

<https://doi.org/10.15255/KUI.2021.048>

KUI-18/2022

Original scientific paper

Received July 6, 2021

Accepted October 15, 2021

# Kinetic Parameters Estimation and Model Evaluation for the Aerobic Bioconversion Process of the Organic Fraction of Municipal Solid Waste

E. Papračanin\*

This work is licensed under a  
Creative Commons Attribution 4.0  
International LicenseDepartment of Chemical Engineering, Faculty of Technology, University of Tuzla, Urfeta  
Vejzagića 8, 75 000 Tuzla, Bosnia and Herzegovina

## Abstract

Aerobic bioconversion is very interesting process for the mathematical modelling and optimisation from the aspect of improving and accelerating the process, which is reflected in a higher organic matter decomposition rate. The aim of this research was to estimate the kinetic parameters in a dynamic model that described aerobic biodegradation of organic fraction of municipal solid waste (OFMSW) with various additions, from an engineering aspect. The presented mathematical model based on heat and mass transfer phenomena is a dynamic model for the gas-liquid-solid system. For the optimization and process simulation, three experiments were performed in three geometrically identical reactor systems at the same time, with different initial composition of composting mixtures. Data obtained experimentally from one reactor were used to optimize kinetic parameters of the model, and data from the other two reactors were used to verify and evaluate the dynamic model. Detailed statistical analysis showed narrow values of 95 % confidence interval for estimated parameters, indicating the appropriate accuracy of parameter estimation. Better data agreement was achieved in the reactor with a smaller ratio of OFMSW and additives, and the most accurately predicted dynamic state variable was the mass of organic matter. Parameter sensitivity analysis showed that the most sensitive parameters were reaction order  $n$  and activation energy  $E$ . Overall, the application of this model with optimised kinetic parameters of the aerobic biodegradation process represents a tool to predict the most important process variables ( $SD = 0.3378$ ).

## Keywords

Mathematical modelling, kinetic parameters, model evaluation, sensitivity analysis, aerobic biodegradation, OFMSW, waste yeast, kieselguhr

## 1 Introduction

The process of aerobic biodegradation (composting) is a very environmentally friendly process, especially when performed in closed systems.<sup>1,2</sup> This is reflected in several aspects: minimal emission of greenhouse gases and unpleasant odours, reduction of landfill formation, destruction of pathogens and pests. Although the trend of development and improvement of techniques for performing aerobic degradation processes in the world has reached a high level, it is still necessary to provide a simple tool that would reliably provide data during and at the end of the process. Maintaining composting systems near to the optimal conditions has been an essential part of most composting system engineering design and study.<sup>3</sup> Considering biological activities, composting is a complex process that involves many physical, chemical, and biological mechanisms.<sup>4</sup> Therefore, it is necessary to develop and/or improve existing mathematical models from the engineering aspect. Mathematical modelling and optimisation in any case facilitate the understanding of any process, even the process of aerobic degradation. The presence and activity

of microorganisms in the process of aerobic biodegradation further complicates the development and optimisation of a mathematical model that would describe this process. In this case, the presence and activity of microorganisms can in some way be neglected by the engineering/macro aspect of the process. A large number of authors have applied this approach with very good results.<sup>5-7</sup>

To make the process more efficient, key parameters such as oxygen concentration, moisture content, pH value, etc., must be considered.<sup>8,9</sup> In the last few decades, researchers have also dealt with the use and optimisation of kinetic parameters within correction functions (for temperature, free air space, moisture content, pH value, and oxygen concentration). General review of the correction functions was given by Mason.<sup>10</sup> Only 46 % of the reviewed models by Walling *et al.*<sup>11</sup> used one or more correction functions, and the number of models that implemented no type of correction was high. The most significant and most modelled corrective function is related to temperature, followed by moisture content, etc.

The increase in parameters can lead to a rise in predictive uncertainty.<sup>12</sup> Some researchers believe that correction functions within the model are not necessary, but their neglect can lead to unreliable results, especially in the case

\* Edisa Papračanin, PhD  
Email: [edisa.papracanin@untz.ba](mailto:edisa.papracanin@untz.ba)

of extreme temperature during thermophilic stage. It is also important to mention dynamic models in which  $n^{\text{th}}$  order kinetics were used (Briški *et al.*,<sup>13</sup> Barneto *et al.*,<sup>14</sup> Papačanin and Petric<sup>8</sup>). Most authors have applied first-order kinetics,<sup>7,15,16</sup> which greatly simplifies modelling, and the results of agreement with experimental data are very poor, especially when it comes to highly heterogeneous systems. In the case of the  $n^{\text{th}}$  reaction order, mathematical models and their optimisation significantly complicate the solution of such systems, but the agreement of the results in relation to the first-order kinetics is much better.<sup>8,13,14,17–19</sup>

The aim of the present study was to modify a dynamic mathematical model of composting process in terms of optimising the kinetic parameters and correction functions that are built into the dynamic model. Presented model was fitted with experimental data for the most important process variables (the mass of organic matter, O<sub>2</sub> consumption, CO<sub>2</sub> production, and temperature). In addition, to confirm the plausibility of describing the actual process, it was necessary to evaluate the model. Model evaluation (maximum and mean difference, R-square, root mean square error) was performed using experimental data obtained from the experiments in identical pilot reactors with different composting mixtures. In order to obtain a clearer view of the process, all measurements of process variables were performed several times and at several heights of the pilot reactor. Sensitivity analysis, as the last phase of this research, was performed for eleven kinetic parameters (variation of  $\pm 2$  %) to obtain insights for future research, and determine which kinetic parameters had the greatest impact on presented mathematical model, and how to manipulate sensitive parameters.

Review of available literature revealed that very few researchers had dealt with the optimisation of kinetic parameters in a dynamic model of the  $n^{\text{th}}$  order, which describes the processes of mass and heat transfer in a three-phase system, gas-liquid-solid. Moreover, it was necessary to check the stability and reliability of the mathematical model with appropriate statistical indicators (e.g., standard deviation, 95 % confidence interval of parameters), independently of the model evaluation with experimental data, which are also one of the objectives and novelties of this study.

## 2 Materials and methods

### 2.1 Experimental setup

Before performing the experiment, a calculation was made for the preparation of a mixture of synthesized solid waste based on the known composition of the components (Table 1). Experiment was performed in three identical reactors at the same time with mixtures of different initial composition.

Specially designed and prepared 57-l (operating volume is about 90 %) pilot reactors were used in the experiments. The pilot reactors were made of high density polyethylene and had the following dimensions: height 686 mm, outer diameter 330 mm, wall thickness 4.8 mm. The reac-

tors were thermally insulated with a layer of polyethylene foam (10 mm thick) on the outside of the rim and bottom of the reactor, as well as on the inside of the lid. The reactors were equipped with two air inlets via fixed taps, one air inlet 20 mm below and one 20 mm above the false bottom, to achieve the best possible aeration of the composting mixture. At a height of 270 mm from the false bottom of the reactor, was an opening 30 mm in diameter, which was closed with a plug, and used for taking samples and measuring the concentrations of carbon dioxide and oxygen. At the same height was an opening 30 mm in diameter for thermocouples. A more detailed description of the reactor system can be found in the paper of Papačanin and Petric.<sup>8</sup>

In all three reactors, the organic fraction of municipal solid waste (OFMSW), and additives: poultry manure, sawdust, waste yeast, and waste kieselguhr from the brewing industry, were used. The role and advantages of used additives are generally known, except the kieselguhr. One of the goals of research was to examine the influence of kieselguhr as an additive in the composting process.

All used waste was collected in Tuzla, Bosnia and Herzegovina. 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 experiments 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 centres in Tuzla. Waste yeast and kieselguhr collected from Tuzla brewery. The role of poultry manure is to adjust the ratio of C/N, and to act as inoculum. Poultry manure was collected from a chicken farm. Sawdust is added to increase aeration of mixture in reactors, while waste yeast was added to adjust the moisture content and C/N ratio.

Basic physical and chemical characteristics of the materials used in the three reactors are shown in Table 1.

