Biomass Conversion and Biorefinery
https://doi.org/10.1007/s13399-020-01014-3

ORIGINAL ARTICLE

Appraisal of information system for evaluation of kinetic parameters of biomass oxidation

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Received: 21 August 2020 / Revised: 31 August 2020 / Accepted: 10 September 2020

Abstract
To understand the decomposition behavior of biomass oxidation, there is need to analyze the process by some models. An e-tracking system was established and modeled by the object-oriented methodology of kinetic parameters of biomass oxidation. The system calculates kinetic parameters of the biomass oxidation through neuro-fuzzy methodology which is the main core of the e-tracking system. The main attempt in this study was to develop a model for tracking of the biomass oxidation based on different input features. Activation energy and reaction order were the kinetic parameters of the biomass oxidation which were used as the output parameters. Fixed carbon and ash are the most influential factors for the activation energy and reaction order respectively. Oxygen concertation has the smallest impact on the activation energy and reaction order. Designed e-tracking system could have potential for practical applications since it could be updated with more input parameters.

Keywords Biomass · Neuro-fuzzy · Oxidation · Fresh weight · E-tracking

1 Introduction

Biomass represents one of the most known renewable energy sources which could serve as substitution for fossil fuel. During biomass growth process, carbon dioxide is captured; hence, the obtained final product is carbon neutral source for bioenergy. For the bioenergy production, there is biomass oxidation process. The biomass oxidation process includes physical and chemical processes. During the process, there are several steps which occur simultaneously with different thermal and oxidization reactivity. Therefore, estimation of the oxidation process of different biomasses is a difficult task which requires advances in computational approaches. In other words, there is need to develop models for the biomass oxidation in order to simulate the process.

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The predicted results in article [1] proved the oxidative mechanism of biomass: the first stage is caused by the decomposition of hemicellulose and cellulose and partially decomposition of lignin, and the second stage is resulted from both the decomposition of the remaining lignin and char combustion. The incineration model in article [2] gave a lead to the sequestration of emissions released during the direct combustion of biomass and the subsequent entrapment of oxides of carbon and the eventual release of abundant hydrogen gas in the entrapment jar. The comparison of reforming technologies showed that an autothermal reformer (ATR) could be an advantage since oxygen is already available from the electrolysis stack and the ATR produced syngas has higher CO/CO_2 ratio, which increases the methanol synthesis's reaction rate [3]. The catalytic depolymerization of lignocellulosic biomass to specialty chemicals is often hampered by challenges, which mainly includes cost of catalyst and degradation of the chemicals as they are produced [4]. Evaluation of an existing biomass Gasifier–SOFC–GT system shows the highest exergy losses in the gasifier, gas turbine, and as waste heat [5]. Partial oxidative gasification in supercritical water is a new technology for hydrogen production from biomass [6]. Performance assessment of a novel energy system integrating both biomass gasification and fuel cell systems has been performed in article [7] thermodynamically through energy and exergy efficiencies and results shown that steam biomass ratio

Table 1 Experimental data samples [14]

