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Mathematical modeling and simulation of the composting process in a pilot reactor

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Abstract: In this paper, a mathematical model for composting process with an engineering approach was presented. The model describes the *n*-th order kinetics of composting process (mesophilic-thermophilic phase) with mass and heat balances in the process. Verification of the model was performed using experimental data obtained from a pilot reactor. Measured dynamic state variables used for a verification of the model were: organic matter mass, water mass in a mixture, amount of oxygen and carbon dioxide, temperature of mixture and the temperature of gas phase. The developed mathematical model was implemented in numerical software package MATLAB. Three kinetic parameters were estimated using the Marquardt method. Global sensitivity analysis and statistical F-test showed that the model is valid for predicting the change in five dynamic state variables. The advantage of the model is that it can be applied to the composting process with mixtures of different compositions in reactors with different volumes.

INTRODUCTION

Waste as a result of human activities which in the modern age, as cities developed, is a serious problem. Waste collection and disposal is necessary, as for hygiene and space reasons, because large quantities of solid waste cover huge areas (Atalia *et al.*, 2015).Waste management is a critical area in practice with regard to increase of pollution. Management techniques for organic waste are carried out in many ways: waste disposal in landfills, incineration, pyrolysis and gasification, composting and anaerobic digestion (Taiwo, 2011).According to the environmental laws of the European Union, organic waste in landfills will have to be reduced to a certain extent, it implies a choice of one of several methods for the treatment of the organic portion of municipal solid waste, of which the cheapest and most effective is composting process.

Composting is a complex biological process, in which the heterogeneous organic waste is converted into humus (compost), under the influence of mixed microbial populations in controlled conditions of moisture, temperature and aeration. The composting process can be characterized as a way of sustainable waste management (Bonoli *et al.*,2012), and the resulting compost can be used to improve soil quality, and can be used for fertilization and soil conditioning (Zaha *et al.*, 2011; Zorpas *e tal.*, 2000).

In order to develop a process that would lead to a more efficient degradation of organic matter and reduce the negative impact of waste on the environment, mathematical modeling provides great opportunities for simulation and optimization of processes. Mathematical modeling provides the understanding of dynamic interaction between the mechanisms and provides the basis for a rational design process (Higgins and Walker, 2001). By the literature review, it can be said that most of the so far published models based on solving equations of heat balance (Bach *et al.*, 1987; Kishimoto *et al.*, 1987; Nakasaki *et al.*, 1987; Haug, 1993; Van Lier *et al.*, 1994; Kaiser, 1996; Stombaugh and Nokes, 1996; Das and Keener, 1997; Mohee *et al.*, 1998; Seki, 2000; Scholwin and Bidlingmaier, 2003; Xi *et al.*, 2005) and massbalance (Keener *et al.*, 1993; Kaiser, 1996; Stombaugh and Nokes, 1996; Das and Keener, 1997; Mohee *et al.*, 1998; Higgins and Walker, 2001). Most of the researchers observed a system for composting at the macro level, with the emphasis on reactor system

