LOCAL AND GLOBAL SENSITIVITY ANALYSIS OF MODEL PARAMETERS FOR COMPOSTING PROCESS

ORIGINAL SCIENTIFIC PAPER

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ABSTRACT: In this paper, a local sensitivity analysis was performed using one at time technique (OAT) on the parameters of the mathematical model for the composting process. An integrated mathematical model for composting process was used, in which kinetic parameters and the reaction order was estimated. The values of the absolute and relative sensitivity of the specified parameters are calculated. The following dynamic variables were selected as the objectives functions for sensitivity analysis: the mass of organic matter at the end of the process, the minimum amount of oxygen, the maximum amount of carbon dioxide and the maximum substrate temperature. The sensitivity analysis showed that the variations of the parameters mostly affect the amount of carbon dioxide, and at least the substrate temperature, and that the most sensitive parameter is the reaction order. ANOVA analysis (one-way and two-way) showed a statistically significant difference between experimental data.

KEYWORDS: mathematical modeling, model parameters, composting, sensitivity analysis, ANOVA.

INTRODUCTION

Composting process is the process of organic matters degradation in aerobic conditions under the influence of microorganisms. The rate and duration of the process are influenced by several parameters, which most important are: initial moisture content, content of organic matter (OM), amount of oxygen, temperature, pH value, C/N ratio, etc. The process parameters that are monitored during the composting process and are important for the matematical modeling of process are: content of organic matters, moisture content, the amount of carbon dioxide generated, then the consumption of oxigen and the temperature of the substrate.

In order to develop a process that would lead to more efficient degradation of organic matter and reduction of the negative impact of waste on the environment, mathematical modeling provides great opportunities for simulation and optimization of the process, which greatly facilitates the work in designing reactor and in situ systems for the composting process. The possibilities of applying numerical simulations influence the reduction of the need for performing expensive experiments, better understanding, control and optimization of the process. The verified mathematical model predict, within certain limits, the characteristics of the process in a laboratory, pilot and full scale [1]. Mathematical modeling of the composting process dates back to 1976, and since then several dozen models have appeared, with researchers which are used different approaches. Most of the models were based on a deterministic approach, and only a few authors dealt with the stochastic approach [2]-[5]. In most models with a deterministic approach, elements of a stochastic approach are also built in. For the past forty years researchers also worked on corrective functions for temperature, free air space, moisture content and oxygen concentration. The review of the literature showed that the most significant and most modeled corrective function is related to temperature. The first corrective function for temperature is based on the modification of the Arrhenius expression [6].

A general review of corrective functions for temperature was given by Mason[1] in his work. In order to verify the stability and reliability of the model, it is necessary to perform the sensitivity analysis of the model parameters. Sensitivity analysis of model parameters can be done before and after model development. Most authors performed a sensitivity analysis of the model after the development, investigating sensitivity of model parameters and their influence on the stability of the model [6]-[9]. In this paper a corrective function for the temperature based on the modification of the Arrhenius expression is used. In the integrated model, three kinetic parameters were evaluated [10]. The sensitivity analysis seeks to determine how the model depends on the assigned values, structure of the model, and the assumptions on which it is set up. Also, sensitivity analysis represents an important method for checking the quality of the proposed model.

The aim of this paper is to assess the relative importance of the selected model parameters by sensitivity analysis and ANOVA analysis of experimental data in two different experiments.

MATERIALS AND METHODS

MATERIALS

The experiments were conducted in a pilot scale reactors (57 liters of volume). During experiments (23 and 15 day), three reactors were used, with mixtures of different initial composition. In both experiments, the organic fraction of municipal solid waste (OFMSW), poultry manure, sawdust, waste yeast and kiselguhr from the beer industry were used. The composition of OFMSW and characterization of the initial mixtures of the first experiment are given in the paper of Paprаćanin & Petric [10]. Composition of OFMSW used in second experiment is shown in Table 1.

