

## Statistical model for prediction of Ash Fusion Temperatures from additive doped biomass

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### INTRODUCTION

The prediction of phase transformation of ashes from the combustion process is a topic often discussed by researchers around the world [1]-[5]. The estimation of the slagging ability of fuels is used in power boilers, waste incineration plants and gasification installations. The excessive occurrence of hardly removable ash deposits reduces the heat exchange steam/flue gases as a result, leading to a decrease in boiler efficiency. Deposits formation is also associated with corrosion and other technical problems. Such models allow estimating the behaviour of ashes subjected to high-temperature processes based on the chemical composition of ash and/or fuel. The prediction of phase transformation of biomass ashes is challenging, due to the highly variable composition of these fuels, as well as complex processes accompanying phase transformations [6]. Until now, a model with high reliability for biomass samples has not been developed. These models mainly use available databases such as [1], [7] [8] with the chemical composition of ash samples combined with experimental results of phase transformations. One of the first is Seggiani models [1]. This model was successfully dedicated to ash from coal. Were built on the basis of multiple regression based on data containing 433 samples of coal ash and some biomass ash. This model calculates characteristic temperatures of phase transitions: IDT – the temperature of initial deformation of ash, ST – softening temperature, HT – hemisphere temperature, FT - flow temperature and  $T_{cv}$  - critical viscosity temperature for coal ash samples. The model is characterized by temperature prediction with a standard error of less than 90°C, using 49 independent variables.

Next one Holubcik model, also use multiple regression to predict the characteristic melting temperatures of biomass ashes with additives [2]. However, in this model, a small population of  $N = 21$  samples with 9 independent variables was used, which may indicate limited applicability of this model for a wider range of biomasses. The standard error of temperature estimation for the Holubcik model was below 70°C. For the prediction of phase transformations, models are made on the basis of neural networks are also used, such as the Miao model [9]. This model predicts softening temperatures ST based on the chemical composition of 200 coal ash samples. In the best version, this model contains 5 variables and allows ST prediction with an average error not exceeding 3.59%. Another author, Yang [4], based his non-linear model on a database containing 77 samples of coal ashes. This model was built based on the SVM (Support Vector Machine) package form MATLAB® software. It calculates the softening temperature ST for tested samples with an accuracy of 86.7%.

Phase transition temperatures can also be determined on the basis of thermodynamic equilibrium calculations, often with using the FactSage® software [5],[10]. The next model uses STA (Simultaneous Thermal Analysis) and equilibrium thermodynamic calculations to predict characteristic fusion temperatures [5]. The predicted temperature of ash sample deformation is near the designated temperature  $T_{30}$  (30% of the mass of the sample occurs in the liquid phase). In the described tests differs by less than 100°C for straw and wood bark. By using the same model, predicted temperatures of ash deformation from miscanthus and beech trees were differed by less than 200°C. Thus, it can be defined that the model is sensitive to the type of biomass and the chemical composition of it.

Model shown in this study is an extension of research on halloysite doped biomass presented in works [10], [11], [12].

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## METHODOLOGY

The AFT model (Ash Fusion Temperature) developed in this work was performed in the STATISTICA 13.1 program. A software package containing statistical analysis using multiple progressive regression was used. This model is divided into 3 separate models, which are designed to predict the characteristic melting temperatures of the ash IDT - deformation temperature, HT - hemisphere temperature, FT - flow temperature and it is based on the chemical composition of fuel and ash as in the standard [13]. IDT, HT, FT temperatures are dependent variables in discussed models. The model calculating shrink temperature SST was not made due to the incomplete database in this area. The regression model was made at the significance level of  $\alpha = 0.05$ . For the discussed models (IDT, HT, FT) a number of coefficients describing multiple regression parameters are presented, such as F - statistical significance level by Fisher-Snedecor test and p - corresponding probability level,  $R^2$  - model determination coefficient, and Se - standard error of estimation. The models are designed to predict AFT for biomass (raw and modified by means of fuel additive).

## BASICS OF MULTIPLE REGRESSION

The multiple regression is one of many ways to match a linear function to empirical data. The least squares method is used in this regression, by means of which the regression line is selected that the sum of squares of the distance for measurement points from the regression line is as small as possible, this can be written as follows (1) [14]:

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2 = \min \quad (1)$$

Through the application of this criterion, it is possible to choose practical structural parameters of the regression model  $\beta_0, \beta_1$ . The multiple regression model is described by equation (2) [1], [2]:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_n X_n \quad (2)$$

where:

$Y$  – dependent variable,

$X_1, X_2, X_n$  – independent variables,

$\beta_0, \beta_1, \beta_n$  – structural coefficients, assigned to successive independent variables.