(Nakasaki *et al.*, 1987; Hogan *et al.*,1989; Keener *et al.*, 1993; Van Lier *et al.*, 1994; Richard *et al.*, 1999; Robinzon *et al.*, 2000; Barrena *et al.*, 2005; Nakayama *et al.*, 2007; Mason, 2008). Physical modeling of processes which helps identifying process in many aspects in laboratory and pilot scale. Opposite the physical modeling, mathematical modeling enables prediction of characteristics of the process, based on the knowledge of independent data on the measured variables and process conditions. Verified mathematical model predicts, within certain limits, the characteristics of the process in the laboratory, pilot and full scale (Mason, 2007). The authors who have applied engineering approach, set the reactor in the focus of research, during which they modeled the process that involves mass balance, heat balance, as well as other processes occurring*in vivo*. Some of the authors who applied engineering approach are: Nakasaki *et al.*, (1987), Hogan *et al.*, (1989), Keener *et al.*, (1993), Van Lier *et al.*, (1994), Richard *et al.*, (1999), Robinzon *et al.*, (2000), Themelis and Kim (2002), Cronje *et al*. (2004), Barrena *et al.*, (2005), Mudhoo and Mohee (2006, 2007), Nakayama *et al.*, (2007), Mason (2008), Kumar *et al*., (2009), Zhang*et al*., (2010), Baptista *et al*., (2010), Petric *et al*., (2015), Shishido and Seki (2015). The thing that the researchers dealt with the last thirty years, is corrective functions for temperature, free space for air, moisture content and oxygen concentration. During literature review, the most important and most modeled corrective function is related to temperature. General review of corrective function for temperature, can be found in Mason (2007). A large number of the researchers modeled composting process with first order kinetics. However, models with first order kinetics are greatly simplified and the results do not agree very well with the data from the experiment, especially in the case of very heterogeneous systems. Very few of researchers described the degradation of the substrate, with kinetics *n*-th order kinetics: Briški *et al*.,(2003a, 2003b, 2007); Petric and Selimbašić (2008); Barneto *et al*.,(2010); Avdihodžić *et al*.,(2011). In their work Barneto *et al*.,(2010), gave an explanation why the composting process can notbe predicted first order kinetics. The objectives of this study are related to possibilities of performing process of aerobic composting of municipal solid waste in pilot reactors, development of an integrated kinetic and reactor mathematical model to describe the decomposition of organic matter, mass transfer and heat, based on existing models, then optimization of kinetic parameters of the proposed model based on experimental data for several dynamic state variables obtained from the pilot reactor and at the end verification and validation of the developed mathematical model, with independent data and testing the sensytivity of the model.

MATERIALS AND METHODS

In the experiments have been used a specially designed pilot reactors (volume 57 dm^3). Pilot reactors are made of high density polyethylene, following dimensions: height 686 mm, outer diameter 330 mm, wall thickness 4.8 mm. Reactors are thermally insulated with a layer of foamed polyethylene thickness of 10 mm. The reactors were equipped with two air inlets and a few aperture for the taking samples. Two taps are attached on the cover of reactors, one tap is used for the continuous exit gas mixture, and the second tap is used for measuring the concentration of carbon dioxide and oxygen in the reactor outlet.

Composting material

Organic fraction of municipal solid waste (OFMSW) were used in the experiment, also with poultry manure, wood chips, waste yeast from the beer industry. Basic physical and chemical characteristics of the material are shown in Table 1. The basic material used in the experiment were OFMSW, which is synthesized by mixing the food waste (42.1 mass.%), paper and cardboard(31.6 mass.%) and garden waste (26.3 mass.%)

Table 1. Basic physical and chemical characteristics of OFMSW, poultry manure, wood chips, waste yeast

Material	Moisture content (% w.b.)	Organic Matter (%d.b.)	pH	Electrical condutivity ($dS\ m^{-1}$)	C/N ratio
OFMSW	72.44	88.17	6.70	1.790	52.73
Poultry manure	77.03	75.13	7.53	2.317	5.83
Wood chips	10.03	99.90	5.31	0.240	77.19
Waste yeast	95.61	91.55	6.46	2.795	21.19

w.b. – wet base, d.b. – drybase

Food waste is collected from restaurants in the Student Center of the University of Tuzla and the main city market in Tuzla. Garden waste which is used in the experiment collected from the city's parks and home gardens in Tuzla. The paper that was used in the experiment, consisting mainly used office paper collected at the Faculty of Technology in Tuzla. Cardboard that was used in the experiment, collected from several shopping centers in Tuzla. The role of poultry manure is to adjust the ratio of C/N, and to act as inoculum. Sawdust is added to increase aeration of mixture in reactors. Table 2 shows the percentage composition of the initial mixtures used in the reactors, and Table 3 shows the physical-chemical composition of the mixture for composting.

