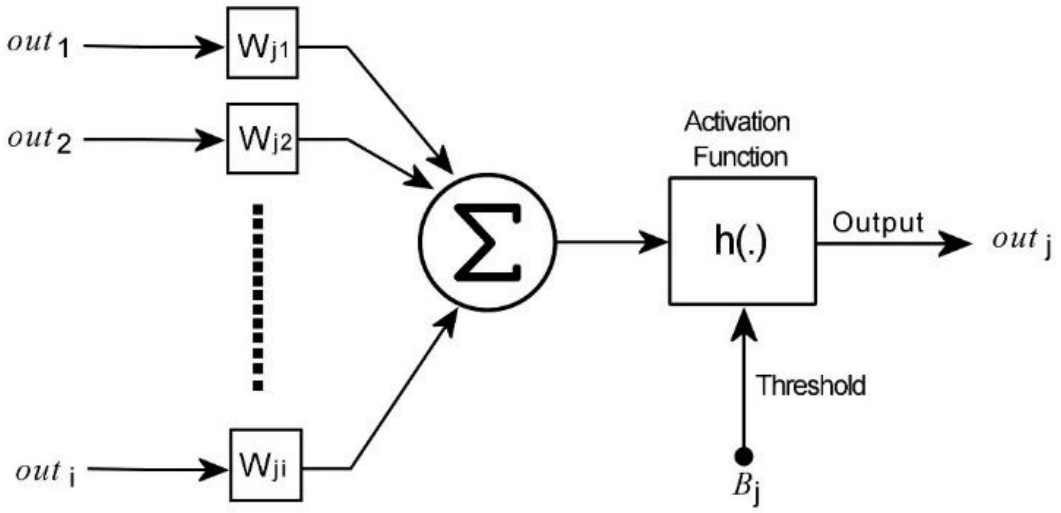

Figure 1. Architecture of an artificial neuron

In this figure, input from the output (out_i) of the preceding layer neuron is multiplied by its weight value (W_{ji}). Then, results of these multiplications are summed with bias value (B_j). The initial weights and biases are usually assigned randomly. The output of a neuron, which is in Figure 1, can be described by Equation 1.

$$out_j = h(\sum_{i=1}^{N}(W)_{ji}X_i + B_j) \quad \text{(Eq. 1)}$$

where h is the activation (transfer) function. The activation function can be found in different forms, either linear or non-linear. In this work, logarithmic sigmoid, h(x), function was used an activation function which defines as:

$$h(x)= 1/(1+\exp(-x)) \quad \text{(Eq. 2)}$$

Bayesian methods are the ideal methods for solving learning problems of neural network (20), which can automatically select the regularization parameters and integrate the properties of high convergence speed of traditional BP and prior information of Bayesian statistics (21). The Bayesian Regularization method changes the error performance function by attaching a standard deviation of the weights and the thresholds (22) and can be expressed by (23):

$$F=\beta E_D+\alpha Ew \quad \text{(Eq. 3)}$$

where α and β are the regularization parameters. Using (Equation 3) to minimize the performance error, enables the network to possess less weights and thresholds. This is

equivalent to reducing the size of the network in such a way that it can respond smoothly, thus reducing overfitting (23).

ANN Model

The exergy value of a solid fuel is related to higher heating values and proximate analysis. Therefore, the correlation between the exergy values of torrefied fuels and their proximate analysis with higher heating values has been examined to develop an artificial neural network model. There are several classes of neural network architectures, classified according to a number of layers, neurons, and their interconnections. In this paper, we adopt a single-output three-layered BP neural network with Bayesian regularization to predict the dry ash free based chemical exergy (e_{DAF}^{CH}) of the torrefied fuels. Figure 2 presents the neural network structure of proposed model.

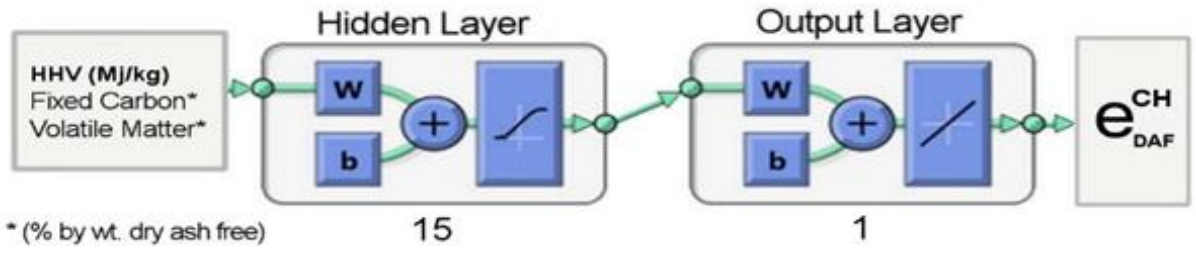

Figure 2. ANN Model

Validation of the correlations

In this study, Coefficient of determination (R^2) is employed to assess correlations for the chemical exergy of torrefied biomass, which is computed as follows:

$$R^2=1-\frac{\sum_i^n(c_i-e_i)^2}{\sum_i^n(c_i-\bar{c})^2} \quad \text{(Eq. 4)}$$

Where e and c denote the estimated and calculated values, respectively. $\bar{c}$ is the calculated average value. R^2 is used as a universal parameter to measure the accuracy of any model. A higher R^2 value means a better estimation and fitting.