There are several assumptions in the regression model. The model assumes the linearity of parameters and the stability of the relationship between the studied phenomena. In addition, the random component is a random variable with a normal distribution  $N(0, \sigma^2)$  [14]. In order to verify the fit of the model to the empirical data, the determination coefficient  $R^2$  is most often used.  $R^2$  is calculated from the following formula (3) [15]:

$$R^2 = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (3)$$

where:

$\hat{y}_i$  – predicted value of the dependent variable,

$\bar{y}$  – average value of dependent variable  $y$ .

The numerator of the above formula defines the variability of  $\hat{y}_i$  and the predicted value, while the denominator checks the variability of the observed values of  $y_i$ . This means that the determination coefficient  $R^2$  is a measure of matching the variable  $y$  to the predicted value. The  $R^2$  coefficient takes values in the range of 0.0-1.0. The closer to 1.0, the better fit of the model to the empirical data. However, using only  $R^2$  is not enough to assess the correctness of model prediction. A suitable parameter is the adjusted determination coefficient  $R^2_{adj}$  (4). It evaluates the number of significant independent variables used in the model. The removal of irrelevant independent variables has the effect of increasing the  $R^2_{adj}$  ratio [15]:

$$R^2_{adj} = 1 - \left( \frac{(1 - R^2)(n - 1)}{n - m - 1} \right) \quad (4)$$

where:

n - number of observations,  
m - number of independent variables in the model excluding the constant.

However, this coefficient always takes values lower than  $R^2$ . Another parameter describing the model fit to the empirical data is the standard error, also called the standard deviation of residues  $S_e$ . It is a very popular statistical parameter and determines the average difference between measured and predicted values. It is described by the following formula (5) [16]:

$$S_e^2 = \frac{\sum_{i=1}^n e_i^2}{n - k - 1} \quad (5)$$

where:

n - number of observations,  
k - the average value of dependent variable y.

The next simple parameters verifying the correctness of model prediction include absolute error  $\Delta x$  (6) and relative error  $\delta$  (7). These parameters are useful when analyzing specific prediction results.

$$\Delta x = |x - x_0| \quad (6)$$

$$\delta = \frac{|x - x_0|}{x} \cdot 100\% \quad (7)$$

where:

x - value from measurement,  
 $x_0$  - predicted value.

One of the basic methods of verifying the statistical significance of the multiple regression model is the use of F Fisher - Snedecor test [18]. It consists of checking whether there is a relationship between the dependent variable and the system of independent variables. The zero hypothesis  $H_0$  is tested for which the independent variables  $\beta_n$  are 0 (hypothesis of no regression). An alternative is a hypothesis  $H_1$   $\beta_n \neq 0$ , for which the regression coefficients reach values different from 0. Hypothesis tests can be symbolically written by equations (8) and (9) [19].

$$H_0: \beta_n = 0 \quad (8)$$

$$H_1: \beta_n \neq 0 \quad (9)$$

Next, the value of the F-Fischer-Snedecor test  $F_{emp}$  is calculated from the equation (10), the  $F_{crit}$  value is read from the Fisher-Snedecor test table and they are compared [18]. If  $F_{emp} > F_{crit}$ , then  $H_0$  must be rejected - the hypothesis of no regression. There is a linear regression relationship between the dependent variable and the independent variables system. If  $F_{emp} < F_{crit}$  then  $H_0$  can not be rejected. It would mean that the regression equation does not have a strong linear relationship. If the value of p (test probability) is lower than the adopted level of statistical significance, the structure of the model is correct and its assumptions are satisfied, the null hypothesis can be rejected. In the designated model, the  $H_0$  hypothesis is a hypothesis of no regression [21].

$$F_{emp} = \frac{\frac{S_{xy}^2}{SS_y} \cdot (n - 2)}{SS_y - \frac{S_{xy}^2}{SS_y}} \quad (10)$$

where:

$SS_x$  - the sum of squared deviations for the X (independent variable),  
 $SS_y$  - the sum of squared deviations for the Y (dependent variable),

$S_{xy}$  - the sum of squared deviations for the X and Y characteristics (dependent and independent variable),

n - the number of freedom degrees.