Table 2. Percentage composition of the starting mixture (mass.%) in the reactors

Reactor	OFMSW	Poultry manure	Wood chips	Waste yeast
1	67.6	10.8	10.8	10.8
2	77.8	5.5	11.1	5.5
3	82.0	5.1	10.3	2.6

Table 3. Basic physical and chemical characteristics of starting mixtures in reactors

Reactor	Moisture content (% w.b.)	Organic matter(% d.b.)	pH	Electrical Conductivity (dS m^{-1})	C/N ratio
1	71.09	90.00	6.72	1.299	71.09
2	63.09	92.96	6.80	1.303	63.09
3	65.65	89.27	6.98	1.280	65.65

Sampling and analysis

After daily mixing of the composting mixtures, samples were taken from different places in the mass (top, middle and bottom, three samples from each places) in order to obtain a representative sample. Moisture content was analyzed by dry oven method at 105°C for 24 h (APHA, 1995). The organic matter (OM) content (volatile solids) was determined after burning in an oven at 550°C for 6 h (APHA,1995). Conversion of organic matter (%) was calculated from the initial and final organic matter mass, according to the following equation:

$$K = \frac{(m_{OTP} - m_{OTK})}{m_{OTP}} \cdot 100 \qquad 1$$

m_{OTP} – mass of organic matter at the beginning of the process (kg),

m_{OTK} – mass of organic matter at the end of the process (kg).

Determination of nitrogen is carried out by the Kjeldahl method (Austrian Standard, 2001). The mass percentage of carbon (%C) is calculated according to the following equation (Haug, 1993):

$$\%C = \frac{\%OM}{1.8} \qquad 2$$

Concentrations of carbon dioxide and oxygen Infrared Gas Analyzer MGA5, VarioPlus Industrial (MRU GmbH, Germany) was used. The electrochemical cell of the analyzer is used to measure the concentration of oxygen in the range of 0 to 21.0% by volume, where the accuracy of ± 0.2 vol.%.

Matematical modeling

All details about the mathematical model (description; assumptions and simplifications; mass balances equations for water, carbon dioxide, oxygen, ammonia and nitrogen; heat balances equations for solid–liquid and gas phases; other supporting algebraic equations, explanations) can be found in the previous paper (Petric *et*. *al*., 2015).

The focus in this paper will be on *n*-thorder kinetics and on effect of temperature on reaction rate. The *n*-th order kinetics was applied, where the reactionrate is equal to the rate of organic matter degradation:

$$\frac{dm_{OT}}{dt} = -k \cdot m_{OT}^{n} \qquad 3$$

Reaction rate constant is the function of temperature, oxygen concentration, pH, moisture content and free air space:

$$k = k_T \cdot k_{O_2} \cdot k_{pH} \cdot k_{H_2O} \cdot k_{SPZ} \qquad 4$$

As a basis for the description of the effect of temperature on reaction rate constants, modified Arrhenius's expression were used, (Fogler, 2005; Sheridan *et al.*, 2012):

$$k_T = A \cdot e^{\frac{E}{R}\left(\frac{1}{293} - \frac{1}{T}\right)} \qquad 5$$

wherein:

A– frequency factor (units depending on the order of reaction),

T – thermodynamic temperature of the substrate (K),

E – activation energy (J/kmol),

R– universal gas constant (J/kmol·K).

This model has been proposed a modified form of the expression (5):

$$k_T = \alpha \cdot e^{\beta\left(\frac{1}{293} - \frac{1}{T}\right)} \qquad 6$$

wherein:

α=*A* *i* β=*E/R* kinetic constants that need to be determined, together with the reaction order *n* in the expression (3). Other equations for correction factors in equation (4) and constants used in model are given in previous paper (Petric *et*. *al*., 2015). Stoichiometric coefficient are determinated later in the paper.

Mathematical model consists of twelve nonlinear ordinary differential equations with twelve dynamic state variables (massof organic matter, mass of dissolved oxygen, mass of dissolved carbon dioxide, mass of dissolved ammonia, mass of water in the composting mixture, mass of oxygen in gas phase, mass of carbondioxide in gas phase, mass of ammonia in gas phase, mass of water vapor in gas phase, mass of nitrogen in gas phase, temperature of gas phase, temperature of solid–liquid phase) and corresponding algebraic equations. All differential equations and algebraic equations are mutually connected and nonlinear and therefore, they have to be solved simultaneously both for the purpose of model calibration and numerical simulation.