Table 1. The composition of the OFMSW used for the second experiment

Waste	Composition (*mass*%)
Food waste	63.6
Paper and cardboard	25.6
Garden waste	10.8

Table 2. Percentage composition of initial mixtures (*mass*%) in reactors (second experiment)

Reactor	OFMSW	PM	S	WY	K
1	67.8	9.2	4.6	9.2	9.2
2	66.6	8.9	6.7	-	17.8
3	73.2	4.9	7.3	-	14.6

PM-Poultry manure,
S-Sawdust, WY-Waste yeast,
K- kiselguhr

Table 3. Characterization of initial mixtures in reactors (second experiment)

Reactor	Moisture (% w.b.)	OM (% d.b.)	pH	C/N
1	67.13	83.09	7.10	43.70
2	59.53	79.30	7.36	40.40
3	62.35	82.35	7.32	34.50

w.b. - wet base,
d.b. - dry base

The percentage composition of the initial composting mixtures in the second experiment is shown in Table 2, and their basic physical and chemical characteristics are given in Table 3. The prepared mixtures took up about 90% of the total volume of the reactors. For the first and second experiment, the reactors was filled with: 26.1 kg, 19.5 kg, 24.4 kg, 19.1 kg, 18 kg and 18.7 kg of the compost mass, respectively. Other details about eksperimental procedure can be found in literature [7], [10]. Sheme of experimental set-up is shown on figure 1.

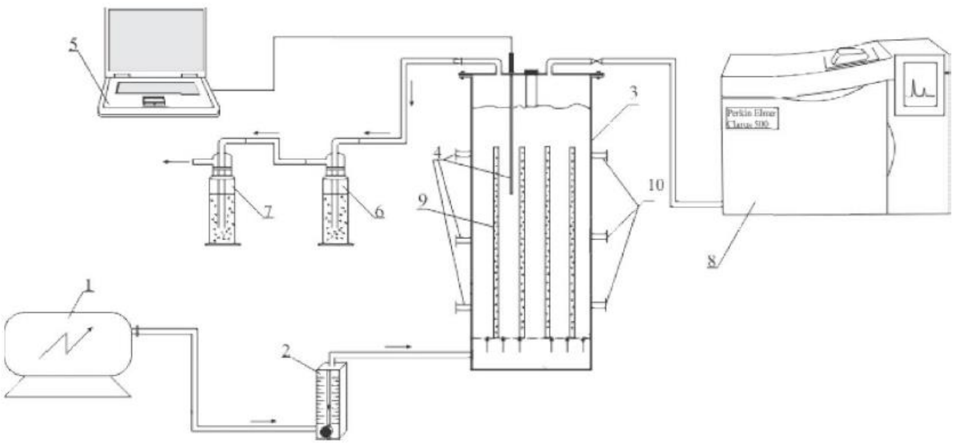

Figure 1. Schematic diagram of the reactor system: 1-compressor, 2-flow meter, 3-reactor, 4 thermocouples, 5-port computer with acquisition module, 6-rinse with sodium hydroxide solution, 7-bottle wash with boric acid solution, 8- chromatograph-gas analyzer, 9-perforated tubes, 10-holes for sampling.

SAMPLING AND ANALYSIS

After daily mixing of the composting mixtures, samples were taken from different places in the reactor (top, middle and bottom, three samples from each places) in order too obtain a representative sample. Moisture content, OM content and pH value was measured daily. Measurment and used methods for composting proces, are standard methods, and can be found in the literature [6], [9], [10], [11]. For measurment of concentrations of carbon dioxide and oxygen concentrations, Infrared Gas Analyzer MGA5, VarioPlus Industrial (MRU GmbH, Germany) was used. Concentrations of CO_2 and O_2 are measured at three heights in the reactor and at the top of the reactor (gas outlet).

Measurement of the air flow was done by rotameters (Cole-Parmer, USA). The temperature in the reactors was measured automatically every 30 minutes for the entire duration of the experiment by thermocouple (type T, Digi-Sense, Cole-Parmer, USA), which are connected to a notebook via the acquisition module (Nomadics, USA). The ambient air temperature in the laboratory was 22.5 ± 2.5 ° C during the experiments.

MATHEMATICAL METHODS

The mathematical model that is used for performing local and global sensitivity analaysis of model parameters, was presented in a previous work [7], [10] also as mathematical methods.

SENSITIVITY ANALYSIS METHODOLOGY

In this study, local sensitivity was defined as the relative change in the system output when a small perturbation (±1%) was imposed on a single kinetic parameter.