Input 1	Input 2	Input 3	Input 4	Input 5	Output 1	Output 2
Fixed carbon	Volatile matter	Ash	O_2 concentration	Air to biomass ratio (L/(g min))	Activation energy, Ea (kJ/mol)	Reaction order, *n*
15.2	73.8	11.1	21	1	96	1.3
15.2	73.8	11.1	21	1	98.4	1.3
15.2	73.8	11.1	21	1	88	1.3
16.1	73	10.8	21	1	94.4	1.3
16.1	73	10.8	21	1	96.3	1.3
16.1	73	10.8	21	1	99.6	1.4
16.8	77.1	6.1	21	1	91.9	1.3
16.8	77.1	6.1	21	1	81.8	1.3
20	76.5	3.5	21	16.7	98.5	1.4
17.2	75.8	7	21	16.7	99.6	1.4
32.7	64.4	2.8	21	16.7	78.8	1.5
10	70	20	21	16.7	114.9	1.2
18.4	54.6	27	21	5	80.8	1.2
8.7	80	11.3	100	10	84.2	1.2
8.7	80	11.3	60	10	85	1.2
8.7	80	11.3	80	10	85	1.2
8.7	80	11.3	40	10	85.8	1.2
8.6	86.6	4.9	21	4	62.6	1.1
8.8	85.8	5.4	21	1	62.5	1.1
8.9	85.1	6	21	1	63.4	1.1
9.1	84.4	6.5	21	1	62.5	1.1
10.2	79.9	9.9	21	1	79.5	1.1
8.5	87.2	4.3	21	2.5	79.8	1.6
18	74.1	7.9	12.5	10	114.4	1.9
20.1	69.8	10.1	5	10	125.9	1.3
20.1	69.8	10.1	10	10	128.3	1.3
20.1	69.8	10.1	15	10	130.4	1.4
18.4	81	0.6	10	10	161.4	1.3
3.6	81.4	15	21	1.3	104.3	1.3
3.6	81.4	15	21	1.3	107.5	1.3
3.6	81.4	15	21	1.3	109.9	1.4
3.6	81.4	15	21	1.3	96.9	1.4
15.8	71.6	12.6	21	10	93.5	1.5
13.3	81.5	5.2	21	10	104	1.5
24	72.3	3.8	21	10	86.8	1.3
24	72.3	3.8	21	10	88.2	1.3
24	72.3	3.8	21	10	89.9	1.3
14.5	82.5	2.9	21	6	102.6	1.5
13.6	82.7	3.6	21	6	99.1	1.4
10.7	74.6	14.8	21	6	108	1.5
18.2	79.3	2.5	60	10	81.6	1.4
24.7	73.5	1.7	21	0.8	97.1	1.2
19.2	70.2	10.7	21	0.8	94.4	1.2
12.2	57	30.8	80	16.7	103	1.4
12.2	57	30.8	70	16.7	102.7	1.4
12.2	57	30.8	50	16.7	103.5	1.4
12.2	57	30.8	40	16.7	102.3	1.4
12.2	57	30.8	20	16.7	102.2	1.4
34.4	55.4	10.3	60	10	87.3	1.2
34.4	55.4	10.3	20	10	86.3	1.2
34.4	55.4	10.3	50	10	86.8	1.2
34.4	55.4	10.3	50	16.7	84.9	1.2
34.4	55.4	10.3	20	16.7	84.2	1.2
15.1	83.9	1	21	10	127.1	1.4
6.4	71.1	22.5	21	6	114.8	1.2
15.1	83.8	1.1	21	10	127	1.4
60.8	30	9.2	21	6.3	136	1.3
35.4	45	19.6	21	25	77.2	1.2
27.4	59.1	13.6	21	25	79.3	1.2
28.5	60.2	11.3	21	25	75.4	1.2
1.4	47.1	51.5	21	16.7	116.7	1.2
2.6	49.4	48	21	16.7	116.7	1.2
3.9	51.7	44.4	21	16.7	120.1	1.3
5.1	54.1	40.8	21	16.7	118	1.3

Table 1 (continued)

Input 1	Input 2	Input 3	Input 4	Input 5	Output 1	Output 2
7.6	58.7	33.7	21	16.7	119.9	1.3
7.6	58.7	33.7	21	16.7	118.7	1.3
7.6	58.7	33.7	21	16.7	119.9	1.3
7.6	58.7	33.7	21	16.7	127.2	1.2
10	63.4	26.6	21	16.7	119.8	1.3
11.3	65.7	23	21	16.7	121.1	1.3
13.1	69.2	17.7	21	16.7	101.6	1.4
13.7	70.4	15.9	21	16.7	92.6	1.5
34.4	55.4	10.3	20	16.7	88.8	1.2
11.3	88.1	0.6	21	4	121.5	1.4
16.4	75.3	8.3	20	16.7	96.2	1.4
13	54.6	32.5	20	2.9	77.7	1.2
9	48.2	42.8	20	2.9	76.8	1.1
6	48.7	45.3	21	10	100.1	1.4
17.6	82.1	0.3	21	12	126.4	1.3
17.6	82.1	0.3	21	12	129.5	1.3
12	87.5	0.4	21	12	127	1.4
12	87.5	0.4	21	12	114.7	1.5
15.5	84.2	0.3	21	12	123.5	1.4
15.5	84.2	0.3	21	12	133	1.4
15.2	83.9	0.9	21	12	106.5	1.5
9.7	79.8	10.5	20	100	121.2	1.3
17	78.9	4.1	15	100	95.7	1.5
19.3	75.7	5.1	15	100	103.9	1.5
30.8	64.1	5.1	10	20	75	1.4
30.8	64.1	5.1	10	20	79.9	1.4
30.8	64.1	5.1	25	20	82.9	1.4
30.8	64.1	5.1	10	20	71.3	1.5
30.8	64.1	5.1	25	20	68.8	1.5
32.2	67	0.9	10	20	82.9	1.5
32.2	67	0.9	10	20	78.5	1.5
19.2	64.6	16.2	21	10	64.4	1.4
19.2	64.6	16.2	21	10	72.9	1.3
19.2	64.6	16.2	21	10	78.7	1.3
17.1	74.4	8.5	21	10	91.5	1.3
17.1	74.4	8.5	21	10	94.6	1.3