Four different categories of data are required in the model: initial values of the dynamic state variables, constants (physical, thermodynamic and stoichiometric), kinetic parameters and operational conditions. Calculation of initial mass values for dissolved oxygen, carbon dioxide and ammonia in interstitial water was based on solubility data from literature (Perry and Green,1997). Initial mole values of gases were calculated using the initial values of molar flows of gases, airflow rate and volume of gas phase.

Applied numerical methods and software

Algorithms for parameter estimation and numerical simulation were implemented in numerical software packages Matlab and Polymath. For numerical solution of system of differential equations, ODE23s solver, modified Rosenbrock method (Shampine and Reichelt,

1997). In order to determine the kinetic parameters, Marquardt method (Marquardt, 1963) was used with application of experimental data. As a criterion of agreement between values obtained by model and experimental data, the following target function *F* was taken as:

$$F = \sum_{j=1}^{m} \sum_{i=1}^{n} W_j \left(Y_{ij,\mathrm{model}} - Y_{ij,eksp} \right)^2 \qquad 7$$

wherein:

W_j – weight coefficient,
$Y_{ij,model}$ – value of dynamic state variables obtained by the model,
$Y_{ij,eksp}$ – value of dynamic state variables obtained by experiment.

After optimization of the kinetic parameters and the order of reaction, stoichiometric coefficients for oxygen, carbon dioxide and water and amount of loss of conductive-convective heat were adjusted. Experimental data used for verification of the model are: substrate temperature, temperature of the gas phase, carbon dioxideand oxygen concentration, mass of organic matter, mass of water in the substrate. The program consists a main file and three sub-routines and one file with experimental values of the dynamic state variables. The main program is used to call experimental data required for optimization, then vector of initial conditions for independent and dependent variables, as a vector of initial assumptions of parameters that need to be optimized. The main program also performs a statistical analysis by calling one of the routines for Statistics and the output is the optimization results numerically and graphically. Linear, multiple linear and nonlinear regression was performed in the software package *Polymath*. Regression is performed in order to obtain of approximate values for the initial vector parameters which are optimized using known values for corrective function of temperature and the experimental data. Sensitivity analysis was performed with the aim of evaluation relative importance of selected model parameters. Global sensitivity analysis was performed by determination the absolute and relative sensitivity of parameters. Details can be found in the previous paper (Petric *et. al*., 2015). F-statistical test, as an indicator of the sensitivity of the model was performed.

RESULTS AND DISCUSSION

Optimization of kinetic parameters

Numerical optimization presents a serious challenge in systems, such as the composting process. Problems that occur during optimization of these "live" system usually related to problems of initial conditions. First of all it is necessary to select an appropriate numerical method that would successfully solve a system of several differential equations and then even further to optimize the unknown parameters. As initial values for the of dynamic state variables in the model, experimental values are used for one of the reactors (reactor 1). The complex biochemical systems and their modeling represent the systems that is basically very difficult to simulate and optimize. The problem of initial conditions for the parameters is solved so that the used data from previous research Avdihodžić (2011). Table 4 showes optimized values of kinetic parameters together with the mean-square deviation. Comparing the value of the standard deviation with the previous work (Petric *et al*., 2015), valued at 0.4958, we can conclude that the selected corrective function of temperature gives significantly better results in the optimization of parameters.

Table4. Optimized values of kinetic parameters in the mathematical model

Parameter	Value	Unit
α	$9.6595 \cdot 10^{-5}$	$\mathrm{kg^{1-n}\,h^{-1}}$
β	$4.9140 \cdot 10^{3}$	K
n	1.5526	-

***SD^2 = 0.1020

Experimental data which has been used to evaluate the model parameters, are shown in Figure 1. Swedish chemist Arrhenius first proposed the dependence of the reaction rate constant of temperature, which was later confirmed through empirical and experimental data for a large number of reactions, including reactions in biological systems (Fogler, 2005). Several authors have used the Arrhenius model for temperature correction, which is a function of the reaction rate constants for the processes of degradation: Benefield and Randall (1980), Haug (1993), Mashauri and Kayombo (2002), Rousseau *et al*., (2004), Marsili-Libelli and Checchi (2005), Nitisoravut and Klomjek (2005), Andreottola *et al*., (2007), Kadlec (2009). Most of the authors used the mentioned corrective function for the first order kinetics, while in this study is used a model of *n*-th order. Model of *n*-th order, is proposed based on the fact that the organic waste consists many different organic compounds which decompose with different rates and different kinetics of reaction orderobtained value of the activation energy is correlated with literature values. Adjusted values for stoichiometric coefficients are: Value for conductive-convective heat loss is 2650 $\mathrm{J \cdot h^{-1}}$.

