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Fuzzy logic modeling of porous carbon body fabrication from cellulose based materials

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Abstract. This research presents a novel process for dry wood parts carbonization to net shape porous carbon body which retains all the wood's anatomical feature. Due to reasonable price, easy shaping and good formability of wood, as a raw material, it can be used in several advanced cellulose-based applications without any special finishing steps. The interpretation of how carbonization parameters such as heat treatment temperature, carbonization time and initial density of wood affects the final solid carbon characteristics is a fundamental step in this technology improvement and is discussed in this study. A fuzzy logic (FL) method was implemented as a powerful and accurate way for predicting the bulk density change in special tree wood samples during carbonization process. Besides, a regression relationship is established between above parameters and subsequently, significance of each one was identified. Scanning electron microscope (SEM) was used to elucidate the porous carbon microstructure of final product.

Introduction

In recent decades, researchers have shown so many interests in discovering new natural sources of raw materials for artificial synthesized products substitution. The shortage and high fabrication cost of available using materials enhance the encouragement of this novel field of materials utilization and application. The use of carbonized wood in engineering fields is being considered in recent researches that it can be used as a matrix for production of cellulose derived composites (CDC) including carbon/polymer, carbon/carbon, carbon/ ceramics and carbon/metal composites [1].This category of composites posses several thermal, mechanical and also tribological applications by using Wood and Carbonized wood as matrix or reinforcement in templates, chops and husks form.Typically, the chemical composition of dry wood sample is: 50 wt.% carbon, 44 wt.% oxygen and 6 wt.% hydrogen. During carbonization, none of wood anatomical features altered while a completely different composition achieved [2]. Wood has several natural polymers in its content which form a complex body of different interconnected long cells. These cells are parallel with central axis of tree trunk. Cellulose, hemicellulose and lignin are the three main polymers of wood material. The most significant one is cellulose. Hemicellulose and lignin are put in the net shape body of cellulose with different ratio depending on the wood sample place in the tree trunk. At heating rate of $5^{O}C\ min^{-1}$, hemicelluloses is decomposed at temperatures ranging from 170 to 240 ^{O}C, cellulose 240–310 ^{O}C, and lignin 320–400 ^{O}C [3]. Aggregation of crystalline cellulose in the cell wall of wood into larger aligned parts shaped elementary fibrils which form narrow aggregates known as microfibrils [4]. Carbon body has several desired properties like stable coefficient of friction (μ), good electromagnetic shielding, low coefficient of thermal expansion (α), high damping capacity and self lubricity [5-6]. Different studies have been done on thermophysical and microstructural aspects of wood carbonizations and its affecting parameters [7-12]. But there are so far only a few researches focused on numerical and soft computational view of process [13-14]. The present study also implements a powerful fuzzy logic model for predicting process operating parameters by considering heat treatment temperature, carbonization time and initial density of wood on the bulk density change of porous carbon during carbonization. Fuzzy logic is a very useful and outstanding computational tool in different complex and nonlinear engineering problem[15]. Since any logical system can be fuzzified and a general logical relationship exists between solid carbon density and above carbonization factors, a fuzzy logic (FL) approach would be very efficient and effective for this case.

Experimental

Samples from oak (scientific name: Quercus), Maple (scientific name: Acer), and Basswood (scientific name: Tilia) tree were prepared in cubic shape using a precise wood cutting instrument. These different types of wood samples have different bulk densities. They have 20 millimeters length and width and 10 millimeters height. In the second stage, two drying steps were carried out for removing structural water of wood in order to avoid fungus affection and spoiling during test period in laboratory atmosphere:

i) Air drying for one week in a warm location.

ii) Drying for 48 hours at 103 ^{O}C in an electrical oven with air circulation mode.