The sensitivity analysis was done in order to assess the relative importance of the selected model parameters. For the numerical simulation of the process, developed program were implemented in Matlab [12] while MS Excel used for graphical representation of the results of the sensitivity analysis. The sensitivity analysis of the parameters was done in two ways [7], [9], [10]. Investigated sensitivity functions of model are: the minimum weight of organic matters, the maximum amount of carbon dioxide and the maximum substrate temperature. Absolute and relative sensitivity of the model was calculated in MS EXCEL, based on the data obtained from simulations and experimental data. The numerical simulation data were obtained in Matlab [12] (ODE23s solver). The absolute sensitivity was obtained by minimizing the variation of the optimized kinetic parameters by creating a "noise" [13]. Obtained kinetic parameters [10] are varied by +1% of their optimum values. Absolutely Parametric Sensitivity (APS) and Relative Parametric Sensitivity (RPS) is calculated as described in literature

$$APS = \frac{\partial f}{\partial k_i} \approx \frac{\Delta f}{\Delta k_i} \qquad (1)$$

where in:
f – optimization function,
k_i – parameter.

Since sensitivity can not be expressed analytically for nonlinear dynamical models, it is possible to use differential approximation. Relative Parametric Sensitivity (RPS) is calculated from the following expression:

$$RPS = \left|\frac{k_i \partial f}{f \partial k_i}\right| \approx \left|\frac{k_i \Delta f}{f \Delta k_i}\right| \qquad (2)$$

Similar to the absolute sensitivity of the parameters, the differential approximation of the equation (1) can also be used to express the relative sensitivity of the parameters. More details can be found in the literature [9].

In order to determine statistical differences between treatments in individual reactors, ONE-WAY ANOVA (variance analysis) was performed. Statistical analysis of data related to organic matter loss, carbon dioxide concentration and substrate temperature was performed. This data relates to the mean height in the reactor. TWO-WAY ANOVA analysis (multi comparison test) was carried out in order to determine statistically significant differences in data obtained at different heights (spatial gradients) in reactors and different treatments in experiments. In both cases (one-way and two-way ANOVA), a T (*Tukey*) statistical test was used. Statistical analysis was performed in Matlab [12].

RESULTS AND DISCUSSION

SENSITIVITY ANALYSIS

Sensitivity analysis is the method of variation of the input parameters of the model within the permitted area and observation of variations of the dependent variables as output of the model. Generally, the sensitivity analysis can be defined as the study of uncertainty in the output of models that can be attributed to different sources of uncertainty in the input model [14]. The sensitivity analysis is used to increase the reliability of the model and its prediction, so that it allows understanding how model variables respond to changes in input parameters [15]. In essence, the sensitivity analysis is performed before optimizing the parameters to determine which parameter affects the reliability and stability of the model, but it is possible to perform the analysis after optimization. One approach to sensitivity analysis is local sensitivity analysis or one-at-one (OAT) techniques. OAT technique analyzes the effect of changing one parameter of model, while the values of other parameters are fixed, which is also applied in this paper. The influence of individual parameters on the objective functions is shown in Figure 2.