has a significant effect on the hydrogen production efficiency and optimal value of 0.677 is calculated for maximum exergy efficiency at the base case condition. An integrated process of biomass gasification and solid oxide fuel cells (SOFC) has been investigated using energy and exergy analyses [8]. In this study [9], biomass straw was used as a reductant and fuel for the reduction of manganese oxide ore at low temperature of up to 600 °C. In thermal energy conversion of biomass, the char conversion rate influences the design of industrial systems, and results in article [10] have been shown the char oxidation rates are strongly overestimated when predicting rates based on single oxidizers, while the detailed model shows a good agreement to the experimental measurements.

Although there is different approach for monitoring and calculation of kinetic parameters of biomass oxidation, the main goal of the study is to implement an object-oriented approach. The main structure of the system was composed of adaptive neuro-fuzzy inference system (ANFIS) [11], which uses for the kinetic parameter's estimation of biomass oxidation based on acquired data. Unified modeling language (ULM) [12, 13] is used for developing of the e-monitoring system.

2 Methodology

2.1 Data sample selection

There are several steps during biomass oxidation chemical reaction. It is expected that the volatile matter mass percentage fixed carbon mass percentage and ash mass percentage to have

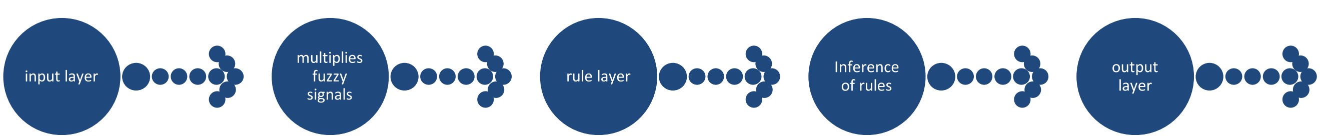

Fig. 1 ANFIS network architecture