In various time sets, Different types of wood samples were heated to different temperatures in order to produce porous carbon body. Among the selected tree samples, Maple has the denser structure with bulk density of 0.75 g/cm^3, Oak posses the second rank with density of 0.7 g/cm^3 and at last; Basswood has the lowest density of all with about 0.5 g/cm^3. Using an Argon atmosphere control electrical furnace, cubic wood samples were carbonized at different temperatures of 400 ^{O}C, 450 ^{O}C and 500 ^{O}C. According to design strategy, the process was conducted in three durations: 1.5, 2 and 2.5 hours. Since the density change of product is the main output of the work, exact value of wood mass and dimensions were measured before and after test by precise balance tools. Table 1 indicates the details of performed experiments and the final measured density of each test run.

Table 1 Carbonization test's design and final carbon density

Test run	Carbonization temperature (°C)	Time period (Hour)	Initial density (g/cm^3)	Carbon density (g/cm^3)
1	400	1.5	0.5	0.146
2	400	1.5	0.7	0.212
3	400	1.5	0.75	0.229
4	400	2	0.5	0.201
5	400	2	0.7	0.283
6	400	2	0.75	0.311
7	400	2.5	0.5	0.245
8	400	2.5	0.7	0.336
9	400	2.5	0.75	0.308
10	450	1.5	0.5	0.189
11	450	1.5	0.7	0.256
12	450	1.5	0.75	0.261
13	450	2	0.5	0.274
14	450	2	0.7	0.318
15	450	2	0.75	0.326
16	450	2.5	0.5	0.361
17	450	2.5	0.7	0.385
18	450	2.5	0.75	0.397
19	500	1.5	0.5	0.333
20	500	1.5	0.7	0.351
21	500	1.5	0.75	0.362
22	500	2	0.5	0.345
23	500	2	0.7	0.374
24	500	2	0.75	0.378
25	500	2.5	0.5	0.498
26	500	2.5	0.7	0.513
27	500	2.5	0.75	0.537

The application of numerical methods in new fields of industrial and engineering topics are getting raised day to day. Soft computation methodology based on the science of artificial intelligence has found its place in modern advanced materials challenges and applications. Artificial neural network (ANN) is the most well-known tool in prediction and classification of complex and multi-dimensional materials properties characterization with its outstanding ability of learning from sets of examples and generalizing the knowledge to new conditions [16].However, above method has many disadvantages that may get the simulation process into trouble; very slow convergence, entrapment in local minimum and of course requirement of large number of data sets are some of ANN problems. Therefore, fuzzy logic can be considered as a better modeling approach[17]. Fuzzy logic theory was first introduced by L. A. Zadeh in 1965 [18]. Fuzzy logic is a powerful problem-solving methodology with a lot of applications in embedded control and materials processing [19-23]. Fuzzy concepts provide a remarkably simple way to draw definite conclusions from vague, ambiguous or imprecise information. In a sense, fuzzy logic resembles human decision making with its ability to work from approximate data and find precise solutions. Unlike classical logic which requires a deep understanding of a system, exact equations, and precise numeric values, Fuzzy logic incorporates an alternative way of thinking, using a higher level of abstraction compromised from our past experiences so it simplifies design complexity and solution implementation. Considering above concepts, deterministic uncertainty in Fuzziness may be confused with nondeterministic probability. Fuzziness describes event ambiguity but probability describes event occurrence. Whether an event occurs is random, the degree to which it occurs is fuzzy. In fuzzy logic, numbers replaced by linguistic variables whose values are words and specific rules. The conventional coding of a classical set (crisp set) has only two values: one uses when a member is in the set; and zero, when it is out of it but in fuzzy logic theory, everything is a matter of degree .Membership function is used for clarifying the value of each element.

The fuzzy logic based modeling is much more in-line with human's interpretation trend, which implements an 'if–then' principle. In the fuzzy theory literature, 'If' usually named premise and 'Then' is the subsequence. Basically, fuzzy logic has three steps: fuzzification, rule evaluation and defuzzification process. Fuzzification is a process that converts numerical values into fuzzy sets. The rule evaluation step contains the ''if...then" phrases that forms linguistic structure of rules. Finally, a defuzzification procedure transforms the fuzzy outputs to crisp ones.