## INDICATORS

Model is base on a number of indicators selected from 103 tested independent variables. Finally, 42 independent variables were chosen for IDT and HT, and 40 for FT. The IDT, HT, FT indicators are presented in Table 1. Independent variables that have a significant statistical impact (for which the probability of test statistic reached  $p < 0.05$ ) are marked in red.

**Table 1** List of independent variables used in regression equations and structural parameters which were assigned to them for IDT, HT, FT models

IDT		HT		FT	
N=92	$\beta$	N=92	$\beta$	N=92	$\beta$
Constant	3209.07	Constant	153.64	Constant	2307.76
(SiO <sub>2</sub> +Al <sub>2</sub> O <sub>3</sub> )·K <sub>2</sub> O	-1.35	K <sub>2</sub> O·SiO <sub>2</sub>	-0.17	Sr	1026.70
P <sub>2</sub> O <sub>5</sub>	-35.62	Fe <sub>2</sub> O <sub>3</sub>	158.02	(SiO <sub>2</sub> +Al <sub>2</sub> O <sub>3</sub> )·K <sub>2</sub> O	-0.16
B/A·BAI	396.66	Na <sub>2</sub> O <sup>2</sup>	-0.67	Fe <sub>2</sub> O <sub>3</sub>	37.94
Na <sub>2</sub> O <sup>2</sup>	-0.66	SiO <sub>2</sub> ·CaO	0.11	P <sub>2</sub> O <sub>5</sub>	-8.00
	-				
2·S <sup>d</sup> /(K <sub>2</sub> O +Na <sub>2</sub> O)	1295.60	P <sub>2</sub> O <sub>5</sub>	0.20	Na <sub>2</sub> O <sup>2</sup>	-0.46
Fu <sup>2</sup>	-0.01	CaO <sup>2</sup>	0.20	SiO <sub>2</sub> ·CaO	-0.10
B/A·fph	0.33	B/A·BAI	-32.31	CaO <sup>2</sup>	0.17
					-
Fe <sub>2</sub> O <sub>3</sub> ·CaO·K <sub>2</sub> O	-0.50	Al <sub>2</sub> O <sub>3</sub>	47.73	Dix	6387.02
					-
Fe <sub>2</sub> O <sub>3</sub> ·MgO	6.73	Dix	9908.07	Fe <sub>2</sub> O <sub>3</sub> ·CaO	-1.94
					-
R250 <sup>2</sup>	2993.99	(CaO+MgO)/Al <sub>2</sub> O <sub>3</sub>	1.68	Al <sub>2</sub> O <sub>3</sub> <sup>2</sup>	-0.05
SiO <sub>2</sub> ·Fe <sub>2</sub> O <sub>3</sub> ·K <sub>2</sub> O	0.18	B/A·Sr	-104.79	B/A·BAI	42.30
SiO <sub>2</sub> /CaO	27.96	K <sub>2</sub> O <sup>2</sup>	-0.22	Fe <sub>2</sub> O <sub>3</sub> ·Al <sub>2</sub> O <sub>3</sub>	-0.09
Cl <sup>d</sup> ·Rs	9.72	MgO <sup>2</sup>	0.02	Fe <sub>2</sub> O <sub>3</sub> ·MgO	6.19
B/A·Fu	0.40	B/A·fph	-1.09	MgO	-43.39
					-
Dr	1785.53	Fe <sub>2</sub> O <sub>3</sub> ·CaO	-1.68	SV	2934.82
Fu	-2.46	B/A·Dix	406.96	B/A·Sr	-87.46