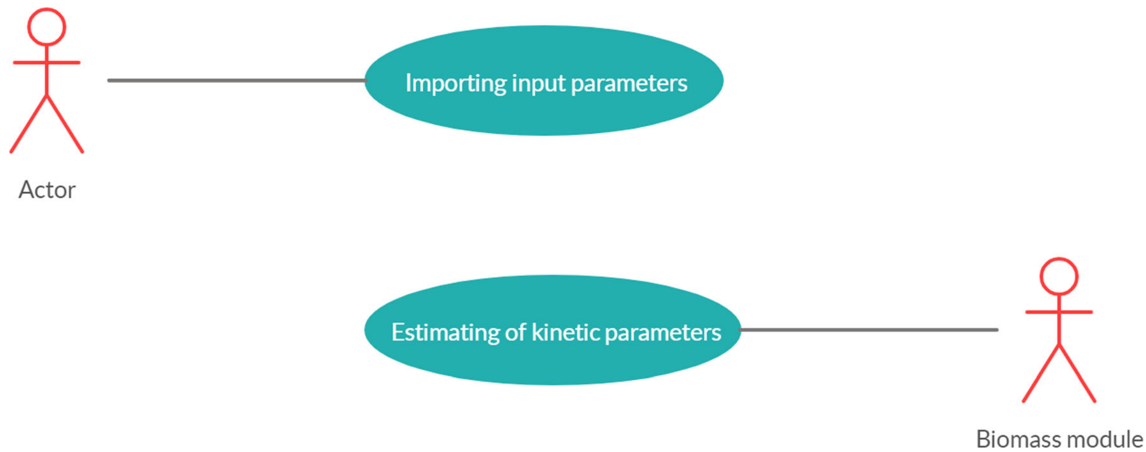

Fig. 2 Main architecture of the e-tracking system

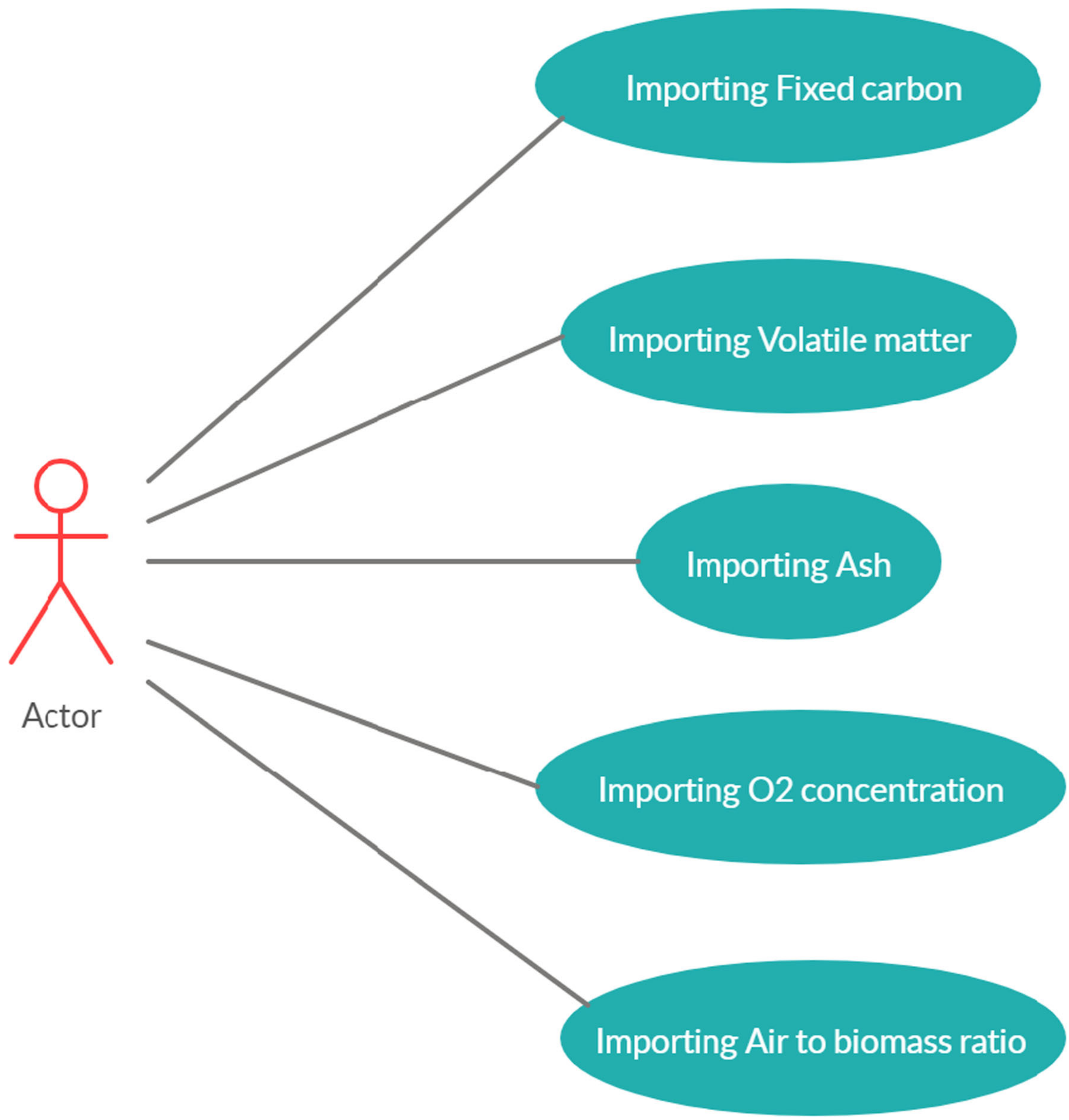

Fig. 3 Use case: importing of input parameters

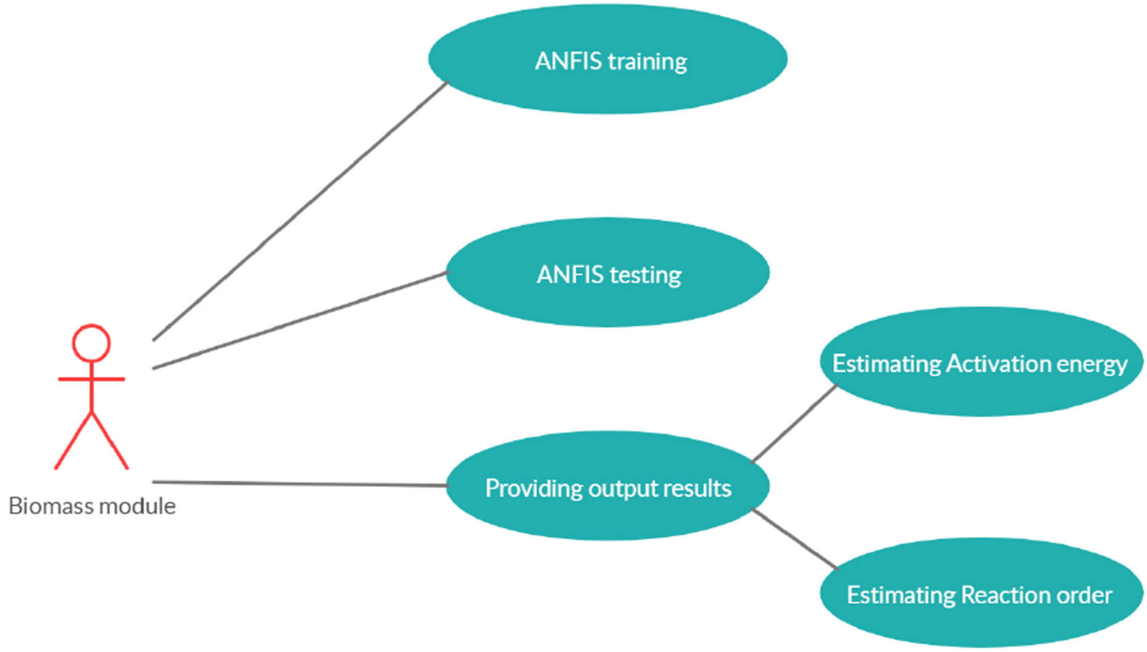

Fig. 4 Use case: tracking of biomass yields

some impact on the reactivity of biomass oxidation according to literature review. Also, oxygen concentration could impact the biomass oxidation process. Therefore, this study selected five input parameters which are considered independent parameters as it was shown in Table 1. As output factors activation energy and reaction order are used which represented kinetic parameters of the oxidation process, there is need to find relationships between the input and output parameters in order to estimate the prediction accuracy of the biomass oxidation. The used dataset selection is arranged according to the single-step decomposition model based on article [14]. The kinetic parameters are extracted from single step decomposition model [14].

2.2 Adaptive neuro-fuzzy inference system

ANFIS network has five layers as it was shown in Fig. 1. The main core of the ANFIS network is fuzzy inference system. Layer 1 receives the inputs and converts them in the fuzzy value by membership functions. In this study, bell-shaped membership function is used since the function has the highest capability for the regression of the nonlinear data.

Adaptive neuro-fuzzy inference system or ANFIS has an architecture composed of five layers as it was shown in Fig. 1. Fuzzy inference system or FIS is the main core of the ANFIS