Sensitivity analysis

With the aim of testing the sensitivity of the model, values of the absolute and relative sensitivity of model parameters were calculated. Absolute and relative sensitivity of the parameters is shown in Table 5. The positive values of APS indicate that all three parameters lead to an increase in the difference between the experimental and simulation results. Sensitivity analysis was performed for a small deviation of model parameters from their optimal values (+1%). Based on the RPS values it can be concluded that the most sensitive parameter is reaction order and it has the greatest impact on the formulation of the entire model. Also, it is necessary to perform the validation of the model from the point of view of data analysis. For this purpose F-test was performed

with the significance level α= 0.05. Table 6 shows the results of the F-distribution data.

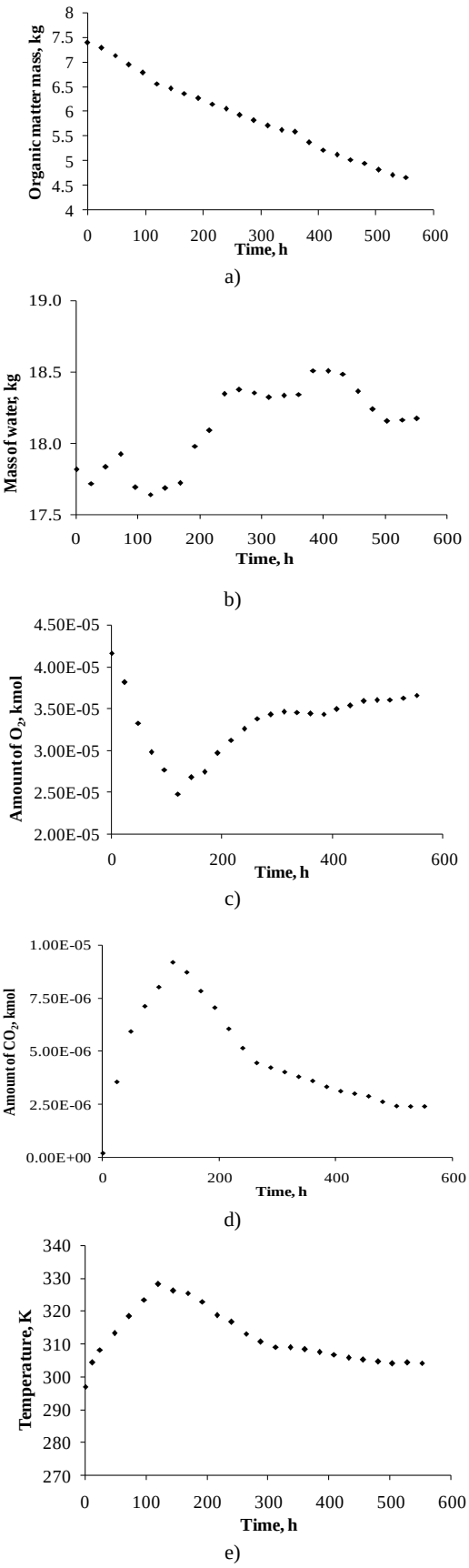

Figure 1. Experimental data from reactor 1: a) mass of organic matter, b) mass of water in substrate, c) amount of O_2, d) amount of CO_2, e) temperature of substrate.

The results of F-distribution show that the model is acceptable for given conditions for the four dynamic state variables. Only for the mass of water, the null hypothesis is rejected. Performing a sensitivity analysis, in terms of data for the mass of water in the substrate, similar results get Neves *et al.* (2007). In the future, it is necessary to perform a sensitivity analysis before the optimization of kinetic parameters in order to obtain more reliable simulation results.