B/A·Sr	102.05	Na <sub>2</sub> O·(B/A)	-3.96	B/A·Dix	375.20
CaO+MgO	-53.80	SO <sub>3</sub>	75.32	Na <sub>2</sub> O·(B/A)	-2.04
SV <sup>2</sup>	7604.73	Na <sub>2</sub> O	20.82	SO <sub>3</sub>	39.85
SiO <sub>2</sub> ·Rs	0.10	Fu <sup>2</sup>	0.00	TiO <sub>2</sub> <sup>2</sup>	-1.26
(SiO <sub>2</sub> +P <sub>2</sub> O <sub>5</sub> +K <sub>2</sub> O)/(CaO+MgO)	-28.57	B/A	3.81	TiO <sub>2</sub>	-94.82
B	39.65	B/A·Fu	-0.01	CaO	-13.46
B/A·Dix	293.00	Fe <sub>2</sub> O <sub>3</sub> ·MgO	1.50	(CaO+MgO)/Al <sub>2</sub> O <sub>3</sub>	1.81
Al <sub>2</sub> O <sub>3</sub> ·CaO·K <sub>2</sub> O	0.12	CaO·MgO	-0.26	Al <sub>2</sub> O <sub>3</sub> ·CaO	0.02
B/A·fcmk	0.00	K <sub>2</sub> O·MgO	0.30	CaO·MgO·K <sub>2</sub> O	0.02
				(Al <sub>2</sub> O <sub>3</sub> +SiO <sub>2</sub> )/(Na <sub>2</sub> O+K <sub>2</sub> O)	-5.65
Na <sub>2</sub> O·(B/A)	-1.23	Cl <sup>d</sup> ·Rs	19.62	O)	0.32
BAI·Fu	-11.37	K <sub>2</sub> O·BAI	-51.85	SiO <sub>2</sub> ·Fe <sub>2</sub> O <sub>3</sub>	1340.11
SiO <sub>2</sub> ·CaO·K <sub>2</sub> O	0.06	Fe <sub>2</sub> O <sub>3</sub> ·Al <sub>2</sub> O <sub>3</sub>	-2.06	SV <sup>2</sup>	-18.00
					-
SV	7785.94	K <sub>2</sub> O·Fe <sub>2</sub> O <sub>3</sub>	-1.57	fph	4.93
exp(10·2·SiO <sub>2</sub> ·Al <sub>2</sub> O <sub>3</sub> )	0.00	K <sub>2</sub> O	31.22	K <sub>2</sub> O·TiO <sub>2</sub>	0.37
Fe <sub>2</sub> O <sub>3</sub> /CaO	-429.15	SiO <sub>2</sub> <sup>2</sup>	0.40	Fu	-0.23
TiO <sub>2</sub>	-4.89	SV	-615.34	K <sub>2</sub> O·SO <sub>3</sub>	7.54
Dr <sup>2</sup>	3363.29	Fe <sub>2</sub> O <sub>3</sub> <sup>2</sup>	-1.27	Cl <sup>d</sup> <sup>2</sup>	-0.34
		Al <sub>2</sub> O <sub>3</sub> ·+SiO <sub>2</sub> /(Na <sub>2</sub> O+K <sub>2</sub> O)		P <sub>2</sub> O <sub>5</sub> <sup>2</sup>	-24.06
Al <sub>2</sub> O <sub>3</sub> ·+SiO <sub>2</sub> /(Na <sub>2</sub> O+K <sub>2</sub> O)	-16.84	O)	-14.49	K <sub>2</sub> O·BAI	-1.41
Cl <sup>d</sup>	40.41	Dr <sup>2</sup>	693.36	Fe <sub>2</sub> O <sub>3</sub> ·Al <sub>2</sub> O <sub>3</sub>	-1.21
P <sub>2</sub> O <sub>5</sub> <sup>2</sup>	-0.26	Al <sub>2</sub> O <sub>3</sub> ·CaO	-0.21	Fe <sub>2</sub> O <sub>3</sub> <sup>2</sup>	
exp(10·4·SiO <sub>2</sub> ·Al <sub>2</sub> O <sub>3</sub> )	2071.35	S <sup>d</sup> <sup>2</sup>	-124.35		