Table 2 ANFIS activation energy (Ea) prediction based on one feature

Ea prediction (one feature)
ANFIS model 1: fixed carbon --> training = 15.8258, checking = 19.6083
ANFIS model 2: volatile matter --> training = 17.3234, checking = 21.2210
ANFIS model 3: ash --> training = 17.5159, checking = 20.5030
ANFIS model 4: O_2 concentration --> training = 18.0173, checking = 20.9812
ANFIS model 5: air to biomass ratio --> training = 16.8953, checking = 19.1268

Italized entries represent the optimal combinations

Table 3 ANFIS activation energy (Ea) prediction based on two features

Ea prediction (two features)
ANFIS model 1: fixed carbon, volatile matter --> training = 12.7803, checking = 24.1353
ANFIS model 2: fixed carbon, ash --> training = 12.4828, checking = 24.8518
ANFIS model 3: fixed carbon, O_2 concentration --> training = 14.3164, checking = 19.0549
ANFIS model 4: fixed carbon, air to biomass ratio --> training = 13.1696, checking = 82.3402
ANFIS model 5: volatile matter, ash --> training = 12.9343, checking = 18.9395
ANFIS model 6: volatile matter, O_2 concentration --> training = 15.4898, checking = 20.6548
ANFIS model 7: volatile matter, air to biomass ratio --> training = 13.6692, checking = 74.8270
ANFIS model 8: ash, O_2 concentration --> training = 15.3932, checking = 38.1668
ANFIS model 9: ash, air to biomass ratio --> training = 13.1112, checking = 547.5914
ANFIS model 10: O_2 concentration, air to biomass ratio --> training = 14.8848, checking = 1126.9617