Results and discussion

The scanning electron microscope images of the carbonized dry wood are illustrated in Fig. 1. These micrographs are taken after two hours of holding in argon atmosphere control furnace at 450 ^{O}C. It can be seen from the micrographs that the wood anatomical feature remains without any considerable change and the shape of porosities in initial wood templates is similar to heated wood in the form of carbon and this leads to the different separated pores in carbon surface. In wood-based carbon matrix composites, by using a vacuum infiltration process, metals, ceramics or even polymers can play the role of reinforcement component and fill these cylindrical porosities.

Basically, density change in wood structure with temperature increasing during carbonization in an inert gas atmosphere condition depends on two thermophysical factors which act just in opposite direction with each other: i) Weight loss due to degradation of some wood component while heating and also evaporation of volatile chemicals in wood. This phenomena decrease the density of solid carbon. ii) Wood cell-wall expansion and shrinkage of wood samples that reduce the pore's diameter and increase density in fabricated product [24]. Approximately, from 400 ^{O}C to 1000 ^{O}C the second effect is dominant mechanism and for more enhanced temperatures the first effect. In current study, in selected temperatures were between 400 ^{O}C and 550 ^{O}C in which density increases with temperature. At a constant temperature, higher carbonization time gets more opportunity to organic wood components to rearrange during heating. This longer times leads to more complete reshape of survived organic chain. Consequently, cell wall expansion process improvement takes place in a better mode. In addition, it had been proved that the density of fabricated solid carbon and dry wood has a linear relation and many operating conditions affect the linear equation slope [2].

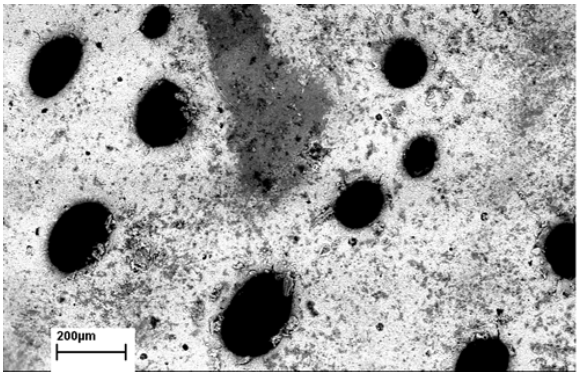

Fig. 1 Microstructure of carbon derived from oak wood

In this research, a number of experiments are carried out for calculation and quantification the final product density in carbonization of wood considering the corresponding parameters including temperature and time of heating and also base wood strain. In order to establish this purpose, carbon density expresses as a non-linear function of its process parameters like the following equation 1.

$$CD = F0 + (F1 \times WD) + (F2 \times TP) + (F3 \times HTT) \quad (1)$$

where, CD is the final carbon density in g/cm^3 and F1 to F4 are equation constants. HTT is the heat treatment temperature (^{O}C), TP is the time period of heating (Hour) and WD is the approximate wood initial density (g/cm^3). The constants are identified using an appropriate regression analysis with a correlation coefficient (r^2) of 0.8981.

$$CD = -0.814 + (0.233 \times WD) + (0.138 \times TP) + (0.00158 \times HTT) \quad (2)$$

Implementation of the fuzzy model applied to density prediction followed the steps listed below:
Fuzzification: choosing the most appropriate membership functions for the three input variables.
Rule evaluation: design of the related rule which link up the three input variables to the single output variable and also assigning membership functions.
Defuzzification: the process of making a fuzzy quantity crisp, with goal of obtaining a real number for next numerical interpretation.
The first phase in the fuzzy system design is assigning a membership function to each variable. Depending on the problem conditions and user's experience, different shapes of membership functions can be used. Membership function can have a symmetrical or asymmetrical shape. In present work, we have chosen triangular fuzzy sets because they are commonly applied because of their simplicity and ability for coding non-linearity. Fuzzy membership converts the notion of binary membership to various degrees of membership value on a two dimensional diagram. Fig. 2 introduces different parts of a typical membership function and Fig. 3 and Fig. 4 illustrates the shape and range of each membership function for inputs and output variables.