RESULTS AND DISCUSSIONS

In order to use an artificial neural network model, one needs first to train the proposed model with training dataset. Figure 3 showed the quality of fit between the chemical exergy values and predicted chemical exergy values of torrefied fuels for training dataset.

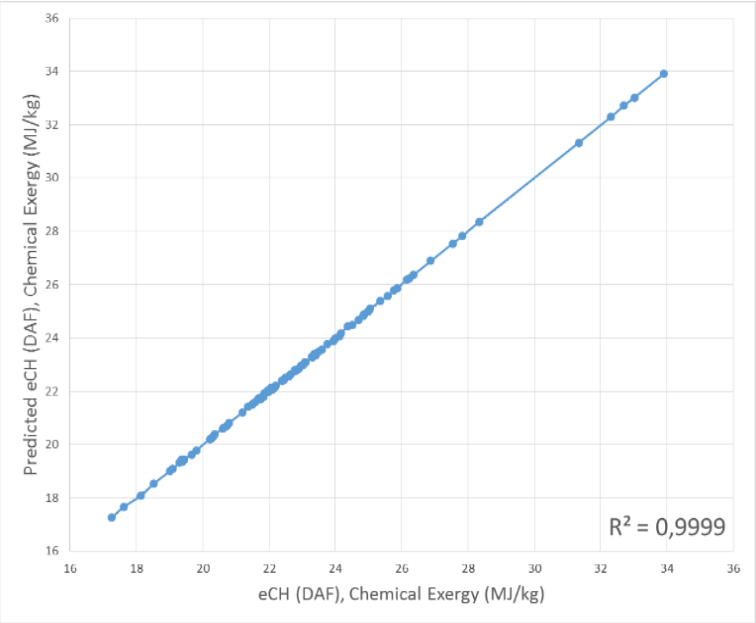

Figure 3. Training dataset

The artificial neural network model was also tested for reliability using the testing dataset (Figure 4).

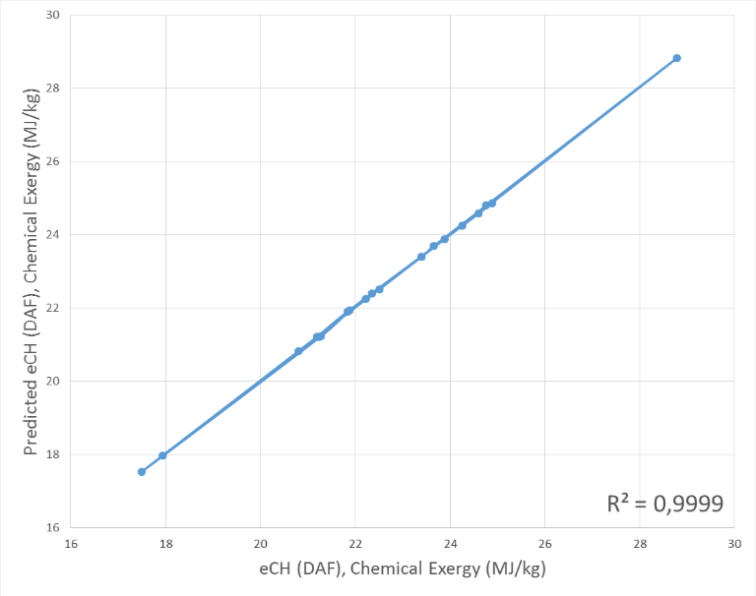

Figure 4. Test dataset

In this study, a high degree of correlation (R^2 = 0,9999) between actual and predicted chemical exergy was observed, as shown in Figure 4, for test datasets of the torrefied lignocellulosic fuels. It can thus be apprehensible that the ANN model used in this study possesses good accuracy and generalization performance.

To ensure the capability and predictive ability of the model, biomass fuel dataset also were used for the robustness of the proposed model. Figure 5 shows plots of the chemical exergy values and corresponding ones estimated by the model in this study.

CONCLUSIONS

A model for chemical exergy prediction of lignocellulosic fuels was developed using artificial neural networks. The high R^2 values and the good fit in testing dataset lead to the conclusion that the artificial neural network model provides accurate predictions of the chemical exergy for a variety of torrefied lignocellulosic fuels. The major advantage of this model is its capability to compute chemical exergy of any torrefied fuels simply from its proximate analysis instead of ultimate analysis. Thereby provides a useful tool for exergy analysis of thermal conversion processes.