Standard methods were used to determine moisture content, organic matter, and pH (Austrian Standard<sup>20</sup>). Representative samples of mixtures for determining the mass of organic matter, moisture content, and pH value were taken every 24 h with 3 replications. Nitrogen content was performed by the Kjeldahl method (at the beginning and end of process), and the concentrations of carbon dioxide and oxygen were measured every 24 h with Infrared Gas Analyser MGA5, VarioPlus Industrial (MRU GmbH, Germany). The concentrations of carbon dioxide and oxygen were measured four times (daily) at different heights: outlet, top, middle, and bottom of reactors. After daily mixing, samples were taken from different heights (490 mm-top, 270 mm-middle, and 50 mm-bottom of the reactors, three samples from each height) in order to obtain a representative sample. Moisture content was analysed by dry oven method at 105 °C for 24 h (APHA<sup>21</sup>). The organic matter (OM) content (volatile solids) was determined after burning in an oven at 550 °C for 6 h.<sup>21</sup> Conversion of organic matter (%) was calculated from the initial and final organic matter mass, according to the literature.<sup>9,22</sup>

Table 1 – Basic physical and chemical characteristics of OFMSW and additives (three replicates, mean value  $\pm$  standard deviation)

Tablica 1 – Osnovne fizikalne i kemijske značajke OFMSW-a i dodataka (tri ponavljanja, srednja vrijednost  $\pm$  standardna devijacija)

	MC/% w.b.	OM/% d.b.	pH	C/N
OFMSW	72.44 $\pm$ 0.41	88.17 $\pm$ 0.21	6.70 $\pm$ 0.07	52.73 $\pm$ 0.45
poultry manure	77.03 $\pm$ 0.86	75.13 $\pm$ 0.56	7.53 $\pm$ 0.04	5.83 $\pm$ 0.37
sawdust	10.03 $\pm$ 0.34	99.90 $\pm$ 0.25	5.31 $\pm$ 0.05	77.19 $\pm$ 0.67
waste yeast	95.61 $\pm$ 0.12	91.55 $\pm$ 0.20	6.46 $\pm$ 0.02	21.19 $\pm$ 0.35
kieselguhr	69.06 $\pm$ 0.48	10.47 $\pm$ 0.41	5.39 $\pm$ 0.11	11.36 $\pm$ 0.23

MC – moisture content; OM – organic matter content; w.b. – wet base, d.b. – dry base

The basic material used in the experiment was an organic fraction of municipal solid waste (OFMSW) that was synthesized by mixing food waste, paper, cardboard, and garden waste. After calculating the composition of the mixtures, individual components such as paper, cardboard, twigs, and other garden waste were crushed and mixed. Composition of synthesized OFMSW used in all three reactors was 25.5 % paper and cardboard, 10.8 % garden waste, and 63.7 % food waste. Synthesized waste was used to prepare three composting mixtures. Mixture 1 (M1) was prepared from 66.65 % OFMSW and 33.35 % additives (8.9 % poultry manure, 6.66 % sawdust, and 17.79 % kieselguhr). The total amount of synthesized mixture in the reactor was 24 kg. Mixture 2 (M2) was prepared in the ratio 68/32, using additives poultry manure (9.2 %), sawdust (4.4 %), waste yeast (9.2 %), and kieselguhr (9.2 %). The amount of mixture M2 was 25.24 kg. The percentage composition of mixture 3 (M3) was 73 % MSW and 27 % additives (7.3 % sawdust, 4.9 % poultry manure, and 14.8 % kieselguhr), with the total amount of mixture being

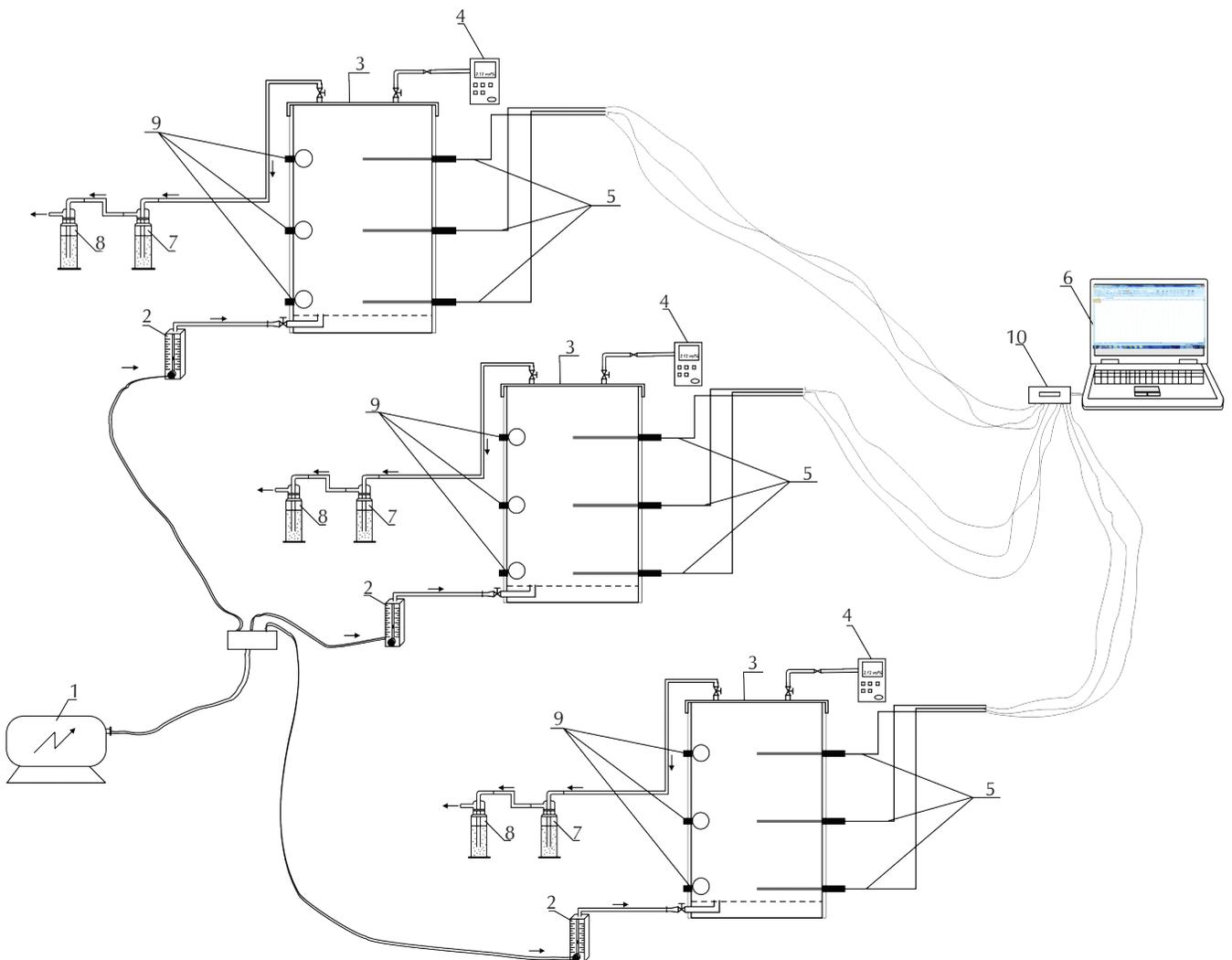


Fig. 1 – Schematic diagram of reactor system for aerobic composting (1 – air compressor, 2 – airflow meter, 3 – reactor, 4 – gas analyzer, 5 – thermocouple, 6 – laptop, 7 – gas-washing bottles with solution of boric acid, 8 – gas-washing bottle with solution of sodium hydroxide, 9 – holes for sampling, and 10 – acquisition module).

Slika 1 – Shematski dijagram reaktorskog sustava za aerobno kompostiranje (1 – kompresor zraka, 2 – mjerac protoka zraka, 3 – reaktor, 4 – analizator plina, 5 – termoelement, 6 – prijenosno računalo, 7 – boca za pranje plina s otopinom borne kiseline, 8 – boca za pranje plina s otopinom natrijeva hidroksida, 9 – rupe za uzorkovanje, 10 – modul za prikupljanje).

20.5 kg. Mixtures that were synthesized in different proportions were prepared in order to obtain large number of data experimentally, which would later be used for verification and evaluation of the mathematical model presented in 2.1. Table 2 shows basic physical and chemical characteristics of the mixtures in the three reactors. Fig. 1 shows a schematic view of the reactor with auxiliary equipment for the process of aerobic degradation.

Table 2 – Basic physical and chemical characteristics of the mixtures in the three reactors

Tablica 2 – Osnovne fizikalne i kemijske značajke smjese u trima reaktorima

Reactor mixture	MC/% w.b.	OM/% d.b.	pH	C/N
M1	67.13	83.09	7.10	43.70
M2	59.53	79.30	7.36	40.40
M3	62.35	82.35	7.32	34.50

MC – moisture content; OM – organic matter content; w.b. – wet base, d.b. – dry base

The airflow ( $0.4 \text{ l min}^{-1} \text{ kg}_{\text{OM}}^{-1}$ ) was calculated by weight of organic matter in accordance with the reference recommendations.<sup>9,23</sup> Measurement of airflow before entering the reactors was performed with rotameters (Cole-Parmer, USA). The temperature in the reactors was measured automatically ( $h = 0.5 \text{ min}$ ) for the entire duration of the experiment using thermocouples (type T, Digi-Sense, Cole-Parmer, USA), which were connected to a portable computer via the acquisition module (Nomadics, USA). The temperature was also measured at three different heights: 490 mm-top, 270 mm-middle, and 50 mm-bottom of the reactor. The ambient air temperature in the laboratory during the experiment was  $22.5 \pm 2.5 \text{ }^\circ\text{C}$ . The experiment lasted 15 days.

## 2.2 Development of mathematical model and assumptions

The mathematical model of the composting process presents the basic principles of process kinetics, the processes of mass and heat exchange in a system of three phases: liquid phase, solid phase, and gaseous phase. In the liquid phase, the processes of gas diffusion take place continuously, which occur during the process of organic matter decomposition, as well as the diffusion of oxygen that is supplied with air. The most important state variables for the composting process are solid-liquid phase temperature, moisture content, and oxygen concentration. The percentage of organic matter decomposition and thus the concentration of carbon dioxide and other gases depend on the mentioned state variables. The airflow in this process has a multiple role; in addition to providing the oxygen necessary for decomposition, the air also dissipates the excess heat generated by the decomposition reaction. In one part, the air has the function of removing moisture, i.e., drying the substrate, because the water vapour continuously condenses and creates ex-

cess moisture in the substrate, which can significantly slow down the process, and ultimately stop because anaerobic conditions are created. The differences between the inlet and outlet oxygen concentrations in the air are minimal and assume that the oxygen concentration inside the reactor is spatially equal. In that case, the reactor model can be approximated by a plug flow reactor model in unsteady-state operation. The model analyses the following heat transfers: heat transfer due to bioreaction, heat transfer from the reactor to the environment, convective heat transfer between phases, and heat transfer during water evaporation. The assumption regarding uniform temperature comes from the fact that there is small or no resistance to heat transfer from the compost matrix to the air in the reactor.<sup>24,25</sup>

The following assumptions were taken into account while developing the model:<sup>8</sup>

1. Volume of gas phase in reactor is constant;
2. Pressure in system (reactor) is constant;
3. Gas phase is saturated with water vapour and airflow is constant;
4. Liquid-solid phase and gas phase have same temperatures;
5. Substrate is a homogeneous mixture of uniform composition at beginning of process.