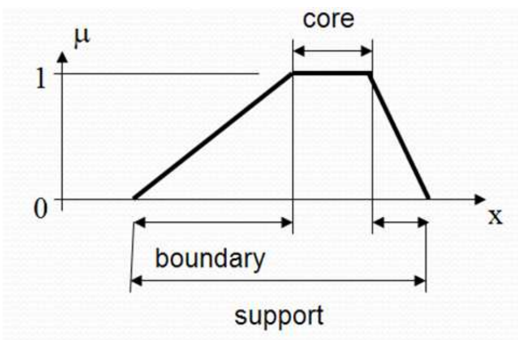

Fig.2 Differnt parts of a membership function

The Core of a membership function is defined as the region that is identified by complete and full membership in the set. . The core consists of elements with unit membership value (μ(x) =1). Boundary is called to the region that is characterized by positive membership in the set. The combination of above two regions is support zone (0≤μ(x) ≤1).

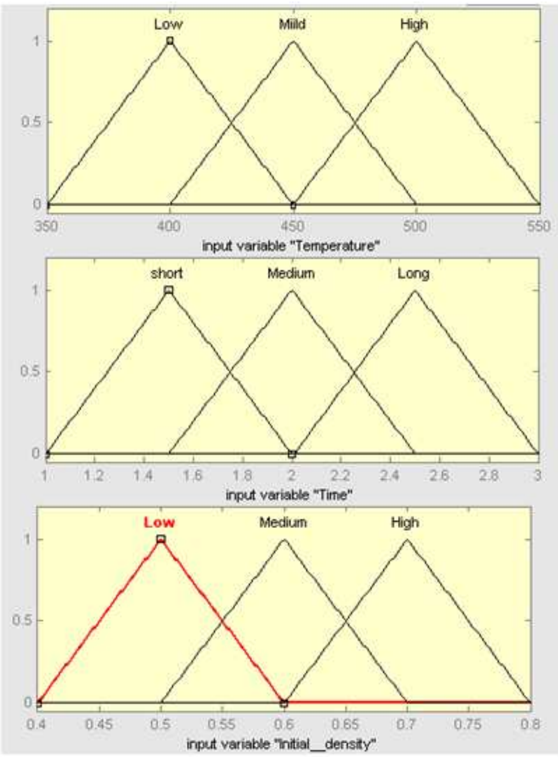

Fig.3 Membership functions for three inputs

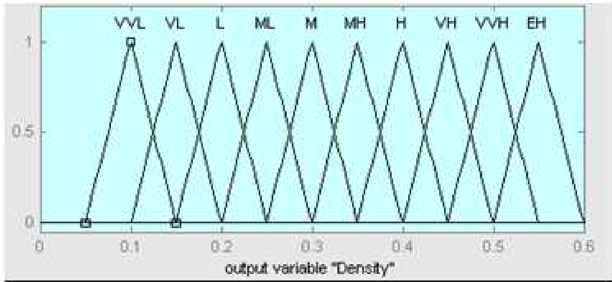

Fig.4 Membership function for single output

The heat treatment temperature is input 1. It has three member functions: low, medium and high. It ranged from 350 to 550 ^{O}C. Carbonization time period, input 2, has three membership functions which are short, medium and long. It ranged from one to three hours and finally initial wood density as third input has three membership functions which are low, medium and high. It ranged from 0.4 to 0.8 g/cm^3. The only output, net shape carbon density, has ten membership functions. It ranged from 0.05 to 0.6 g/cm^{3}and includes very very low(VVL), very low(VL), low(L), medium low(ML), medium(M), medium high(MH), high(H), very high(VH), very very high(VVH) and extra high(EH). Rule evaluation is second step in constructing a fuzzy system .The goal is to establish a connection among multiple inputs and final density of carbon. Table 2 shows 17 accomplishing 'if–then' rules. Deffuzification is the ending process in the fuzzy logic analysis. Many defuzzification methods can be utilized including centre-of-area, weighted average, Max-membership or Height method and Center of sums. We choose the first one of above as one of the most common defuzzification method named centre-of-area or centroid. Fuzzy model results and real carbon density values obtained from experimental tests were compared in Fig. 5 for verifying the accuracy of model in prediction of density changes. The comparison of the actual and fuzzy model value with R^2=0.9781 shows the trustable ability