Table 4 ANFIS activation energy (Ea) prediction based on three features

Ea prediction (three features)
ANFIS model 1: fixed carbon, volatile matter, Ash --> training = 6.9323, checking = 496.6899
ANFIS model 2: fixed carbon, volatile matter, O_2 concentration --> training = 8.2141, checking = 163.1457
ANFIS model 3: fixed carbon, volatile matter, air to biomass ratio --> training = 9.2503, checking = 829.0704
ANFIS model 4: fixed carbon, ash, O_2 concentration --> training = 9.1417, checking = 73.6573
ANFIS model 5: fixed carbon, ash, air to biomass ratio --> training = 7.6868, checking = 917.9579
ANFIS model 6: fixed carbon, O_2 concentration, air to biomass ratio --> training = 9.6392, checking = 160.4402
ANFIS model 7: volatile matter, ash, O_2 concentration --> training = 8.9612, checking = 117.4240
ANFIS model 8: volatile matter, ash, air to biomass ratio --> training = 8.8099, checking = 2735.2453
ANFIS model 9: volatile matter, O_2 concentration, air to biomass ratio --> training = 9.4588, checking = 801.3475
ANFIS model 10: ash, O_2 concentration, air to biomass ratio --> training = 10.2653, checking = 391.3387

network. Each of the layers of the network has specific function. Input signals are normalized in the first layer throughout of membership functions. The functions are selected before training procedure of the ANFIS network. Bell-shaped membership functions are used in this study since the functions have the best regression capabilities for nonlinear data

Table 5 ANFIS reaction order (n) prediction based on one feature

n prediction (one feature)
ANFIS model 1: fixed carbon --> training = 0.1115, checking = 0.1344
ANFIS model 2: volatile matter --> training = 0.1070, checking = 0.1357
ANFIS model 3: ash --> training = 0.1013, checking = 0.1395
ANFIS model 4: O_2 concentration --> training = 0.1130, checking = 0.1411
ANFIS model 5: air to biomass ratio --> training = 0.1069, checking = 0.1378

[15–18]. The first layer has number of neurons according to the number of inputs. The second, third, and fourth layers have two neurons each while the fifth layer has one neuron which represents the output value. Takagi-Sugeno fuzzy model is used for the fuzzy inference system.

Performances of the proposed ANFIS models are estimated by root mean square error (RMSE) as follows:

1) RMSE

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}} \tag{1}$$

where P_i and O_i are experimental and predicted values, respectively, and n is the total number of data samples.

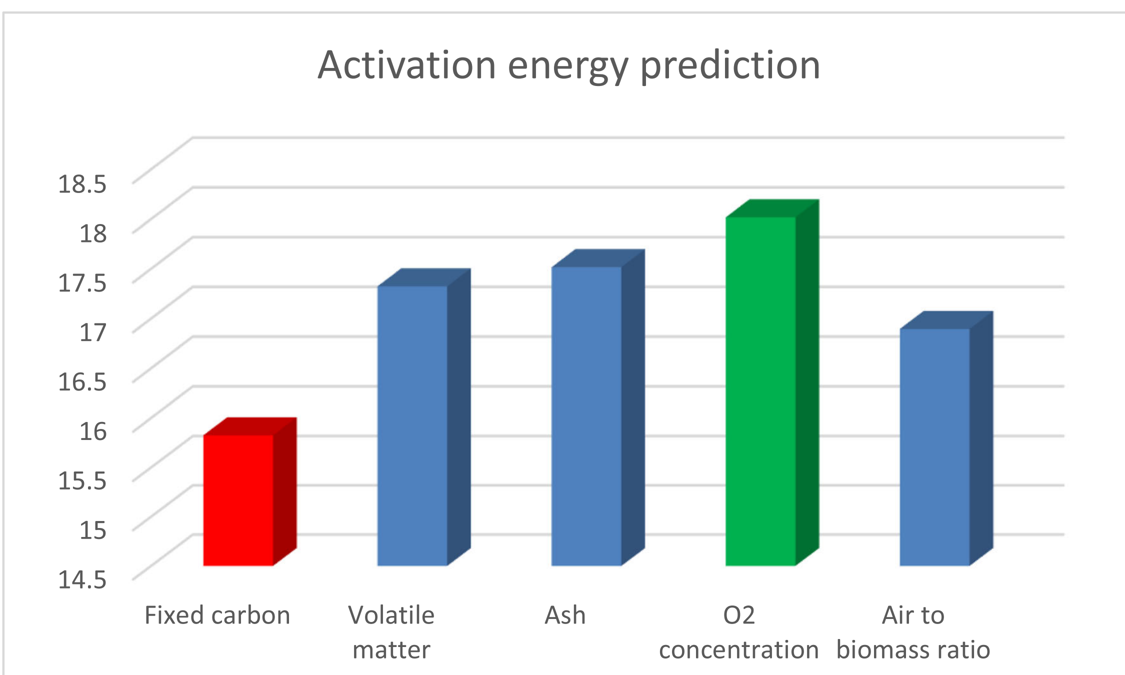

Fig. 5 Activation energy prediction based on single feature (red, the highest influence; green, the smallest influence)