The rate of composting is expressed as the rate of organic matter decomposition and can be described using the following expression:

$$\frac{dm_{\text{OM}}}{dt} = -k \cdot m_{\text{OM}}^n \quad (1)$$

where  $m_{\text{OM}}$  is mass of organic matter (kg),  $t$  is time (h),  $n$  represents the reaction order, and  $k$  is reaction rate constant ( $\text{kg}^{1-n} \text{ h}^{-1}$ ). The rate constant is a function of temperature, oxygen, pH, moisture, and free space for air:<sup>26</sup>

$$k = k_T \cdot k_{\text{O}_2} \cdot k_{\text{pH}} \cdot k_{\text{H}_2\text{O}} \cdot k_{\text{FAS}} \quad (2)$$

Parameters in these functions (Eq. (2)) present the focus of this work. The expressions of the mentioned functions are described below.

For the temperature correction function, a modified Arrhenius expression was used:<sup>8,26,27</sup>

$$k_T = \alpha \cdot e^{\beta \left( \frac{1}{293} - \frac{1}{T} \right)} \quad (3)$$

where  $\alpha = A$  and  $\beta = E/R$  are kinetic constants that need to be determined, together with the reaction order  $n$  in the Eq. (1),  $A$  is frequency factor (units depending on the order of reaction),  $T$  is thermodynamic temperature of the substrate (K),  $E$  is activation energy ( $\text{J kmol}^{-1}$ ) and  $R$  the universal gas constant ( $\text{J kmol}^{-1} \text{ K}^{-1}$ ).

The following term was used for oxygen correction:<sup>7</sup>

$$k_{\text{O}_2} = \frac{\text{O}_2}{k_{\text{O}_2(0)} \cdot (\text{K}_{\text{O}_2} + \text{O}_2)} \quad (4)$$

where  $\text{O}_2$  is oxygen concentration (% v/v),  $k_{\text{O}_2(0)}$  presents the correction for oxygen concentration of the oxygen in

the atmospheric air (20.95 %, v/v), and  $K_{O_2}$  is half rate constant for oxygen (% , v/v). This function is one of the most commonly used functions for oxygen correction.<sup>11</sup>

For moisture correction function, the following equation was used:<sup>22</sup>

$$k_{H_2O} = \frac{1}{e^{-17.684 \cdot (1-S_m) + 7.0622} + 1} \quad (5)$$

Eq. (5) was modified as:

$$k_{H_2O} = \frac{1}{e^{-\gamma \cdot (1-S_m) + \Delta} + 1} \quad (6)$$

where  $S_m$  is fractional dry matter content of the composting material, and  $\gamma$  and  $\Delta$  are constants.

The Eq. (7) relates to free air space correction function.<sup>22</sup>

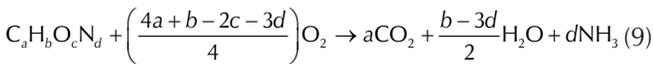
$$k_{FAS} = \frac{1}{e^{-23.675 \cdot FAS + 3.4945} + 1} \quad (7)$$

The proposed form of this function is:

$$k_{FAS} = \frac{1}{e^{-\chi \cdot FAS + \omega} + 1} \quad (8)$$

where  $\chi$  and  $\omega$  are constants.

For the known initial elementary composition of the substrate, organic matter degradation in the substrate can be calculated using the following equation:<sup>22,24</sup>



This expression is also used to calculate theoretical stoichiometric coefficients for water vapour, oxygen, and ammonia. Only stoichiometric coefficient for  $CO_2$  ( $\gamma_{CO_2}$ ) was not calculated using this formula. The reason for this was the significant deviations in the verification of the model by experimental data and the heterogeneity of the composting mixtures used in experiments. Stoichiometric coefficient

for  $CO_2$  exists in the relation of mass balance of  $CO_2$  dissolved in water:

$$\frac{dm_{CO_2}}{dt} = +\gamma_{CO_2} \cdot \frac{dm_{OM}}{dt} - k_L a_{CO_2} \cdot (He_{CO_2} \cdot f_{CO_2} \cdot X_{CO_2} - p_{CO_2}) \quad (10)$$

wherein  $k_L a_{CO_2}$  – mass transfer coefficient for  $CO_2$  ( $kg\ h^{-1}\ Pa^{-1}$ ),  $He_{CO_2}$  – Henry's constant for  $CO_2$  (Pa),  $f_{CO_2}$  – gas dissociation factor of  $CO_2$  in aqueous solution (–),  $X_{CO_2}$  – molar fraction of  $CO_2$  dissolved in water (–),  $p_{CO_2}$  – partial pressure of  $CO_2$  in the gas phase (Pa).

The literature review showed that one of the problems affecting the simulation of the composting process was the value of the amount of heat dissipated into the environment through the walls of the reactor. Since this was a reactor system in which an exothermic reaction would take place on the one hand, while on the other hand, the reactor was located in a space where variations in temperature would occur (depending on atmospheric conditions), it was necessary to correct/obtain the conductive-convective amount of heat lost in the environment. The relation describing temperature of the solid–liquid phase, in this case, was described by the following relation :

$$\frac{dT}{dt} = \frac{Q_{cw} + Q_G - Q_c^T - \sum_i (\max\{0, V_0 \bar{R}_i^T\} \cdot \bar{h}_i(T) + \min\{0, V_0 \bar{R}_i^T\} \cdot \bar{h}_i(\psi)) - (T - 273.15) \cdot \left( c_{pw} \cdot \frac{dm_w}{dt} + c_{pOM} \cdot \frac{dm_{OM}}{dt} \right)}{c_{pw} \cdot m_w + c_{pOM} \cdot m_{OM} + c_{pNT} \cdot m_{NT}} \quad (11)$$

where  $Q_c^T$  is heat transferred by convection,  $c_{pw}$ ,  $c_{pOM}$  and  $c_{pNT}$  are specific heat capacities of water, organic and inorganic matter, respectively;  $\bar{h}_i(T)$  and  $\bar{h}_i(\psi)$  are molar enthalpies of gas at temperature of solid–liquid and gas phase, respectively.  $Q_{cw}$  is the heat transfer through the reactor walls and  $Q_G$  is the biochemical heat generation.

Table 3 shows the differential equations built into the presented mathematical model and used to calculate the amount of dissolved gases in the composting material, the amount of gases in the gas phase, the temperature of the gas phase, etc. All other details of the mathematical model

Table 3 – Differential equations  
Tablica 3 – Diferencijalne jednačnje

Description	Equations
Equation for calculating dissolved gases ( $CO_2$ , $O_2$ , and $NH_3$ ) in water of a composting material (three differential equations).	$\frac{dm_i}{dt} = \pm \gamma_i \cdot \frac{dm_{OM}}{dt} - k_L a_i \cdot (He_i \cdot f_i \cdot \frac{M_w}{M_i} \cdot \frac{m_i}{m_w} - \frac{n_i \cdot R \cdot \psi}{V_g})$
Equation for calculating the mass of water in a composting material.	$\frac{dm_w}{dt} = -\gamma_w \cdot \frac{dm_{OM}}{dt} - k_L \cdot a_w \cdot (10^{(22.443 - 2795/\psi - 1.6798 \cdot \ln \psi)} - \frac{n_w \cdot R \cdot \psi}{V_g})$
Equation for calculating the amount of gases in gas phase (five differential equations).	$\frac{dn_i}{dt} = F_{i,0} + V_0 \bar{R}_i^T - \frac{R \cdot \psi}{P \cdot V_g} \cdot \left( F_{T,0} + \sum_i V_0 \bar{R}_i^T \right) \cdot n_i - \frac{n_i}{\psi} \cdot \frac{d\psi}{dt}$
Equation for calculating gas phase temperature.	$\frac{d\psi}{dt} = \frac{Q_c^T + (\psi_0 - \psi) \cdot \left( \sum_i c_{pi} \cdot F_{i,0} \right) + (T - \psi) \cdot \sum_i c_{pi} \cdot \max\{0, V_0 \bar{R}_i^T\}}{\sum_i n_i \cdot c_{pi}}$

(description; assumptions and simplifications; other supporting algebraic equations, explanations) can be found in the literature.<sup>8,18</sup>

### 2.3 Numerical methods for optimisation and simulations

The proposed mathematical model describes twelve dynamic state variables (nonlinear differential equations). Other equations of the mathematical model, some of which are described in Section 2.1, are algebraic linear and nonlinear. These equations describe the kinetic relations, the functional dependences of individual parameters on the temperature, and composition of the substrate, followed by the molar flows of the gas phase, flows during the transfer of mass from liquid to gas phase, etc.