R250	4298.52	Sr	1015.75	K <sub>2</sub> O·P <sub>2</sub> O <sub>5</sub>	0.33
Al <sub>2</sub> O <sub>3</sub> ·CaO	-1.41	fph	7.61	MgO <sup>2</sup>	0.30
abs(B/A-1)	-80.32	SV <sup>2</sup>	857.03	K <sub>2</sub> O·CaO	-0.26
MgO <sup>2</sup>	-0.43	2S <sup>d</sup> /(K <sub>2</sub> O+Na <sub>2</sub> O)	492.90		
Al <sub>2</sub> O <sub>3</sub>	40.42	SiO <sub>2</sub> +Al <sub>2</sub> O <sub>3</sub>	-33.15		

Below, there are indicators that have more complex equations (11-22) which were taken from the literature [1], [2], [6], [22], [11]:

$$D_r = \frac{CaO + MgO}{SiO_2 + CaO + K_2O + MgO + Al_2O_3} \quad (11)$$

$$D_{ix} = \frac{SO_3 + S^d}{S^d + SO_3 + Fe_2O_3 + 100} \quad (12)$$

$$f_{ph} = \frac{CaO + MgO + K_2O}{SiO_2 + Al_2O_3} \quad (13)$$

$$f_{CMK} = \frac{CaO + MgO}{K_2O} \quad (14)$$

$$SV = \frac{SiO_2}{SiO_2 + Fe_2O_3 + CaO + K_2O + MgO} \quad (15)$$

$$R250 = \frac{SiO_2 + Al_2O_3}{SiO_2 + Al_2O_3 + Fe_2O_3 + CaO} \quad (16)$$

$$B = Fe_2O_3 + CaO + MgO + Na_2O + K_2O + P_2O \quad (17)$$

$$A = SiO_2 + Al_2O_3 + TiO_2 \quad (18)$$

$$BAI = \frac{Fe_2O_3}{Na_2O + K_2O} \quad (19)$$

$$R_s = \frac{B}{A} \cdot S^d \quad (20)$$

$$Fu = \frac{B}{A} \cdot (Na_2O + K_2O) \quad (21)$$

$$Sr = \frac{SiO_2 \cdot 100}{SiO_2 + Fe_2O_3 + CaO + MgO} \quad (22)$$

## FUEL DATABASE

To build the AFT model, a database describing 104 biomass samples of various types were taken from [22]. Each sample is characterized by complete data set (complete ash oxide analysis, AFT experiment results for IDT, HT, FT, sulfur and chlorine content in fuel). Incomplete analysis of samples was omitted. In addition, the database was extended by 4 samples of biomass tested in this work without the addition of halloysite: DS0, BZ0, SPK0, DM0, and also 4 with the addition of halloysite: DS4, BZ2, SPK4, DM4. Detail ash characterisation of biomass with and without halloysite addition was presented in [11] and [12]. Next Table 2 shows the values of min and max individual ranges for entered data. They are a criterion for using the model. The ranges of data entered are very wide, eg. the content of silica in the ash is in the range of 0.00-94.48%, the potassium content: 0.23- 63.90%, the phosphorus content: 0.00-40.94%, the sodium content 0.00-29.82%, the sulfur content: 0.01-2.33%, chlorine content: 0.00-3.13% etc. This demonstrates the potentially wide applicability of the AFT model for biomass with different chemical composition, as well as for biomass with fuel additives.

**Table 2** Min and max content of individual ash and fuels components

Name	Formula	Min	Maks
Silica content in ash	SiO <sub>2</sub> (%)	0.00	94.48
Calcium content in ash	CaO (%)	0.97	72.39

Potassium content in ash	K <sub>2</sub> O (%)	0.23	63.90
Phosphorus content in ash	P <sub>2</sub> O <sub>5</sub> (%)	0.00	40.94
Glin content in ash	Al <sub>2</sub> O <sub>3</sub> (%)	0.01	25.02
Magnesium content in ash	MgO (%)	0.19	38.22
Iron content in ash	Fe <sub>2</sub> O <sub>3</sub> (%)	0.00	36.27
Sulfur content in ash	SO <sub>3</sub> (%)	0.36	45.89
Sodium content in ash	Na <sub>2</sub> O (%)	0.00	29.82
Titanium content in ash	TiO <sub>2</sub> (%)	0.00	21.96
Sulfur content in fuel	S <sub>d</sub> (%)	0.01	2.33
Chlorine content in fuel	Cl <sup>d</sup> (%)	0.00	3.13

## MODEL LIMITATIONS

To calculate the temperatures IDT, HT, FT, complete oxidic composition should be given and normalized to 100% (SiO<sub>2</sub> + CaO + K<sub>2</sub>O + P<sub>2</sub>O<sub>5</sub> + Al<sub>2</sub>O<sub>3</sub> + MgO + Fe<sub>2</sub>O<sub>3</sub> + SO<sub>3</sub> + Na<sub>2</sub>O + TiO<sub>2</sub> = 100%), as well as the sulfur content in the fuel in dry state S<sup>d</sup> (%) and chlorine content in dry fuel Cl<sup>d</sup> (%). Below, assumptions for model limits were described.