Table 6 ANFIS reaction order (*n*) prediction based on two features

n prediction (two features)
ANFIS model 1: fixed carbon, volatile matter --> training = 0.0853, checking = 0.3624
ANFIS model 2: fixed carbon, ash --> training = 0.0874, checking = 0.2565
ANFIS model 3: fixed carbon, O_2 concentration --> training = 0.1064, checking = 0.1328
ANFIS model 4: fixed carbon, air to biomass ratio --> training = 0.0944, checking = 0.1857
ANFIS model 5: volatile matter, ash --> training = 0.0856, checking = 0.1815
ANFIS model 6: volatile matter, O_2 concentration --> training = 0.0957, checking = 0.1431
ANFIS model 7: volatile matter, air to biomass ratio --> training = 0.0877, checking = 0.3258
ANFIS model 8: ash, O_2 concentration --> training = 0.0912, checking = 0.1577
ANFIS model 9: ash, air to biomass ratio --> training = 0.0889, checking = 0.1632
ANFIS model 10: O_2 concentration, air to biomass ratio --> training = 0.0928, checking = 11.8848

2.3 E-tracking of kinetic parameters of biomass oxidation

Modeling of e-tracking system for kinetic parameters of biomass oxidation could include all environmental or weather factors which have impact on the biomass oxidation. The proposed e-tracking system has 5 inputs based on abovementioned section and Table 1. Unified modeling language (UML) is used for the modeling purpose.

Table 7 ANFIS reaction order (*n*) prediction based on three features

n prediction (three features)
ANFIS model 1: fixed carbon, volatile matter, ash --> training = 0.0698, checking = 6.5620
ANFIS model 2: fixed carbon, volatile matter, O_2 concentration --> training = 0.0764, checking = 0.3451
ANFIS model 3: fixed carbon, volatile matter, air to biomass ratio --> training = 0.0606, checking = 19.4324
ANFIS model 4: fixed carbon, ash, O_2 concentration --> training = 0.0781, checking = 0.5185
ANFIS model 5: fixed carbon, ash, air to biomass ratio --> training = 0.0652, checking = 6.5036
ANFIS model 6: fixed carbon, O_2 concentration, air to biomass ratio --> training = 0.0778, checking = 9.3422
ANFIS model 7: volatile matter, ash, O_2 concentration --> training = 0.0771, checking = 0.5240
ANFIS model 8: volatile matter, ash, air to biomass ratio --> training = 0.0634, checking = 9.0591
ANFIS model 9: volatile matter, O_2 concentration, air to biomass ratio --> training = 0.0750, checking = 2.3769
ANFIS model 10: ash, O_2 concentration, air to biomass ratio --> training = 0.0772, checking = 9.9244

3 Results

3.1 Architecture of the e-tracking system

Figure 2 shows the architecture of the e-tracking system for the kinetic parameters based on the use case model. There are two subjects in the system: users and biomass module. The users could import of biomass parameters based on Table 1. The biomass module is responsible for kinetic parameter's estimation based on the data samples in Table 1. To estimate the kinetic parameters, it is need to incorporate the ANFIS model in the biomass module. In this article, ANFIS model is used for the kinetic parameter's calculation based on biomass parameters in Table 1.

Figure 3 shows the architecture of the importing of input parameters. The use case has five activities. The activities belong to the importing of the biomass parameters according to Table 1.

Figure 4 shows the architecture of estimating the kinetic parameters of biomass oxidation. The use case is based on the proposed ANFIS model.

3.2 ANFIS models

ANFIS methodology was used for feature prediction based on Ea and *n* prediction accuracy. Higher prediction accuracy leads to a higher influence of the selected feature. Dataset was divided in two groups for ANFIS training (50%) and checking (50%) respectively. Training errors are used for tracking of prediction accuracy while checking errors are used for tracking of potential overfitting between training and checking errors. As can be seen in Table 2, there are five ANFIS models according to the single inputs. Prediction of activation energy (Ea) has the highest accuracy for ANFIS model 1 or fixed carbon as the input feature. Figure 5 shows prediction of the activation energy based on the single inputs where one can see visually difference between the prediction accuracy of the activation energy for the single features. Table 3 shows activation energy prediction based on two features combinations. The combination of fixed carbon and volatile matter is the most optimal combination of the two features for the ANFIS prediction of activation energy. Table 4 shows activation energy prediction based on three feature combinations. The combination of fixed carbon, volatile matter, and ash is the most optimal combination of the three features for the ANFIS prediction of activation energy.