Given that the proposed mathematical model was impossible to solve analytically, the proposed model was implemented in a numerical software package *Matlab*. Optimisation of kinetic parameters was performed by the Marquardt method,<sup>28</sup> which applies the Gauss-Newton technique, together with multivariate nonlinear regression analysis, i.e., interpolates between the Gauss-Newton algorithm (GNA) and the decreasing gradient method.<sup>29</sup> The parameters were simultaneously calibrated by minimising the error of the model concerning the experimental data based on the objective function (Eq. 12), using the Levenberg–Marquardt algorithm to solve the nonlinear least-square problem with a parameter tolerance of  $1e^{-6}$  in *MATLAB*.

This algorithm is one of the most commonly used algorithms for optimisation of nonlinear systems. As a criterion for matching the values obtained by numerical optimisation and experimental data, the following objective function was taken:

$$F = \sum_{j=1}^m \sum_{i=1}^n W_j \left| Y_{ij, \text{model}} - Y_{ij, \text{exp}} \right|^2 \quad (12)$$

where  $W_j$  is weight coefficient,  $Y_{ij, \text{model}}$  is value of dynamic state variables obtained by the model, and  $Y_{ij, \text{exp}}$  represents value of dynamic state variables obtained experimentally.

The relative importance of the variables was expressed by applying the appropriate weighting coefficients:

$$W_j = \frac{1}{\frac{1}{\sum_{i=1}^v n_i} \cdot \frac{1}{\sum_{j=1}^n \left| Y_{ij, \text{exp}} - \bar{Y}_{j, \text{exp}} \right|^2}} \quad (13)$$

$\bar{Y}_{j, \text{exp}}$  is mean value of the state variable obtained experimentally,  $n_i$  is number of experimental data for each variable, and  $v$  is number of variables to be adjusted.

Using experimental data (mass of organic matter, oxygen consumption, carbon dioxide production, and temperature, at different heights in the pilot reactor), 11 kinetic and other parameters were estimated, and shown in Table 4.

Table 4 – Parameters in model for optimisation  
Tablica 4 – Parametri u modelu za optimizaciju

No	Parameter	Equation
1	$\alpha$	(3)
2	$\beta$	(3)
3	$n$	(1)
4	$Y_{\text{CO}_2}$	(10)
5	$Q_c$	(11)
6	$k_{\text{O}_1(0)}$	(4)
7	$K_{\text{O}_2}$	(4)
8	$\gamma$	(6)
9	$\Delta$	(6)
10	$\chi$	(8)
11	$\omega$	(8)

In the *MATLAB*, a main file and three sub-routines, as well as one file with experimental values of the dynamic state variables were created. The main program was used to call: experimental data required for optimisation, vector of initial conditions for independent and dependent variables, a vector of initial assumptions of parameters that need to be optimised. The main program also performed a statistical analysis by calling one of the routines for Statistics (standard deviation and 95 % confidence interval), and gave the output of the optimisation results numerically and graphically. Calculation of the correlation coefficients between the parameters was performed within the statistical analysis in *MATLAB*. For model evaluation, R-square ( $R^2$ ) and root mean square error (RMSE) were also calculated.<sup>28,29</sup> For numerical solution of system of differential equations (numerical simulations), ODE23s solver, modified Rosenbrock method,<sup>30</sup> and STIFF method were used.<sup>31</sup> Sensitivity analysis was performed by parameter variations ( $\pm 2\%$ ) around their optimal values, and by monitoring their influence on selected objective functions (maximum organic matter conversion, minimum  $\text{O}_2$  concentration, maximum  $\text{CO}_2$  concentration, and maximum substrate temperature). Simulations were performed in *MATLAB*.

## 3 Results and discussion

### 3.1 Parameter estimation

The most complex mathematical models incorporate the solid phase in the water film covering the particles, and its solubilisation.<sup>32</sup> Additional model complexities have been found in the case of integrated dynamic models describing mass and heat exchange, including kinetics in a solid-liquid-gas system. Simple models based on kinetics and mass change process offer only a partial insight into the mechanisms that take place during the biodegradation process. Composting models with certain correction factors (temperature, humidity, oxygen, and free air space) offer a tool for dynamically understanding the mechanism of heating up and thermal equilibrium as a process.<sup>22</sup> Mathemati-

cal composting process models help predict how control measures impact various process conditions such as pollution, length of the composting regime, temperature, and compost characteristics themselves during the process.<sup>33</sup> On the other hand, solving such complex mathematical problems requires certain knowledge and tools. The selection of software and appropriate numerical methods facilitate researchers' efforts in obtaining relevant information.

To solve the model, it was necessary to enter the vector of the initial values of the measured variables, as well as the values of these variables during the process. Experimental values were required to calculate the value of the objective function (Eq. 12) for optimising the parameters. Experimental data from reactor 1 (M1) were used as initial values of the dynamic variables in the model, and to estimate the kinetic parameters. Data selection for the kinetic parameters estimation was performed by random selection because the model needs to be verified with the remaining data, so it does not matter which data were used for the estimation. Vector of initial data for experimentally measured variables: mass of organic matter 6.3 kg, mass of water in reactor 11.35 kg, amount of O<sub>2</sub> and CO<sub>2</sub>  $5.84 \cdot 10^{-5}$ ,  $5 \cdot 10^{-6}$  kmol, respectively, and mixture temperature 295 K. Estimated values and statistical analysis of parameters are given in Table 5. The values shown in Table 5 were obtained in *Matlab*. Table 5 shows the values for the 95 % confidence interval for each estimated parameter (lower and upper values). The estimated parameters with a lower value of the standard deviation generated narrower confidence intervals. The narrower the interval, the more precise is the estimate. Most of the eleven estimated parameters have very narrow confidence intervals, only parameters  $\gamma$ ,  $\Delta$ , and  $\chi$  have slightly wider confidence intervals.

As seen from Table 4, the optimised reaction order value is  $\approx 1.9$ . This value is consistent with the results obtained in paper of *Briški et al.*<sup>13</sup> and *Papačanin and Petric.*<sup>8</sup> The

$n^{\text{th}}$  order model was proposed based on the fact that the organic waste used for the composting process consisted of a large number of organic compounds that decompose at different rates (kinetics with a different reaction order). Since the composition of organic waste included carbohydrates, lipids, lignin, cellulose and hemicellulose, it may be concluded that these were compounds with different properties and thus different degrees of decomposition during the process. The obtained value of activation energy (Eq. (3)) was 37.78 KJ mol<sup>-1</sup>. In the paper by *Xi et al.*<sup>34</sup>, household waste and microbiological kinetics were used, and the obtained activation energy value was 29 KJ mol<sup>-1</sup>. Most authors have mainly dealt with the optimisation of parameters in the model, mainly in models with first-order kinetics. *Hamelers*<sup>35</sup> concluded that modelling of the process by  $n^{\text{th}}$  order kinetics should be considered because significant changes in the activation energy occur during the process. Obtained value of the stoichiometric coefficient for CO<sub>2</sub> was higher relative to the theoretically calculated value from relation 9 (calculated value 1.86). When it comes to heat exchanged by conduction, the value obtained in this paper is also consistent with the results of other researchers.<sup>36</sup> Among other parameters, which exist in the corrective functions in relation (4), obtained values were significantly different from the values obtained by *Baptista et al.*<sup>7</sup> Value obtained for the correction of oxygen concentration in atmospheric air was 0.96 (Table 4). As the authors noted, this value was obtained by varying the temperature and moisture content, and represents the mean value obtained in previous studies. That is, the  $K_{O_2}$  value was obtained independently of the integrated model and experimental data. As previously described, several corrective functions were included in this study, where the optimisation was performed based on the experimental data in the integrated model. Other parameters have approximate values given in the original research.

In addition, as a measure of model performance, root mean square error (RMSE) was calculated.<sup>37</sup> RMSE for the

Table 5 – Estimated values of parameters in model and statistical analysis

Tablica 5 – Procijenjene vrijednosti parametara u modelu i statistička analiza

No.	Parameter	Value	Unit	Standard deviation	95 % confidence interval	
					Lower value	Upper value
1	$\alpha$	$1.2688 \cdot 10^{-5}$	kg <sup>-0.5</sup> · h <sup>0.5</sup>	$7.66 \cdot 10^{-7}$	$1.1228 \cdot 10^{-5}$	$1.4244 \cdot 10^{-5}$
2	$\beta$	4544.1	K <sup>-1</sup>	70.5	4401.4	4678.6
3	$n$	$\approx 1.9$	–	0.0262	1.6469	2.1039
4	$Y_{CO_2}$	3.1716	kg <sub>CO<sub>2</sub></sub> kg <sub>OT</sub> <sup>-1</sup>	0.1022	2.9621	3.3644
5	$Q_c$	1753.3	J kg <sub>OM</sub> <sup>-1</sup>	23.3	1704.2	1795.8
6	$k_{O_2(0)}$	0.1554	–	0.0134	0.1291	0.1816
7	$K_{O_2}$	0.8683	%, v/v	0.2703	0.3718	1.3648
8	$\gamma$	17.795	–	3.677	11.539	24.050
9	$\Delta$	6.8565	–	1.4066	4.0890	9.6240
10	$\chi$	23.671	–	2.793	18.156	29.147
11	$\omega$	3.5040	–	0.1765	3.1568	3.8512

SD = 0.3378

mass of organic matter was 0.23 kg,  $O_2$  consumption and  $CO_2$  production was  $1.96 \cdot 10^{-6}$  and  $4.17 \cdot 10^{-7}$  kmol, respectively, and RMSE for temperature was 0.32. The root mean square error was calculated for the experimental data used to estimate the parameters and output of the model. The range of measured values were as follows: mass of organic matter from 6.3 to 4.4 kg, amount of  $O_2$  and  $CO_2$   $5.84 \cdot 10^{-5} - 3.53 \cdot 10^{-5}$ ,  $5 \cdot 10^{-6} - 2.2 \cdot 10^{-5}$  kmol, respectively, and mixture temperature from 295 to 331.7 K. Based on these values, it may be concluded that RMSE indicates a good accuracy of estimation. The number of models that did not implement any type of correction was high.<sup>11</sup> The reason being that the aim was a model with a minimal amount of parameters, and operation at non-optimal conditions. The focus of this paper were the corrective functions that mitigate the extreme phenomena occurring in the process and during the simulation of the composting process.