- The analytical biomass sample should be fired in a muffle furnace at 550 ° C in accordance with PN-EN ISO 18122: 2016-01 [23],
- Oxide analysis of the ash sample must be in accordance with the procedure described in [24] and normalized to 100%,
- The content of individual ash components must be in the min/max range, which is given in Table 2,
- Analysis of sulfur and chlorine content in the fuel must be in accordance with the procedure described in [25] and given in % of the dry matter content,
- The model calculates the characteristic fusion temperatures (IDT, HT, FT) of the ash sample under oxidation atmosphere in the temperature range 700<sup>0</sup>C≤x≤1500<sup>0</sup>C (AFT experiment range [11], remaining results should be rejected as unreliable.

## RESULTS AND DISCUSSION

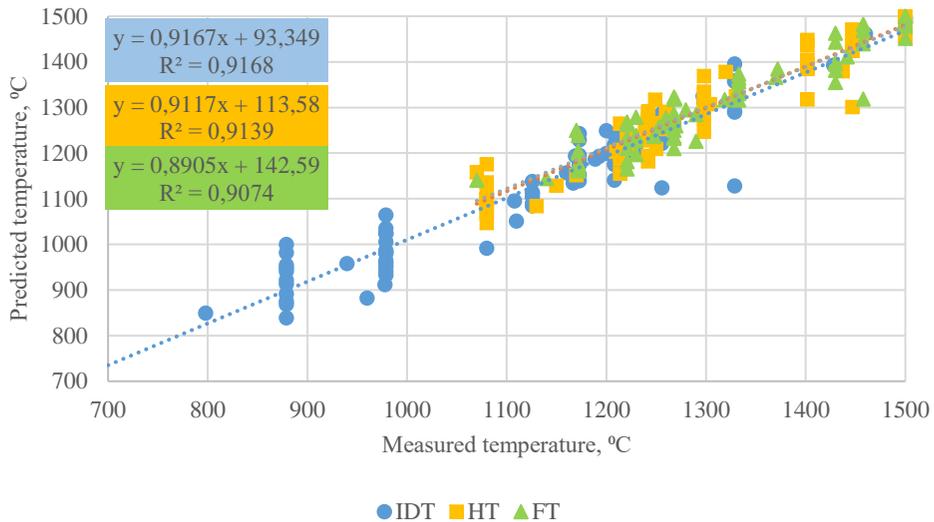
The prediction of characteristic ash fusibility temperatures is a complicated issue due to the complex processes occurring during combustion and the interaction of ash components between them. It is possible to predict phase transitions of ash from biomass based on its chemical composition, but only with a certain approximation. Table 3 shows the results for three separate models IDT, HT, FT. For all models, the value of the statistics made with the Fisher-Snedecor F<sub>emp</sub> test is in the range of 11.10-10.20 above F<sub>crit</sub> with probability levels p < 0.05. This shows the statistical significance of the linear regression model, which means that one can reject H<sub>0</sub> with no regression. Obtained R<sup>2</sup> determination coefficients for IDT, HT, FT are 0.907; 0.906; 0.897, which means that the variability of the model dependent variables were explained in 90.7% for IDT; 90.6% for HT, 89.7% of FT.

**Table 3** Summary of AFT regression results for temperatures: IDT, HT, FT

	IDT		HT		FT
R multiple	0.952	R multiple	0.952	R multiple	0.947
R <sup>2</sup> multiple	0.907	R <sup>2</sup> multiple	0.906	R <sup>2</sup> multiple	0.897
R <sup>2</sup> <sub>adj</sub>	0.825	R <sup>2</sup> <sub>adj</sub>	0.825	R <sup>2</sup> <sub>adj</sub>	0.816
F <sub>emp</sub> (42.49)	11.12	F <sub>emp</sub> (42.49)	11.20	F <sub>emp</sub> (40.51)	11.10
p	4.98E-14	p	2.68E-14	p	1.74E-14
S <sub>e</sub>	70.05	S <sub>e</sub>	51.98	S <sub>e</sub>	47.52