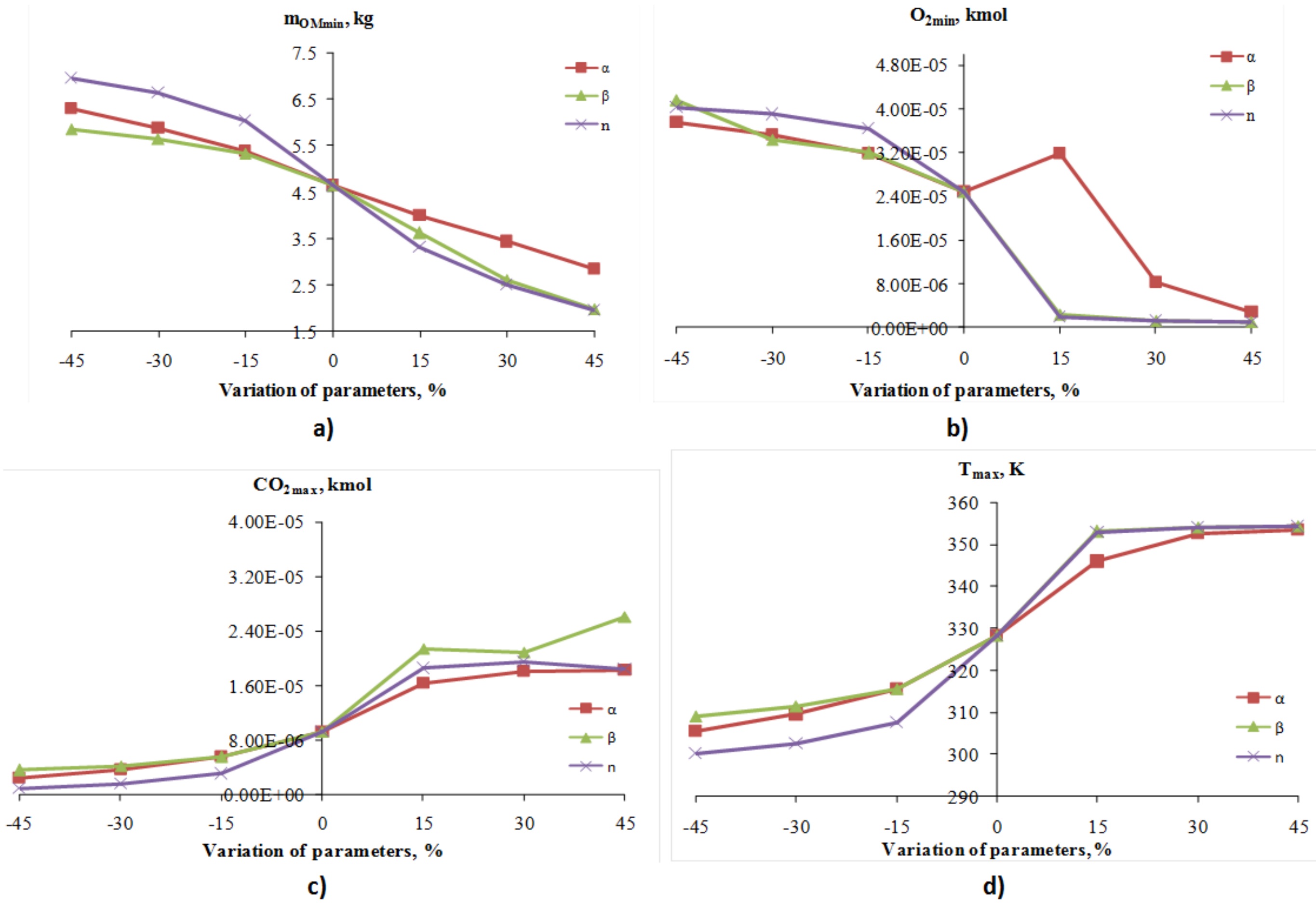

Figure 2. The influence of variation of parameters on:
a) the mass of organic matter at the exit; b) a minimum amount O_2;
c) the maximum amount CO_2; d) the maximum substrate temperature

Figure 2 shows that the parameter that most affects the selected objective functions is the reaction order *n*, that is, the parameter that shows the largest amplitude of the deviation. Negative variations of parameters significantly increase the values of the mass of organic matters at the output and the minimum amount of oxygen. Since the mass of organic matters and the amount of oxygen are practically reactants in the reaction of degradation, it can be concluded that, due to less degradation of organic matter and less oxygen consumption, a smaller amount of carbon dioxide is generated and a lesser amount of heat due to the biological reaction is distinguished. Also, it can be seen that positive variation of parameters, or their increase, results in higher production of carbon dioxide and maximum substrate temperature during the process. Positive variations of all three parameters show an "unusual" trend of changing the function of the target, because the first drop is seen, and then the value is increased. Negative variations of parameters show a "proper" behavior trend that can be explained and linked to the actual process. After the reaction order *n*, a significant influence is given by the parameter *β*, especially when it comes to the minimal amount of organic matter and the minimum amount of oxygen as a objective function. Obtained values of kinetic parameters of the model can be found in paper

Paprаćanin & Petric [10]. The α parameter has the least effect on the selected objective function, especially when it comes to small temperature changes. For all three parameters variations of the objective functions are greater in the case of positive variations of the parameters. Increasing the value of kinetic parameters and the reaction order significantly influences on the stability and reliability of the data obtained as output from the model. The smallest influence of parameter variation has on substrate temperature values, while the greatest influence is observed in the amount of carbon doxide. The variations of +30% and +45% give the values of the objective functions, which have no physical meaning.

Local sensitivity analysis was also carried out in previous work [7]. Several authors performed the sensitivity analysis in the same way [9], [16], [17], [18], whereby the came to the conclusion that only one of several parameters has a significant influence on the model output. The absolute sensitivity of the parameters is characterized by the direction in which the observed parameter is changed. Its positive value leads to an increase in the difference between the model and the experimental data, while its negative value reduces the difference between the model and the experimental data.