### 3.2 Model evaluation

Simulation models are approximate imitations of real systems, which can never exactly imitate the real system. Therefore, the model should be checked and validated to

a certain extent, depending on the purpose and application of the model.<sup>38</sup>

As Roache<sup>39</sup> stated: "Verification deals with mathematics". Validation addresses the accuracy of the conceptual model as compared to the "real world", i.e., experimental measurements.<sup>40</sup> In order to evaluate the proposed model, numerical simulations were performed in which data for M2 and M3 were used as initial values in the model. Figs. 2 and 3 show the results of numerical simulations and experimental data during 360 h. Since the equality between the temperature of the liquid and gas phases was used as a constraint in the model (due to the rapid heat exchange), the evaluation was performed for the bulk temperature. Figs. 2 and 3 show the experimental data as the mean values at three different heights in the reactor (three replications each) along with the standard deviation (SD). The exception is the bulk temperature, since a large number of measurements were performed so that the data for each height are displayed.

Figs. 2a) and 3a) show the verification of the model for oxygen consumption. The agreement of the model is better in the case of data simulation for M2, where the highest oxygen consumption was experimentally achieved after

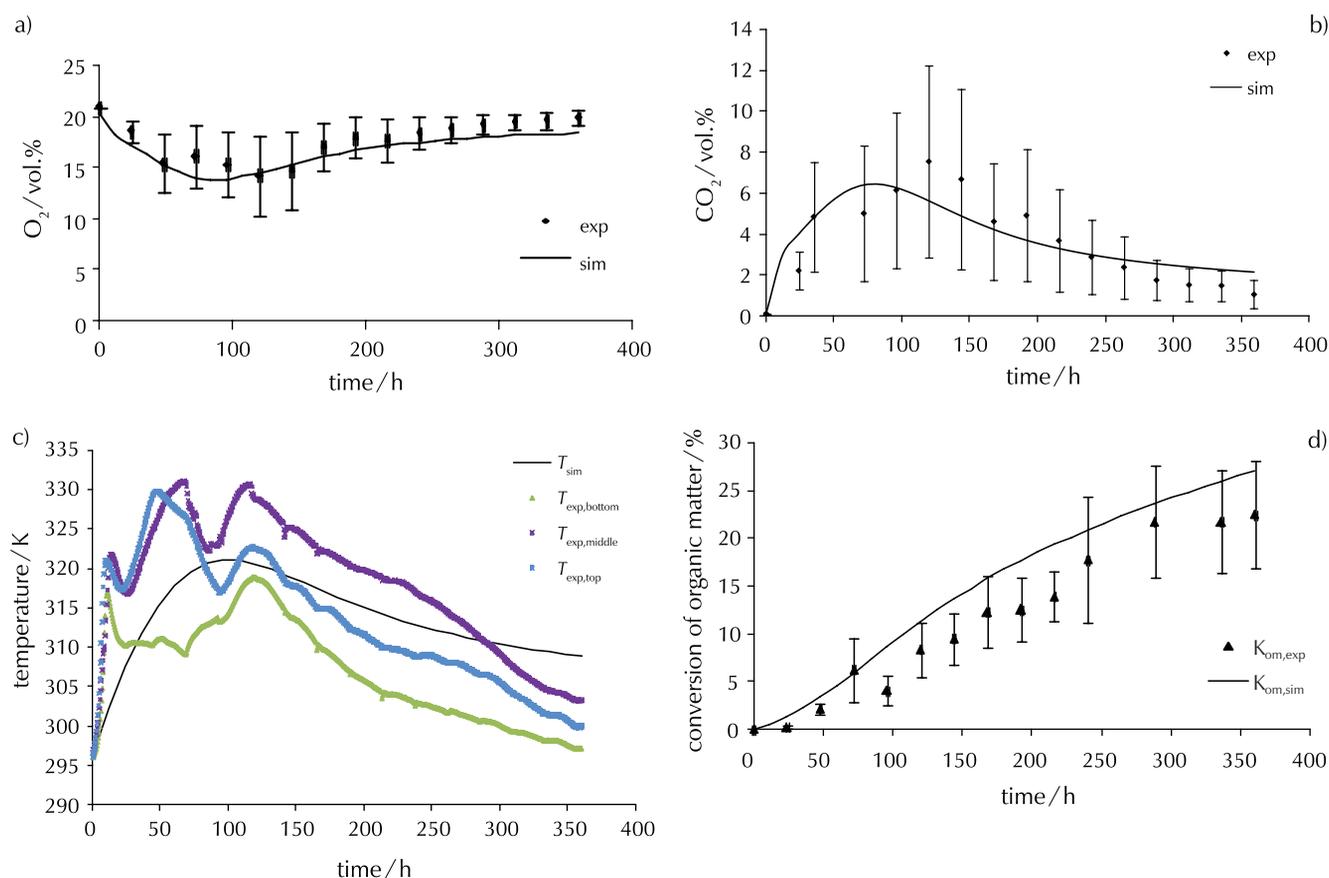


Fig. 2 – Model verification for M2: a)  $O_2$  (vol.%); b)  $CO_2$  (vol.%); c) bulk temperature (K); d) conversion of organic matter (%). Marks sim and exp indicate data obtained by simulation or experimentally. Indexes: bottom, middle, and top, indicate position in the reactor at which the temperature was measured.

Slika 2 – Verifikacija modela za M2: a)  $O_2$  (vol. %); b)  $CO_2$  (vol. %); c) temperatura smjese (K); d) pretvorba organske tvari (%). Oznake sim i exp ukazuju da li su podatci dobiveni simulacijama ili eksperimentalno. Indeksi bottom, middle i top, označavaju da li je temperatura izmjerena na dnu, sredini ili vrhu reaktora. temperatura.

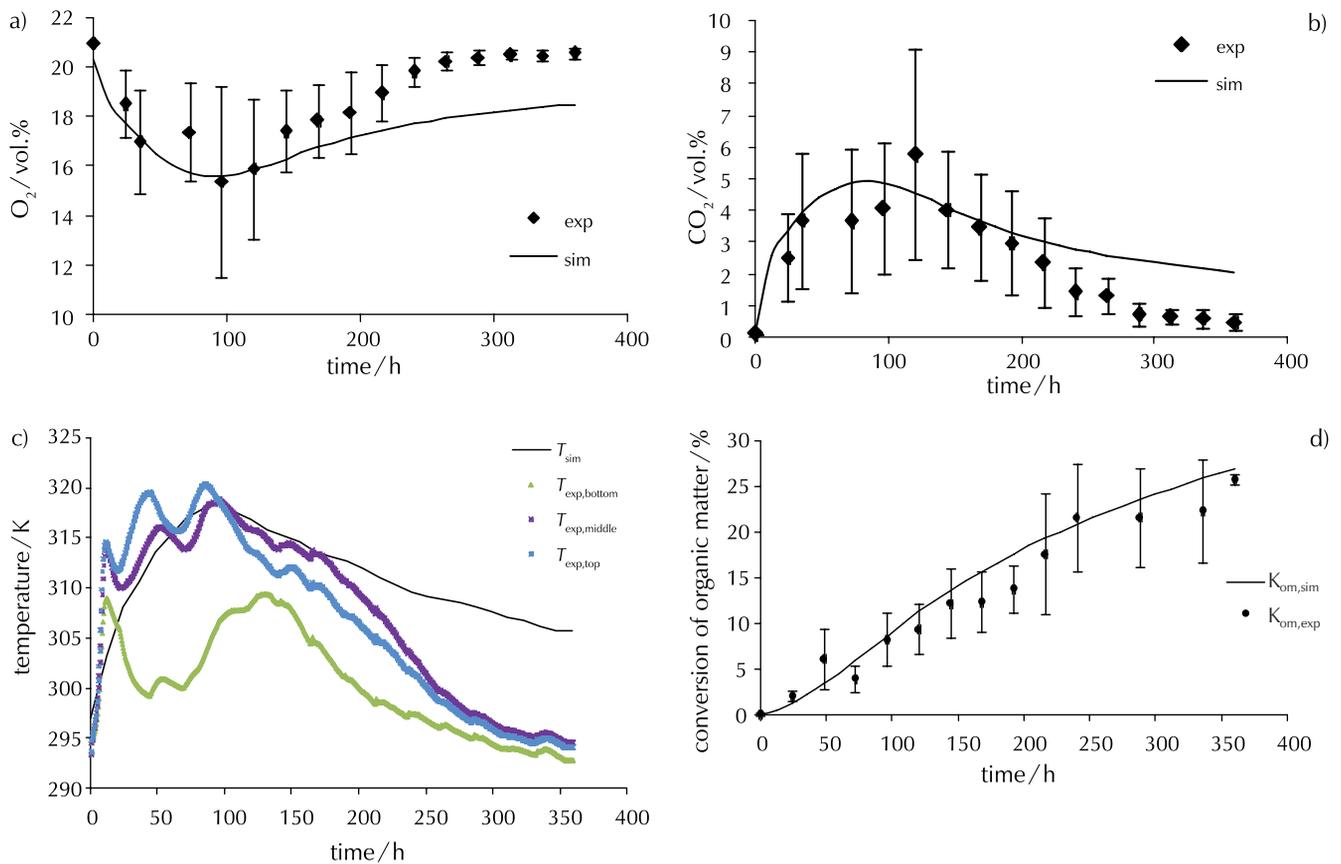


Fig. 3 – Model verification for M3: a)  $O_2$  (vol. %); b)  $CO_2$  (vol. %); c) bulk temperature, K; d) conversion of organic matter, %. Indexes sim and exp indicate data obtained by simulation or experimentally. Indexes: bottom, middle and top, indicate position in the reactor at which the temperature was measured.