Table 5. Parameters of the model and values of the sensitivity analysis

Parameter of the model	Value	APS	RPS
α	$9.65\cdot10^{-5}$	1147578	0.08932
β	4914.0	0.037635	0.14070
n	1.5526	22647.63	23.7114

[a]APS-*eng*. absolute parameter sensitivity
[b]RPS-*eng*. relative parameter sensitivity

Table 6. Results of the statistical analysis of data

Dynamic state variable	σ^a_{exp}	σ^b_{sim}	Value of F-test	Testing the hypothesis
Mass of organic matter	0.7047	0.7422	1.0532	$1.0532 \leq 2.0144$
Mass of water	0.0866	0.9848	11.366	$11.366 > 2.0144$
Amount of O_2	$1.57\cdot10^{11}$	$2.24\cdot10^{11}$	1.4290	$1.4290 \leq 2.0144$
Amount of CO_2	$5.52\cdot10^{12}$	$6.29\cdot10^{12}$	1.1385	$1.1385 \leq 2.0144$
Temperature of gas phase	71.94	65.25	1.1026	$1.1026 \leq 2.0144$
Temperature of substrate	71.94	65.62	1.0962	$1.0962 \leq 2.0144$

a-variance of experimental data
b- variance of simulation data

Verification of the model

Predictive simulation models are approximate imitation of real systems, which can never accurately describe the actual system. Verification of the model was performed with data from two different reactors for five dynamic variables of state (subsection 2.5). Verification of the model with experimental data for the mass of organic matter are shown in Figure 2, mass of the water in supstrate are shown in Figure 3, the amount of gases (CO_2 i O_2) are shown in Figure 4 and results for the temperature of the substrate (measured values are the same and the values calculated by model differ in the maximum 0.5°C) are shown in Figure 5. A comparison of experimental results and the numerical simulation showed good agreement throughout the entire process except when it comes to the mass of water in the substrate, where they observed certain deviations. The model shows a normal trend but experimental data shows an unusual distribution. One of the reasons why there is an unusual trend of experimental dat, is the

possibility of generation of air pockets in which there has been a condensation of water vapor wich the samples were taken.

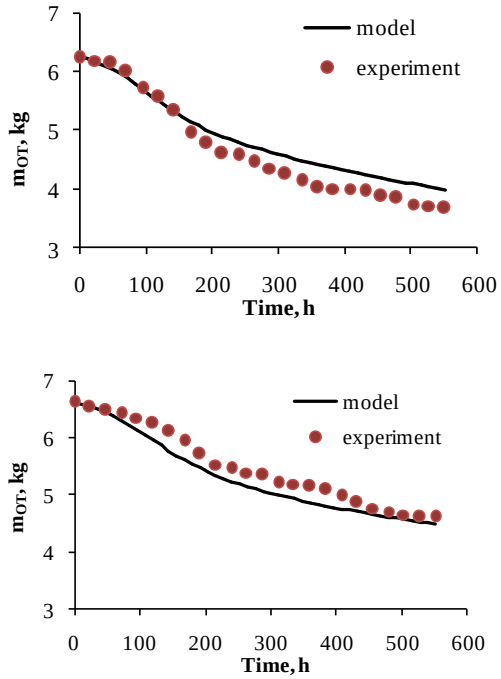

Figure 2. Verification of the model for the mass of OM: a) data from reactor 2, b) data from reactor 3.