Prediction of reaction order (*n*) has the highest accuracy for ANFIS model 3 or ash as the input feature as can be seen in Table 5. Figure 6 shows prediction of the reaction order based

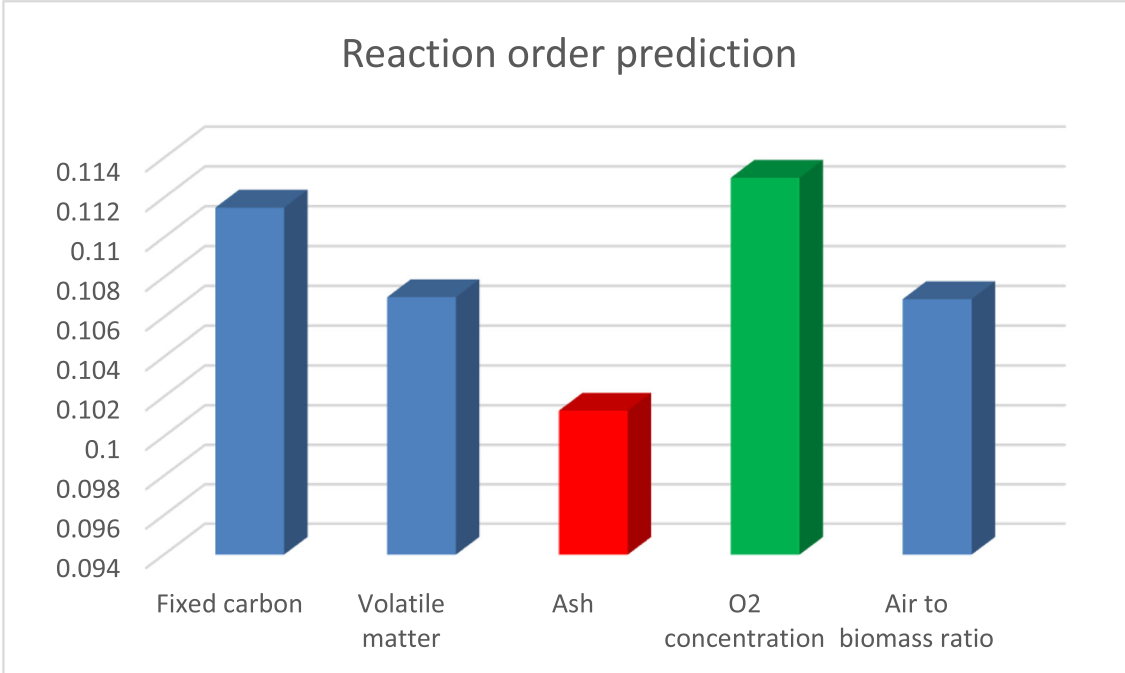

Fig. 6 Reaction order prediction based on single feature (red, the highest influence; green, the smallest influence)

on the single inputs where one can see visually the difference between the prediction accuracies of the activation energy for the single features. Table 6 shows reaction order prediction based on two features combinations. The combination of fixed carbon and volatile matter is the most optimal combination of two features for the ANFIS prediction of reaction order. Table 7 shows reaction order prediction based on the three feature combinations. The combination of fixed carbon, volatile matter, and air to biomass ratio is the most optimal combination of the three features for the ANFIS prediction of reaction order.

4 Conclusion

E-tracking system was established by object-oriented methodology to track the kinetic parameters of biomass oxidation. The system calculates kinetic parameters of the biomass oxidation through neuro-fuzzy methodology which is the main core of the e-tracking system. The system presents a novel approach for the estimation of the kinetic parameters of the biomass oxidation.

Feature selection process could be very important task in order to improve prediction accuracy of the biomass oxidation. Different parameters have an impact on the biomass oxidation; hence, suitable feature selection is a necessary task to improve predictive models. In this study, adaptive neuro-fuzzy inference system (ANFIS) was used as a tool for the feature selection of the biomass oxidation prediction. The ANFIS is suitable for highly nonlinear data pairs. Activation energy and reaction order were the kinetic parameters of the biomass oxidation which were used as the output parameters. According to the feature selection results, fixed carbon and ash are the most influential factors for the activation energy and reaction order respectively. Oxygen concertation has the smallest impact on the activation energy and reaction order.

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