Slika 3 – Verifikacija modela za M3: a)  $O_2$  (vol. %); b)  $CO_2$  (vol. %); c) temperatura smjese, K; d) pretvorba organske tvari, %. Indeksi sim i exp ukazuju na to da su podatci dobiveni simulacijama ili eksperimentalno. Indeksi dno, sredina i vrh, označavaju mjesto u reaktoru na kojoj je izmjerena temperatura.

120 h (12.43 %  $O_2$ ) compared to the model where the highest oxygen consumption (13.82 %  $O_2$ ) was observed after 84 h. Based on these values, it maybe concluded that after 84 h, the maximum degradation of easily degradable organic substances began, but this can be determined with certainty by taking into account other characteristics of process variables. For the case of M3 mixture, both the model and the experiment showed the highest oxygen consumption over 96 h, although the maximum difference in this case was 2.27 %. Also noticeable is that the model showed a higher degradation after reaching the maximum difference compared to the experimental data, which indicated that the composting process was very close to the end (the value of oxygen concentration approached the value of 21 vol.%). The mean difference value for M2 was 1.19 %, while that for M3 was 1.34 %. It is important to note that the presented experimental data were measured at three different heights in the reactors and the reactor outlets (for both  $O_2$  and  $CO_2$ ), and that the highest values for SD were in the period of maximum degradation and activity of microorganisms. After reviewing the literature, most researchers verified the model with data measured at the reactor outlet or near the top of the reactor, with better agreement in some cases.<sup>17,41,42</sup> Since  $O_2$  and  $CO_2$  concentrations were measured not only at the top of the reactors,

but also at the bottom of the reactors, where there was very little space for airflow and gas retention, very low concentrations were obtained, which significantly increased the standard deviation from the output of the model. As carbon dioxide production is directly related to oxygen consumption, the deviations related to the amount of produced carbon dioxide are related to the deviations observed for oxygen consumption. The maximum difference for M2 was 1.25 %, while for M3 it was 1.9 % (Figs. 2b) and 3b)). One of the reasons for the better data agreement may be the composition of mixture M2, in which waste yeast was added (see section 2.2) unlike the M3 mixture. Waste yeast is rich in nitrogen and has high water content, so it can contribute to improving the characteristics of the composting mixture and significantly speed up the process. Heterogeneous systems such as substrate used in this study, are difficult to describe with constant values of stoichiometric coefficients for the whole process. In the proposed model, the value of the stoichiometric coefficient for  $CO_2$  was adjusted, which still indicated insufficient agreement with the experimental data. Since gas accumulation occurs at the top of the reactor (free air space, FAS), the actual concentration of  $O_2$  consumption and  $CO_2$  production is lower, as the model shows. The continuous formation and dissolution of gases in water take place within the mix-

ture, so the amount of gases in the mixture should be taken into account. In addition, it should be emphasised that the trend of O<sub>2</sub> consumption or CO<sub>2</sub> production shown by the model was almost identical to the experimental data. Experimental data for temperature (Figs. 2c) and 3c) show a logical trend in reactor heights. Similar results have been reported in the literature.<sup>43</sup> Also, in the mentioned paper, the equality of gas-phase temperatures and bulk temperatures was observed, as is the case in this research. Since fresh ambient air was continuously introduced to the bottom of the reactor, the lowest temperature value was expected to be at the bottom of the reactor, because the cooling of the system, in this case, was more intense compared to the other parts of the reactor. The temperature profiles were higher towards the top of the reactor. The model showed no “sharp” peak in temperature, but the appearance of milder curve, without the classical peak, which was characteristic of models that use the Arrhenius correction function. The temperature profile obtained by numerical simulations showed the trend of the aerobic decomposition process as reported in the literature.<sup>44</sup> The model predicted slightly slower cooling than did the experimental data. A similar observation has been reported,<sup>32,45</sup> but the deviations in their work were much higher. In both cases, the experimental temperature data showed two “peaks”, with the appearance of the M3 curves being somewhat milder and visually more similar to the model, except for the temperatures measured at the bottom of the reactor. In addition, when it comes to the data for M3 measured at the top and in the middle of the reactor, the obtained values were in accordance with the data obtained by the simulation. The difference in maximum temperatures was 0.185 K (compared to the mean value of the temperatures measured at the top and in the middle of the reactor), while the maximum difference at the end of the process (360 h) was 11.9 K. For M2, the deviations were slightly greater, and the difference in maximum temperatures was about 9 K, which was also the maximum difference. Such deviations between M2 and M3 can be explained by the amount of substrate in the reactors. The mass of mixture M2 was significantly higher compared to M3 in a reactor of the same dimensions, indicating that the mass in the second reactor was much denser, *i.e.*, that the aeration was weaker compared to the third reactor (M3). In this case, the cooling of the mass was much slower and higher temperatures had occurred. It is also important to point out once again that the optimised parameters in the proposed model were obtained based on the mean values measured at different heights in the reactors, which certainly leaves room for better insight into the processes taking place in the reactors. Larger deviations were expected in the case of temperatures, precisely because the simulated data were verified by data from three heights, individually and not as a mean. Regardless of these discrepancies, these results are consistent with previous research that had significantly more limitations in the proposed models and experimental data.<sup>12,46</sup> Table 6 shows the values of the maximum and mean differences between the model and the mean values of the measured temperatures.

Achieving maximum temperatures is the basis for the efficiency of the composting process, and significantly contributes to high decomposition rates during the compost-

Table 6 – Maximum and mean temperature difference (K)  
Tablica 6 – Maksimalna i srednja temperaturna razlika (K)

	Bulk temperature difference /K	
	max	mean
M2	3.86	1.93
M3	4.02	2.74

ing process. On the other hand, during the thermophilic decomposition period, the destruction of most pathogens occurs.<sup>47</sup> In order to evaluate the model, RMSE was calculated and the values are shown in Table 7.

Table 7 – Calculated RMSE values for model evaluation with independent data

Tablica 7 – RMSE vrijednosti evaluacije modela neovisnim podacima

Variable	RMSE	
	M2	M3
mass of organic matter /kg	0.20	0.21
O <sub>2</sub> consumption /vol%	1.17	3.29
CO <sub>2</sub> production /vol%	1.05	1.18
temperature /K	2.89	2.21

The square error between the data for M2 and the output of the model was  $R^2 = 0.91$ , while the square error for the case of mixture M3 was  $R^2 = 0.72$ . As mentioned previously in this section, the better data agreement of M2 mixture was probably due to the initial composition of the composting mixture. The M2 mixture was prepared in a smaller ratio of OFMSW and additives, and additives were used in a ratio of 1 : 1 : 1 (see section 2.2).

Comparisons of the experimental data and numerical simulation results (Figs. 2d) and (3d) for the conversion of organic matter, given the fact that the mixtures used for composting were very heterogeneous, show excellent agreement. In both cases, the model follows the degradation trend in accordance with the experiment, with the model showing a higher decomposition of organic matter. Modelling with  $n^{\text{th}}$  order kinetics offered significantly better results regarding the decomposition of organic matter from the point of view of biochemical processes that take place. This has been confirmed by Zhang *et al.*<sup>48</sup> and Kulcu.<sup>49</sup>

Modelling of food waste composting processes is essential for supporting the prediction of system performance under various operating conditions, and thus quantifying relationships between control actions and process efficiencies.<sup>50</sup>

The fact that the model well described experimental data confirmed that the model was valid for use indifferent experimental conditions, which is one of the goals of mathematical modelling. With small modifications, referring to the initial conditions, this model can successfully simulate

Table 8 – Sensitivity analysis of the model  
 Tablica 8 – Analiza osjetljivosti modela