of proposed approach for evaluating the porous structure of carbon product. Fig. 5 presents a regression graph which shows the fuzzy and actual results compression. There is no considerable difference between the predicted and the actual data. In conclusion, the fuzzy model showed better performance and accuracy rather than the regression model with the higher R^2.

Table 2 Rules for the fuzzy inference system

Num	Rule
1	If (Temperature is Low) and (Time is short) and (Initial density is Low) then (Density is VVL)
2	If (Temperature is Low) and (Time is Medium) and (Initial density is High) then (Density is M)
3	If (Temperature is Low) and (Time is Long) and (Initial density is Low) then (Density is MH)
4	If (Temperature is Low) and (Time is Medium) and (Initial density is Medium) then (Density is ML)
5	If (Temperature is Low) and (Time is Long) and (Initial density is High) then (Density is M)
6	If (Temperature is Mild) and (Time is short) and (Initial density is Low) then (Density is VL)
7	If (Temperature is Low) and (Time is short) and (Initial density is Medium) then (Density is L)
8	If (Temperature is Mild) and (Time is Long) and (Initial density is High) then (Density is H)
9	If (Temperature is Mild) and (Time is Medium) and (Initial density is Medium) then (Density is M)
10	If (Temperature is High) and (Time is Long) and (Initial density is High) then (Density is VVH)
11	If (Temperature is High) and (Time is Long) and (Initial density is High) then (Density is EH)
12	If (Temperature is Mild) and (Time is Long) and (Initial density is Low) then (Density is MH)
13	If (Temperature is High) and (Time is Long) and (Initial density is Medium) then (Density is VVH)
14	If (Temperature is High) and (Time is short) and (Initial density is Low) then (Density is M)
15	If (Temperature is Mild) and (Time is short) and (Initial density is High) then (Density is ML)
16	If (Temperature is High) and (Time is Medium) and (Initial density is Low) then (Density is MH)
17	If (Temperature is Mild) and (Time is short) and (Initial density is Medium) then (Density is ML)