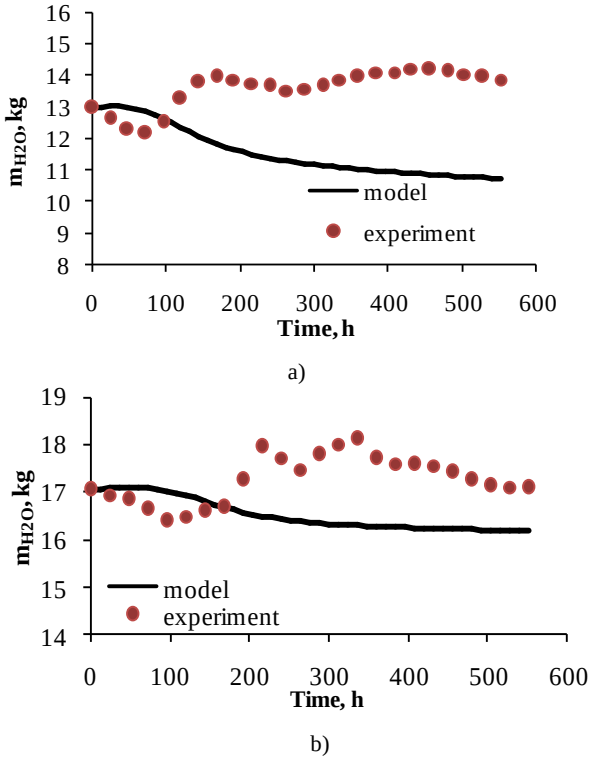

Figure 3. Verification of the model for the mass of water in the substrate: a) data from reactor 2, b) data from reactor 3.

Reaching the maximum temperature is the basis for the efficiency of the composting process (Finstein i Morris, 1975; Finstein *et al.*, 1986b) and during the period of thermophilic degradation leads to the destroying largest number of pathogens (Diaz, 2007). Temperature profiles in pilot reactors can reliably predict the temperature profiles in the processes taking place in full scale. This fact is one of the advantages of this model. The fact that the model well described experimental data confirms that the model is valid for use on different experimental conditions, which is one of the goals of mathematical modeling. With small modifications, referring to the initial conditions, this model can successfully simulate the process of decomposition of organic solid waste with different additions. No matter what kind of substrate is used in the composting process, this model can well predict the degradation process, especially in the active stage of the process.

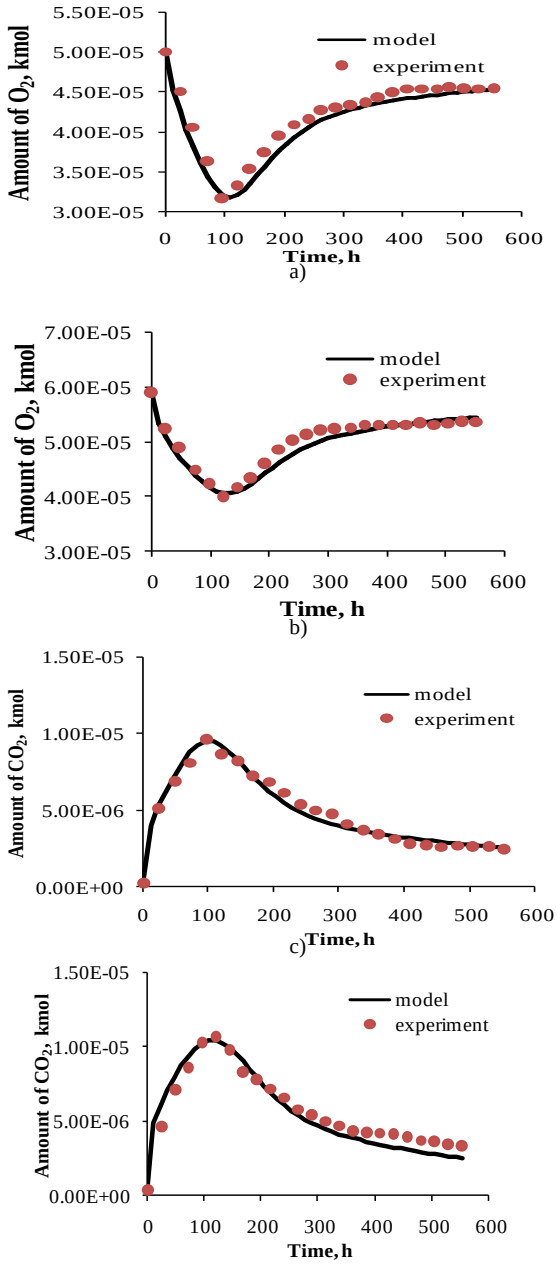

Figure 4. Model verification of the amount of gases: a) and b) verification for amount of O_2 for data from reactor 2 and 3. c) and d) verification for amount of CO_2 for data from reactor 2 and 3.