Parameter	Change / %	Variation			
		$K_{om}/\%$	$O_2/\text{vol.}\%$	$CO_2/\text{vol.}\%$	$T/K$
$A$	$\pm 2$	-0.69/0.70	0.20/-0.20	-0.19/0.18	-0.79/0.78
$E/R$	$\pm 2$	-0.77/0.72	0.27/-0.23	-0.24/-0.23	-1.00/0.90
$n$	$\pm 2$	-2.26/2.16	0.77/-0.62	-0.69/-0.62	-2.83/2.47
$Y_{CO_2}$	$\pm 2$	0.01/-0.01	0.01/-0.01	0.01/-0.01	0.03/-0.03
$Q_c$	$\pm 2$	0.20/-0.21	0	0	0.40/-0.41
$k_{O_2(0)}$	$\pm 2$	0.67/-0.72	0	0	0.74/-0.82
$K_{O_2}$	$\pm 2$	0.07/-0.10	0	0	0.09/-0.12
$\alpha$	$\pm 2$	-0.10/0.09	0.03/-0.03	-0.03/0.02	-0.12/0.12
$\beta$	$\pm 2$	0.05/-0.06	0	0	0.06/0.00
$\gamma$	$\pm 2$	-0.01/-0.00	0	0	0.01/0.00
$\Delta$	$\pm 2$	-0.01/-0.01	0	0	-0.01/-0.01

Table 9 – Matrix of correlation coefficients for model parameters  
 Tablica 9 – Matrica koeficijena korelacije za parametre modela

Parameter											
$\alpha$	1										
$\beta$	0.38*	1									
$n$	-0.38*	-0.34*	1								
$Y_{CO_2}$	-0.06	0.00	0.26	1							
$Q_c$	0.31*	0.40*	-0.82***	-0.32*	1						
$k_{O_2(0)}$	0.00	-0.29	0.78***	0.11	-0.71**	1					
$K_{O_2}$	0.51**	0.90***	-0.22	-0.02	0.30	-0.15	1				
$\gamma$	-0.82***	-0.31*	0.11	-0.19	-0.07	0.03	-0.42*	1			
$\Delta$	0.01	-0.78***	0.21	0.04	-0.28	0.21	-0.77***	-0.16	1		
$\chi$	-0.48*	-0.62**	0.09	0.06	-0.22	-0.11	-0.73**	0.19	0.46*	1	
$\omega$	0.42*	0.18	-0.50*	-0.08	0.45*	-0.56**	0.14	-0.52**	0.13	-0.02	1

\* poor correlation (positive or negative); \*\* moderate correlation (positive or negative); \*\*\* very good to excellent correlation (positive or negative)

the process of degradation of organic solid waste with different additions. The results showed that the used volume of pilot-scale reactor with provided thermal insulation allowed self-heating of the substrate, and thus the simulation of full-scale composting.

### 3.3 Sensitivity analysis

The sensitivity analysis was performed by variation of obtained parameters (see Table 5) of  $\pm 2$  % of their optimal value. Since the statistical analysis of parameter estimation (Table 5) showed reliable values for most parameters, no greater deviations of the parameters (e.g.  $\pm 5$  %) were necessary in order to determine their impact on objective functions. In case of parameter variations of  $\pm 1$  % not yielding a noticeable influence on the selected objective functions, the value of 2 % was chosen.

As objective functions, maximum conversion ( $K_{om}$ ), maximum consumption of  $O_2$ , maximum production of  $CO_2$ , and maximum temperature were selected. Table 8 shows the results of the sensitivity analysis.

As maybe seen, the most sensitive parameter was reaction order  $n$ , followed by activation energy  $E$ , and coefficient  $A$ . Parameters  $E$  and  $A$  exist in the expression for temperature correction, and together with the reaction order, most affect the speed of the decomposition process. Table 8 also reveals that the variation of these parameters had the greatest effect on the conversion of organic matter and temperature, and less on the concentrations of oxygen and carbon dioxide. It is also noticeable that some parameters had no or very little effect on the selected objective functions, and these parameters could be omitted in some future research in terms of optimising their values. One of the parameters that had no effect on the model was the

stoichiometric coefficient for  $\text{CO}_2$ . A potential parameter that causes sensitivity of the model is a constant half-velocity for oxygen, which should be considered in the future. The results of the sensitivity analysis are consistent with the research (Zhang et al.,<sup>51</sup> Petric et al.,<sup>19</sup> Papačanin<sup>52</sup>). Table 9 shows the values of the correlation coefficients of the optimised parameters. These values are shown in order to obtain information of the interaction among parameters for  $p > 0.05$ , since a local sensitivity analysis was conducted in the study. There is a strong correlation between several parameters ( $n$  and  $Q_c$ ,  $K_{O_2}$  and  $Q_c$ ) *apropos*, simultaneous parameter variations need to be performed. For example, a strongly negative correlation between the reaction order  $n$  and the heat transferred by convection  $Q_c$  indicates that it is necessary to increase the reaction order and decrease the heat transferred by convection, and *vice versa*. In the future, influence of simultaneous variations of parameters with a strong correlation coefficient on selected objective functions, e.g., maximum conversion of organic matter, need to be investigated.

This indicates the need to perform a global sensitivity analysis in future research.

## 4 Conclusions

A novelty in this paper is the optimisation of a large number of kinetic and other parameters in an integrated dynamic model, including the reaction order, stoichiometric coefficient, etc., where a large amount of experimental data were used to verify the model. Simplifications and limitations in the proposed model were minimised, and the parameters fitted with experimental data for several dynamic state variables. The experiments were performed in detail and with a large number of measurements (in time and space). Detailed statistical analysis showed good parameter estimation based on 95 % confidence interval values. Verification and validation of the model showed good agreement with independent experimental data. The advantage of this model is reflected in the fact that, with small changes, which refer to the initial conditions, it can successfully simulate the process of decomposition of organic solid waste with various additives. Sensitivity analysis of parameters showed that reaction order  $n$ ,  $E$ , and  $A$ , were the most sensitive parameters based on the maximum conversion, maximum consumption of  $\text{O}_2$ , maximum production of  $\text{CO}_2$ , and maximum temperature. The model is very effective in simulating the composting process, instantly predicting the output parameters, and simple in obtaining initial input parameters for a researcher to use the model.

In future research, it is necessary to optimise the key process parameters for aerobic biodegradation, and this model could be used for simulation to obtain relevant data during and at the end of the process, which would save time and money. In addition, before process parameters optimisation, it is necessary to perform a global sensitivity analysis.

## List of abbreviations and symbols Popis kratica i simbola

$A$	– frequency factor (units depending on the order of reaction)
$c_{pw}$	– specific heat capacity of water
$c_{pOM}$	– specific heat capacity of organic matter
$c_{pNT}$	– specific heat capacity of inorganic matter
$c_{pi}$	– specific heat capacity of gas $i$ , $\text{J kmol}^{-1} \text{K}^{-1}$
d.b.	– dry base
$E$	– activation energy, $\text{J kmol}^{-1}$
$f_{\text{CO}_2}$	– gas dissociation factor of $\text{CO}_2$ in aqueous solution
$f_i$	– gas dissociation factor $i$ in aqueous solution, –
$F_{i,0}$	– molar flow at inlet for component $i$ , $\text{kmol h}^{-1}$
$F_{T,0}$	– total molar gas flow at outlet, $\text{kmol h}^{-1}$
$He_i$	– Henry's gas constant $i$ , Pa
$He_{\text{CO}_2}$	– Henry's constant for $\text{CO}_2$ , Pa
$\bar{h}_i(T)$	– molar enthalpy of gas at temperature of solid–liquid
$\bar{h}_i(\psi)$	– molar enthalpy of gas at temperature of gas phase
$k$	– reaction rate constant, $\text{kg}^{1-n} \text{h}^{-1}$
$k_{\text{FAS}}$	– correction factor for free air space (FAS)
$k_{\text{H}_2\text{O}}$	– correction factor for moisture content
$k_{i,a_w}$	– mass transfer coefficient for water, $\text{kg h}^{-1} \text{Pa}^{-1}$
$k_{i,a_{\text{CO}_2}}$	– mass transfer coefficient for $\text{CO}_2$ , $\text{kg h}^{-1} \text{Pa}^{-1}$
$k_{i,a_i}$	– mass transfer coefficient for gas $i$ , $\text{kg h}^{-1} \text{Pa}^{-1}$
$k_{\text{O}_2}$	– correction factor for oxygen
$k_{\text{O}_2(0)}$	– correction for oxygen concentration in atmospheric air (20.95 %, v/v)
$k_{\text{pH}}$	– pH correction
$k_T$	– effect of temperature on reaction rate constant
$K_{\text{O}_2}$	– half rate constant for oxygen, %, v/v
$K_{\text{OM}}$	– organic matter conversion
$\max\{0, V_0 \bar{R}_i^T\}$	– expression used to determine the direction of mass transfer
$m_{\text{OM}}$	– mass of organic matter, kg
MSW	– municipal solid waste
$n$	– reaction order, –
$n_i$	– number of experimental data for each variable
$\text{O}_2$	– oxygen concentration, %, v/v
OFMSW	– organic fraction of municipal solid waste
OM	– organic matter content
$p_{\text{CO}_2}$	– partial pressure of $\text{CO}_2$ in the gas phase, Pa
$p_i$	– partial pressure of gas and in the gas phase, Pa
$Q_c^T$	– heat transferred by convection
$Q_{cw}$	– heat transfer through the reactor walls
$Q_G$	– biochemical heat generation
$R$	– universal gas constant, $\text{J kmol}^{-1} \text{K}^{-1}$
$R^2$	– square error