Part of the results of performed sensitivity analysis was presented in the paper Paprаćanin & Petric [10]. The difference in the order of the size of the APS value is related to the order of the size of the model parameters. The lower value of the parameter gives a higher APS value and The sensitivity analysis was performed for a slight deviation of the model parameters from their optimal values (+1%) [10]. Therefore, increasing the value of the parameters leads to an increase in the difference between the experimental and the results obtained by the mathematical model as shown in the paper Paprаćanin & Petric [10].

The F-distribution results show that the model is acceptable for the given conditions with a degree of significance α=0.05 for seven dynamic state variables[10].

Most authors have tested the influence of one fundamental parameters on the model, using a variety of methods and techniques for sensitivity analysis [19]. Researchers performed sensitivity analysis in models with microbiological kinetics [20], [21] or the sensitivity analysis were limited to only one segment of the process [19], [22], [23]. Very few researchers performed the sensitivity analysis in the integrated model [7], [24] so that there is enough space for future research in this direction. More precisely, it is possible to perform a sensitivity analysis before optimizing the kinetic and process parameters in order to obtain more reliable simulation results. Also, special attention should be paid to the optimization of the reaction order, which has the greatest influence on the differences between model and experimental data.

STATISTICAL ANALYSIS

The first part of the statistical analysis refers to data obtained from two experiments (three reactors in each experiment) which were measured in the middle height of the pilot scale reactor. The data were statistically analyzed by one-way ANOVA ($p<0.05$).

Measured and statistically analyzed variables are: mass of organic matter, the amount of carbon dioxide and substrate temperature.

The second part of the statistical analysis refers also to the data obtained from the same experiments but measured at different heights in the reactor (50 mm, 270 mm, 490 mm). For the second part of the analysis, "two-way" ANOVA was performed, with multiple data comparison.

The first part of the analysis was done separately, due to the fact that optimization of the kinetic parameters, as well as the verification of the proposed model using on these data [10] (used date were measured at medium height). For a better understanding data obtained from each reactor are numbered from 1 to 6. The first three groups from 1 to 3 refer to the data obtained from first experiment, while groups 4, 5, and 6 refer to data from second experiment.

Table 4 summarizes the results of the *p*-value for: mass of organic matter, amount of carbon dioxide and substrate temperature in all six reactors, measured at middle height. It can be said that there is a statistically significant difference ($p<0.05$) between the reactors for mass of organic matters and amount of carbon dioxide.

Table 4. Results of one-way ANOVA analysis

Measured variable	p
Mass of organic matter	**$3.86 \cdot 10^{-6}$**
Amount of carbon dioxide	**0.007**
Substrate temperature	0.3905

Since the organic matters and the temperature of the substrate were measured at three heights in the reactors, and the carbon dioxide concentration was additionally measured at the top (free air space), a two-way ANOVA analysis with multiple comparison was performed. Statistical data processing for the mass of organic matters and substrate temperature from six reactors to three heights, and data analysis for the concentration of carbon dioxide in six reactors at four heights.

Analysis of the data for the mass of organic matters showed that the data by reactors statistically significantly differ (p=8.65·10^{-6}), while the data in height do not statistically differ (p=0.631873). Results of multiple comparison test are showed in Table 5 (only groups that are statistically significantly differ) .

Table 5. Results of multiple comparison test for mass of organic matters

Groups		Lower value for 95%	Mean	Upper value for 95%
1	**2**	-0.2586	-0.1436	-0.0285
2	**3**	0.1038	0.2188	0.3338
2	**6**	0.0024	0.1174	0.2324
3	**4**	-0.2500	-0.1350	-0.0200

Since data from different heights are not statistically significantly, results are not showed. Based on these it could be concluded that the material is well homogenized since there are no statistically significant differences in heights.

Comparison of data for the amount of carbon dioxide by reactors at four levels (three heights and the top of the reactor) showed that, in opposite to organic matter, the data by reactors do not statistically differ, while they differ significantly in heights (p=1.5·10^{-28}). Multiple comparison showed that the data per reactor differ significantly only in the case of reactors 4 and 6 (lower limit of 95% is 0.2924 and upper limit for 95% is 2.2858), but when it comes to heights, five significant statistical differences can be noticed. The results of multiple comparison test for groups of heights that are statistically different are shown in Table 6. Since the measurements are made at different heights and that it is a gaseous phase, it is logical that there are significant statistical differences. Considering facts that the gas phase flow through the material in the reactor (tree heights) relative to the data from group 4 (free air space, where the concentration is highest) and between each other