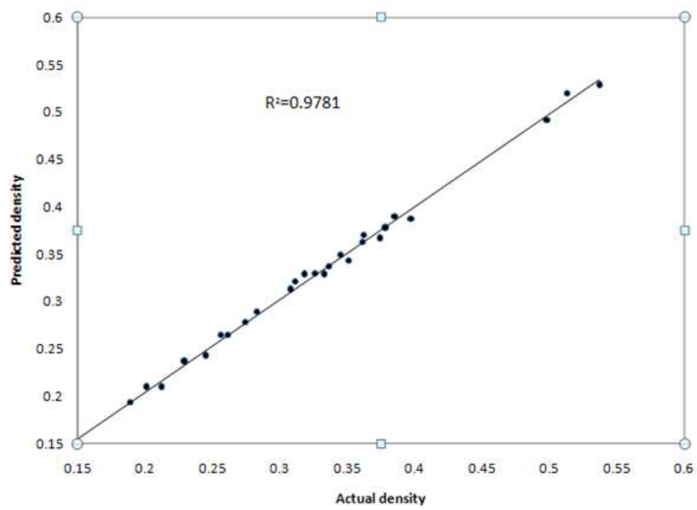

Fig. 5 Regression plot of fuzzy system prediction

Conclusion

In current study different samples of forest plants were used for fabricating porous carbon using an atmosphere control carbonization process in various times and temperatures. The prediction ability of the fuzzy logic and simple regression model for evaluating the experimental bulk density of wood-based carbon considering heat treatment temperature, carbonization time and initial density of wood, as three input parameters, has been performed. The graphs show that the fuzzy logic is a useful tool in estimation of non-linearity in porous carbon density. In addition, linguistic concepts in the form of fuzzy logic are proved to be simpler, more efficient and effective in modeling multi-dimensional complex problems.

References

[1] C.E. Byrne, D.C. Nagle, Mater. Res. Innovations Vol. 1 (1997), p. 137-144.
[2] C.E. Byrne, D.C. Nagle, Carbon Vol. 35 (1997), p. 259-266.
[3] S.-M. Kwon, N.-H. Kim, D.-S. Cha, Wood Sci. Technol. Vol. 43 (2009), p. 487-498.
[4] C.E. Byrne, D.C. Nagle, Carbon, 35 (1997) 267-273.
[5] T.-C. Wang, T.-X. Fan, D. Zhang, G.-D. Zhang, Carbon Vol.44 (2006), p. 900-906.
[6] T.-C. Wang, T.-X. Fan, D. Zhang, G.-D. Zhang, Mater. Lett. Vol. 60 (2006), p. 2695-2699.
[7] P. Gao, M. Wu, B. Li, Y. Liu, Mater. Res. Bull. Vol. 44 (2009), p. 644-648.
[8] K. Ishimaru, T. Hata, P. Bronsveld, Y. Imamura, J. Mater. Sci. Vol. 42 (2007), p. 2662-2668.
[9] D. Özçimen, A. Ersoy-Meriçboyu, Fuel Process. Technol. Vol. 89 (2008), p. 1041-1046.
[10] O. Paris, C. Zollfrank, G.A. Zickler, Carbon Vol. 43 (2005), p. 53-66.
[11] Y.-R. Rhim, D. Zhang, M. Rooney, D.C. Nagle, D.H. Fairbrother, C. Herman, D.G. Drewry Iii, Carbon Vol. 48 (2010) , p. 31-40.
[12] C.S.M. Turney, D. Wheeler, A.R. Chivas, Geochim. Cosmochim. Acta Vol. 70 (2006), p. 960-964.
[13] N. Grioui, K. Halouani, A. Zoulalian, F. Halouani, Thermochim. Acta Vol. 440 (2006), p. 23-30.
[14] N. Grioui, K. Halouani, A. Zoulalian, F. Halouani, Energy Conversion and Manage. Vol. 48 (2007), p. 927-936.
[15] G. Kranthi, A. Satapathy, Comput. Mater. Sci. Vol. 49 (2010), p. 609-614.
[16] M. Kor, E. Abkhoshk, D. Tao, G.L. Chen, H. Modarres, Miner. Eng. Vol. 23 (2010), p. 713-719.
[17] L.A.Zadeh, Inf. control Vol. 8 (1965), p. 338-353.
[18] Y.M. Ali, L.C. Zhang, J. Mater. Process. Technol. Vol. 89-90 (1999), p. 561-568.
[19] D. Chatterjee, G. Sutradhar, B. Oraon, J. Mater. Process. Technol. Vol.200 (2008), p. 212-220.
[20] S. Ramanathan, R. Karthikeyan, M. Gupta, J. Mater. Process. Technol. Vol. 183 (2007), p. 104-110.
[21] S. Raßbach, W. Lehnert, Comput. Mater. Sci.Vol. 16 (1999) , p. 167-175.
[22] O. Ünal, F. Demir, T. Uygunoglu, Building and Environment Vol. 42 (2007), p.3589-3595.
[23] P. Ehrburger, J. Lahaye, E. Wozniak, Carbon Vol. 20 (1982), p. 433-439.

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