In turn, The R<sup>2</sup><sub>adj</sub> parameter was obtained at the level of 0.825 for IDT and HT and 0.816 for FT, which describes the influence of significant independent variables used in the model on obtained results of characteristic ash fusibility temperatures. Predicted with models temperatures IDT, HT and FT are characterized by the following standard estimation errors: 70.05; 51.98; 47.52. One can conclude that the use of the AFT model allows for the prediction of the temperature with an average error of <± 70.5<sup>0</sup>C for IDT; <± 51.98<sup>0</sup>C for HT; <± 47,52<sup>0</sup>C for HT. Results of the IDT, HT and FT models (which were presented in Table 3) describe models with results which are out of the scope of the AFT experiment (700<sup>0</sup>C≤x≤1500<sup>0</sup>C). For models, IDT, HT, FT respectively 12, 11 and 13 prediction results were out of range. Prediction results of characteristic fusion temperatures are shown in Fig. 1, where on the abscissa

there are results from the experiment and on the ordinate, there are results of the predicted temperature using the model. After removal of predicted values outside the experimental range AFT  $700^{\circ}\text{C} \leq x \leq 1500^{\circ}\text{C}$ , the determination coefficient  $R^2$  for IDT, HT and FT was 91.7%; 91.4%; 90.7%. Then, the standard error of estimation  $S_e$  was determined, which for IDT, HT, FT was respectively:  $48,62^{\circ}\text{C}$ ;  $37,15^{\circ}\text{C}$ ;  $34,02^{\circ}\text{C}$ .



**Fig. 1** Experimental results of AFT against the temperature predicted by the model

The model is characterized by a more accurate adjustment to empirical data (high coefficient of determination) and small standard estimation error compared to models which were discussed in Chapter 1. The negative features of the model include a small number of observations ( $N = 92$ ) on which the model was created with a large number of independent variables 40 - 42. This is mainly due to difficulties in finding complete databases for biomass that meet the criteria given in Chapter 5.

For the biomass studied in this paper, the results of temperatures of ash phase transitions as well as their predicted values using the AFT model were presented in Table 4. In some cases, eg. DS0 and SPK0 with IDT prediction, quite significant absolute errors of  $88.5^{\circ}\text{C}$  and  $77.4^{\circ}\text{C}$  were obtained. They are higher than the average difference between the measured temperature and the designated model ( $S_e(\text{IDT}) = 70,05^{\circ}\text{C}$ ). For the predicted HT temperature, SPK0 also exceeds the standard error of  $51.98^{\circ}\text{C}$ . For the last projected HT temperature, values greater than the average difference between  $S_e$  values were determined for DS0, SPK0 and BZ2.

**Table 4** Measured and predicted by the model temperatures for biomass without and with the addition of halloysite

Sample number	IDT				HT				FT			
	Observed value ( $^{\circ}\text{C}$ )	Predicted value ( $^{\circ}\text{C}$ )	$\Delta x$ ( $^{\circ}\text{C}$ )	$\delta$ (%)	Observed value ( $^{\circ}\text{C}$ )	Predicted value ( $^{\circ}\text{C}$ )	$\Delta x$	$\delta$ (%)	Observed value ( $^{\circ}\text{C}$ )	Predicted value ( $^{\circ}\text{C}$ )	$\Delta x$ ( $^{\circ}\text{C}$ )	$\delta$ (%)
DS0	1080	991.54	88.5	8.19	1150	1128.97	21.0	1.83	1290	1226.38	63.6	4.93
BZ0	1110	1051.40	58.6	5.28	1130	1083.80	46.2	4.09	1140	1144.03	4.0	0.35
DM0	940	958.11	18.1	1.93	1170	1151.83	18.2	1.55	1260	1258.68	1.3	0.10
SPK0	960	882.58	77.4	8.06	1070	1158.44	88.4	8.27	1170	1249.88	79.9	6.83
BZ2	1230	1204.67	25.3	2.06	1250	1209.26	40.7	3.26	1070	1140.75	70.7	6.61

SPK4	1200	1249.10	49.1	4.09	1260	1290.66	30.7	2.43	1280	1294.52	14.5	1.13
DS4	1160	1156.90	3.1	0.27	1210	1202.70	7.3	0.60	1260	1277.12	17.1	1.36
DM4	1210	1214.55	4.6	0.38	1260	1252.65	7.4	0.58	1270	1259.96	10.0	0.79

## SUMMARY

This article describes the statistical model of AFT prediction for characteristic ash melting temperatures from biomass using multiple regression. The possibility of predicting the phase transformation of ash based on its chemical composition as well as the content of sulfur and chlorine in the fuel was shown. Models can also be used for biomass with modified composition using additives.  $R^2$  adjustments for empirical data for IDT, HT, FT models were obtained, respectively 90.7%; 90.6%; 89.7%. After removing calculated temperature values outside the AFT experiment range, determination coefficients  $R^2$  increased to 91.7%; 91.4%; 90.7%, and standard error of estimation  $S_e$  reached the value below 50°C.

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