Table 6. Results of multiple comparison test for data by height for amount CO_2

Heights		Lower value for 95%	Upper value for 95%	The difference in mean values
1	**2**	1.8174	3.2847	2.5510
1	**3**	-1.5305	-0.0632	-0.7968
2	**3**	-4.0816	-2.6143	-3.3478
2	**4**	-3.4368	-1.9695	-2.7031

Two way ANOVA for substrate temperature by reactors and hights are showed that there is a statistically significant difference in both cases (Table 7). Results of multiple comparison test showed that the all three groups (three heights) different from each other. Results of multiple comarison test of six groups (reactors), for groups that are statistically different are shown in Table 8.

Table 7. Results of two-way ANOVA analysis for substrate temperature

	SS^a	dF^b	SS/dF^c	F	p	Fc
Height	12059	2	6029	102.5	4.3·10^{-42}	3.00
Reactor	16051	5	3210	54.6	1.4·10^{-51}	2.22
Interaction	2725	10	272	4.6	1.6·10^{-6}	1.87

a-sum of squares;
b-degrees of freedom;
c-mean square deviation

The Table 7 shows, beside that the substrate temperature data are statistically significantly different both in reactors and in height, and that there is strong interaction between the reactors and the heights.

Such results can be explained by the fact that substrate mixing was not carried out, so in some parts of the reactor there was a mass overheating because the temperature of the substrate has the highest value in the center of the mass. Other authors also performed a one-way and two-way analysis of the variance for different reactor treatments. For example, Schloss and Walker [25] have investigated the effect of the active sludge addition as an inoculum, resulting in significant deviations in substrate temperature. Some authors investigated the effects of various additives, the influence of mixing, particle size and various types of inoculum, on the substrate temperature, amount of carbon dioxide, organic matter content [26], [27]. Rebollido [28] have studied the influence of temperature, pH, electrical conductivity and moisture content on the concentration of microorganisms, and concluded that pH and temperature significantly influence (p <0.01) on bacteria, fungi and actinomycetes.

Table 8. Results of multiple comparison test for data by reactors for substrate temperature

Groups		Lower value for 95%	Mean	Upper value for 95%
1	**3**	2.6489	4.7366	6.8244
1	**5**	0.3310	2.1187	4.2065
1	**6**	7.1188	9.2066	11.2943
2	**3**	4.0368	6.1245	8.2123
2	**4**	0.4187	2.5065	4.5942
2	**5**	1.4189	3.5066	5.5942
2	**6**	8.5067	10.5945	12.6822
3	**6**	-5.7058	-3.6181	-1.5303
3	**5**	-4.7056	-2.6179	-0.5301
3	**6**	2.3822	4.4699	6.5577
4	**6**	6.0002	8.0880	10.1758
5	**6**	5.0001	7.0878	9.1756

Komilis and Tziouvaras [29] investigated various types of vegetable seed supplements, concluding that compost on some seed species may have a phytotoxic effect, while other species can influence this to accelerate germination and growth. Kalamdhad [30] analyzed the results of the ANOVA, concluding that the reduction of carbon dioxide production significantly varied over the time (p<0.0001) and treatments (different C/N ratio), (p=0.0013). Wang [31] also carried out an equivariant analysis of the variance, but in order to examine the effects of different treatments on the maturity and composition of the finished compost.

CONCLUSION

Local sensitivity analysis has shown that variation of parameters mostly affects the amount of carbon dioxide, and at least the substrate temperature, and that the most sensitive kinetic parameter is the reaction order. A global sensitivity analysis has shown that the variations of all three parameters influence the increase in the differences in the agreement between the model and the experiment, and that the reaction order is the parameter that affects the stability and the sensitivity of the model to the greatest extent.

The analysis of the variance (ANOVA) for the mass of organic matters and aomunt of carbon dioxide, showed statistically significant difference between the reactors. Two-way ANOVA for the mass of organic matter showed that the data by reactors statistically significantly differ (p=$8.65\cdot10^{-6}$), while the data in heights do not statistically differ (p=0.631873). Comparison of data for the amount of carbon dioxide by reactors at four levels (three heights and the top of the reactor) showed that, in opposite to organic matter, the reactor data does not statistically significantly differ, while they differ significantly in heights (p=$1.52\cdot10^{-28}$). Substrate temperature data are statistically significantly different in both cases, reactors and heights, and there is strong interaction between reactors and heights.

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