REFERENCES

1. Rousset P, Aguiar C, Labbe N, Commandre JM. Enhancing the combustible properties of bamboo by torrefaction. Bioresource Technology. 2011 Sep; 102(17): 8225-8231.

2. Song GH, Shen LH, Xiao J. Estimating Specific Chemical Exergy of Biomass from Basic Analysis Data. Industrial & Engineering Chemistry Research. 2011 Aug 17; 50(16): 9758-9766.

3. Parikh J, Channiwala SA, Ghosal GK. A correlation for calculating HHV from proximate analysis of solid fuels. Fuel. 2005 Mar; 84(5): 487-494.

4. Estiati I, Freire FB, Freire JT, Aguado R, Olazar M. Fitting performance of artificial neural networks and empirical correlations to estimate higher heating values of biomass. Fuel. 2016 Sep 15; 180: 377-383.

5. Nhuchhen DR. Prediction of carbon, hydrogen, and oxygen compositions of raw and torrefied biomass using proximate analysis. Fuel. 2016 Sep 15; 180: 348-356.

6. Arias B, Pevida C, Fermoso J, Plaza MG, Rubiera F, Pis JJ. Influence of torrefaction on the grindability and reactivity of woody biomass. Fuel Processing Technology. 2008 Feb; 89(2): 169-175.

7. Bridgeman TG, Jones JM, Williams A, Waldron DJ. An investigation of the grindability of two torrefied energy crops. Fuel. 2010 Dec; 89(12): 3911-3918.

8. Chen DY, Zhou JB, Zhang QS, Zhu XF, Lu Q. Upgrading of Rice Husk by Torrefaction and its Influence on the Fuel Properties. Bioresources. 2014 Nov; 9(4): 5893-5905.

9. Eseltine D, Thanapal SS, Annamalai K, Ranjan D. Torrefaction of woody biomass (Juniper and Mesquite) using inert and non-inert gases. Fuel. 2013 Nov; 113: 379-388.

10. Ibrahim RHH, Darvell LI, Jones JM, Williams A. Physicochemical characterisation of torrefied biomass. Journal of Analytical and Applied Pyrolysis. 2013 Sep; 103: 21-30.

11. Pala M, Kantarli IC, Buyukisik HB, Yanik J. Hydrothermal carbonization and torrefaction of grape pomace: A comparative evaluation. Bioresource Technology. 2014 Jun; 161: 255-262.

12. Pohlmann JG, Osorio E, Vilela ACF, Diez MA, Borrego AG. Integrating physicochemical information to follow the transformations of biomass upon torrefaction and low-temperature carbonization. Fuel. 2014 Sep 1; 131: 17-27.

13. Soponpongpipat N SD, Sae-Ueng U. Higher heating value prediction of torrefaction char produced from non-woody biomass. Front Energy. 2015; 9(4): 461-471.

14. Strandberg M, Olofsson I, Pommer L, Wiklund-Lindstrom S, Aberg K, Nordin A. Effects of temperature and residence time on continuous torrefaction of spruce wood. Fuel Processing Technology. 2015 Jun; 134: 387-398.

15. Wannapeera J, Fungtammasan B, Worasuwannarak N. Effects of temperature and holding time during torrefaction on the pyrolysis behaviors of woody biomass. Journal of Analytical and Applied Pyrolysis. 2011 Sep; 92(1): 99-105.

16. Wannapeera J, Worasuwannarak N. Upgrading of woody biomass by torrefaction under pressure. Journal of Analytical and Applied Pyrolysis. 2012 Jul; 96: 173-180.

17. Yin CY. Prediction of higher heating values of biomass from proximate and ultimate analyses. Fuel. 2011 Mar; 90(3): 1128-1132.

18. Ozveren U. An artificial intelligence approach to predict a lower heating value of municipal solid waste. Energy Sources Part a-Recovery Utilization and Environmental Effects. 2016; 38(19): 2906-2913.

19. Fausett LV. Fundamentals of neural networks : architectures, algorithms, and applications. Prentice-Hall; 1994 3.

20. Heydecker BG, Wu J. Identification of sites for road accident remedial work by Bayesian statistical methods: an example of uncertain inference. Advances in Engineering Software. 2001 Oct-Nov; 32(10-11): 859-869.

21. Sun Z, Chen Y, Li XY, Qin XL, Wang HY. A Bayesian regularized artificial neural network for adaptive optics forecasting. Optics Communications. 2017 Jan 1; 382: 519-527.

22. Li X, Wang DS. A Sensor Registration Method Using Improved Bayesian Regularization Algorithm. International Joint Conference on Computational Sciences and Optimization, Vol 2, Proceedings. 2009: 195-199.

23. Monteiro RVA, Guimaraes GC, Moura FAM, Albertini MRMC, Albertini MK. Estimating photovoltaic power generation: Performance analysis of artificial neural networks, Support Vector Machine and Kalman filter. Electric Power Systems Research. 2017 Feb; 143: 643-656.