This conclusion can be justified by modeling the process kinetics of *n*-th reaction order. Modeling the process of *n*-th order kinetics, gives significantly better results when it comes to degradation of organic matter from the

standpoint of biochemical processes that occur. This was confirmed by Zhang *et al*., (2012) and Kulcu (2015).

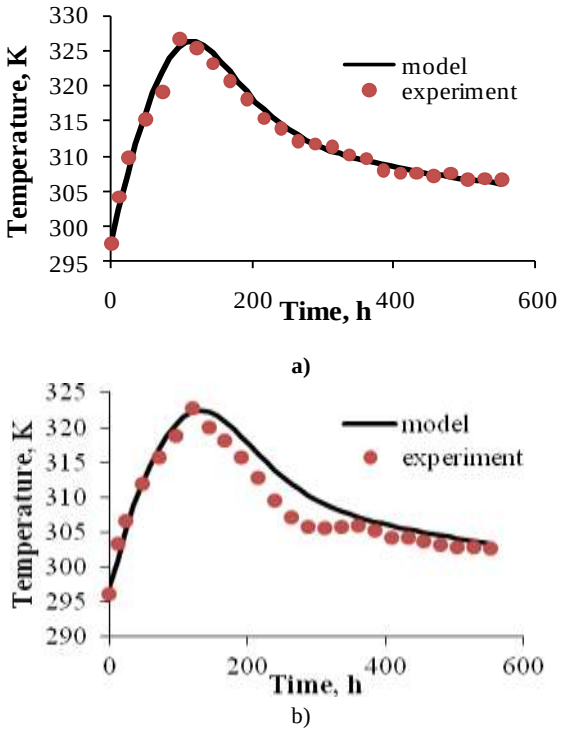

Figure 5. Verification of the model for the temperature of the substrate: a) data from reactor 2, b) data from reactor 3.

CONCLUSIONS

In this paper, the biggest problems related to mathematical modeling of the process, during the initiation of the developed mathematical model. The problem of initial conditions is solved by using data from previous studies. In the developed mathematical model the activation energy for the degradation process of waste were determinate (40855 kJ/kmol). Besides the activation energy, frequency factor is estimated ($9.6595 \cdot 10^{-5}$ kg^{1-n} h^{-1}) and reaction order (1.55). Global sensitivity analysis showed that variations of all three parameters affect the increase in the difference in the agreement between the model and experimental data. Reaction order is most sensitive parameter. Results of the F-distribution show that the model is acceptable for given conditions with the level of significance α= 0.05, except of mass of water in the substrate. Verification of the model was performed for five measured dynamic state variables. The variety of initial conditions in two reactors is important for the verification of the model. The fact that the model very well describes experimental data shows that the model is valid for use on different experimental conditions. Advantage of this model is reflected in the fact that with small changes, referring to the initial conditions, can successfully simulate the composting process of organic solid waste with different additions. Heterogeneous systems, such as the material used in this study are difficult to describe with constant values stoichiometric coefficients for entire process in the future should pay attention just to the values of stoichiometric coefficients and their changes during the process. In the future, should collect data from the plant in full scale with the aim of checking the validity of the proposed model.

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Summary/Sažetak

U ovom radu je predstavljen matematički model procesa kompostiranja sa inženjerskim pristupom. Model je opisan kinetikom *n*-tog reda (mezofilno-termofilna faza) zajedno sa bilansom mase i topline u procesu. Verifikacija modela je izvedena korištenjem eksperimentalnih podataka dobijenih iz pilot reaktora. Mjerene dinamičke varijable, korištene za verifikaciju modela su: masa organskih tvari, masa vode u supstratu, količina kisika i ugljičnog dioksida, temperatura smjese i temperature gasne faze. Razvijeni matematički model implementiran je u numerički softverski paket MATLAB, pri čemu su određena su tri kinetička parametra korištenjem Marquardt metode.Globalna analiza osjetljivosti i *F*-statistički test su pokazali da je model validan za predviđanje pet dinamičkih varijabli stanja. Prednost ovog modela se ogleda u čijenici da se ovaj model može primijeniti na proces kompostiranja smjesa različitog sastava u reaktorima različitih volumena.