RMSE	– root mean square error
SD	– standard deviation
$S_m$	– fractional dry matter content of composting material, –
$t$	– time, h
$T$	– thermodynamic temperature of substrate, K
$v$	– number of variables to be adjusted
$V_0\bar{R}_i^T$	– molar flow of component $i$ at outlet of liquid phase, kmol h <sup>-1</sup>
$V_g$	– volume of gas phase, m <sup>3</sup>
w.b.	– wet base
$W_j$	– weight coefficient
$X_{CO_2}$	– molar fraction of CO <sub>2</sub> dissolved in water, –
$X_i$	– molar fraction of gas dissolved in water, –
$Y_{CO_2}$	– stoichiometric coefficient for CO <sub>2</sub>
$Y_i$	– stoichiometric coefficient
$Y_{ij,exp}$	– value of dynamic state variables obtained experimentally
$Y_{ij,model}$	– value of dynamic state variables obtained by the model
$\bar{V}_{exp}$	– mean value of state variable obtained experimentally
$\psi$	– gas phase temperature, K

## References Literatura

1. *D. Alain*, Technical document on municipal solid waste organics processing, Environment Canada, 2013.
2. *M. Gavrilescu*, Environmental biotechnology: achievements, opportunities and challenges, *Dyn. Biochem. Process Biotechnol. Mol. Biol.* **4** (1) (2010) 1–36.
3. *R. Alkarimiah, F. Suja*, Effects of technical factors towards achieving the thermophilic temperature stage in composting process and the benefits of closed reactor system compared to conventional method—a mini review, *Appl. Ecol. Environ. Res.* **17** (4) (2019) 9979–9996, doi: [https://doi.org/10.15666/aeer/1704\\_99799996](https://doi.org/10.15666/aeer/1704_99799996).
4. *B. Seng, R. A. Kristanti, T. Hadibarata, K. Hirayama, K. Katayama-Hirayama, H. Kaneko*, Mathematical model of organic substrate degradation in solid waste windrow composting, *Bioproc. Biosyst. Eng.* **39** (2016) 81–94, doi: <https://doi.org/10.1007/s00449-015-1492-6>.
5. *N. J. Themelis, Y. H. Kim*, Material and energy balances in a large-scale aerobic bioconversion cell, *Waste Manage. Res.* **20** (3) (2002) 234–242, doi: <https://doi.org/10.1177/0734242X0202000304>.
6. *I. G. Mason*, An evaluation of substrate degradation patterns in the composting process. Part 2, Temperature-corrected profiles, *Waste Manage.* **28** (10) (2008) 1751–1765, doi: <https://doi.org/10.1016/j.wasman.2007.06.019>.
7. *M. Baptista, F. Antunes, M. S. Gonçalves, B. Morvan, A. Silveira*, Composting kinetics in full-scale mechanical–biological treatment plants, *J. Waste Manage.* **30** (10) (2010) 1908–1921, doi: <https://doi.org/10.1016/j.wasman.2010.04.027>.
8. *E. Papačanin, I. Petric*, Mathematical modeling and simulation of the composting process in a pilot reactor, *Bull. Chem. Technol. Bosnia Herzegovina* **47** (2016) 39–48.
9. *R. Kulcu, O. Yaldiz*, Determination of aeration rate and kinetics of composting some agricultural wastes, *Bioresour. Technol.* **93** (1) (2004) 49–57, doi: <https://doi.org/10.1016/j.biortech.2003.10.007>.
10. *I. G. Mason*, A Study of Power, Kinetics, and Modelling in the Composting Process, PhD Thesis, University of Canterbury, New Zealand, 2007.
11. *E. Walling, A. Trémier, C. Vaneckhaute*, A review of mathematical models for composting, *Waste Manage.* **113** (2020) 379–394, doi: <https://doi.org/10.1016/j.wasman.2020.06.018>.
12. *M. Ajmal, S. Aiping, S. Uddin, M. Awais, M. Faheem, L. Ye, Y. Shi*, A review on mathematical modeling of in-vessel composting process and energy balance, *Biomass Convers. Biorefin.* **113** (2020) 1–13, doi: <https://doi.org/10.1016/j.wasman.2020.06.018>.
13. *F. Briški, M. Vuković, K. Papa, Z. Gomzi, T. Domanovac*, Modelling of Composting of Food Waste in a Column Reactor, *Chem. Papers* **61** (1) (2007) 24–29, doi: <https://doi.org/10.2478/s11696-006-0090-0>.
14. *A. G. Barneto, J. A. Carmona, J. A. C. Ferrer, M. J. D. Blanco*, Kinetic study on the thermal degradation of a biomass and its compost: Composting effect on hydrogen production, *Fuel*. **89** (2) (2010) 462–473, doi: <https://doi.org/10.1016/j.fuel.2009.09.024>.
15. *D. P. Komilis, R. K. Ham*, Carbon dioxide and ammonia emissions during composting of mixed paper, yard waste and food waste, *Waste Manage.* **26** (2006) 62–70, doi: <https://doi.org/10.1016/j.wasman.2004.12.020>.
16. *S. Pommier, D. Chenu, M. Quintard, X. Lefebvre*, Modelling of moisture-dependent aerobic degradation of solid waste, *Waste Manage.* **28** (2008) 1188–1200, doi: <https://doi.org/10.1016/j.wasman.2007.05.002>.
17. *F. Briški, N. Horgas, M. Vuković, Z. Gomzi*, Aerobic composting of tobacco industry solid waste—simulation of the process, *Clean Technol. Environ. Policy* **5** (2003) 295–301, doi: <https://doi.org/10.1007/s10098-003-0218-7>.
18. *I. Petric, V. Selimbašić*, Development and validation of mathematical model for aerobic composting process, *Chem. Eng. J.* **139** (2) (2008) 304–317, doi: <https://doi.org/10.1016/j.cej.2007.08.017>.
19. *I. Petric, E. Avdihodžić, N. Ibrić*, Numerical simulation of composting process for mixture of organic fraction of municipal solid waste and poultry manure, *Ecol. Eng.* **75** (2015) 242–249, doi: <https://doi.org/10.1016/j.ecoleng.2014.12.003>.
20. Austrian Standard S 2023, Analytical Methods and Quality Control for Waste Compost, Vienna: Austrian Standardization Institute, Austria, 1986.
21. APHA (American Public Health Association), Standard Methods for the Examination of Water and Wastewater, APHA, Washington, DC, 1995.
22. *R. T. Haug*, The practical handbook of compost engineering, Lewis Publishers, Boca Raton, 1993, pp. 385–436.
23. *M. A. Vining*, Bench-scale compost reactors system and the self-heating capabilities, Master thesis, Louisiana State University, Baton Rouge, 2002.
24. *C. W. Higgins, L. P. Walker*, Validation of a new model for aerobic organic solids decomposition: simulations with substrate specific kinetics, *Process Biochem.* **36** (2001) 875–884, doi: [https://doi.org/10.1016/S0032-9592\(00\)00285-5](https://doi.org/10.1016/S0032-9592(00)00285-5).
25. *K. Nakasaki, J. Kato, T. Akiyama, H. Kubota*, A New Composting Model and Assessment of Optimum Operation for Effective Drying of Composting Material, *J. Ferment. Technol.* **65** (4) (1987) 441–447, doi: [https://doi.org/10.1016/0385-6380\(87\)90141-5](https://doi.org/10.1016/0385-6380(87)90141-5).

26. H. S. Fogler, *Elements of Chemical Reaction Engineering*, Prentice Hall USA, 2005.
27. C. Sheridan, J. Petersen, J. Rohwer, On modifying the Arrhenius equation to compensate for temperature changes for reactions within biological systems, *Water SA* **38** (1) (2012) 149–151, doi: <https://doi.org/10.4314/wsa.v38i1.18>.
28. D. W. Marquardt, An Algorithm for least Squares Estimation of Nonlinear Parameters, *J. Soc. Ind. Appl. Math.* **11** (1963) 431–441, doi: <https://doi.org/10.1137/0111030>.
29. H. Gavin, The Levenberg-Marquardt method for nonlinear least squares curve-fitting problems, Department of Civil and Environmental Engineering, Duke University, 2019, url: <https://msulaiman.org/onewebmedia/LM%20Method%20matlab%20codes%20and%20implementation.pdf>
30. L. F. Shampine, M. W. Reichelt, The Matlab Ode Suite, *Siam J. Sci. Comp.* **18** (1) (1997) 1–22, doi: <https://doi.org/10.1137/S1064827594276424>.
31. W. H. Press, P. B. Flannery, S. A. Teukolsky, W. T. Vetterling, *Numerical Recipes, 2*, Cambridge University Press, Cambridge, 1992.
32. F. Solé-Mauri, J. Illa, A. Mag, F. Prenañeta-Boldú, X. Flotats, An integrated biochemical and physical model for the composting process, *Biores. Technol.* **98** (17) (2007) 3278–3293, doi: <https://doi.org/10.1016/j.biortech.2006.07.012>.
33. P. B. Woodford, In-vessel composting model with multiple substrate and microorganism types, Doctoral dissertation, Kansas State University This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors, 2009.
34. B. Xi, Z. Wei, H. Liu, Dynamic Simulation for Domestic Solid Waste Composting Processes, *J. Am. Sci.* **1** (1) (2005) 34–45.
35. H. V. M. Hamelers, Modeling composting kinetics: A review of approaches, *Reviews Environ. Sci. Biotechnol.* **3** (4) (2004) 331–342, doi: <https://doi.org/10.1007/s11157-004-2335-0>.
36. M. Sharara, S. Sadaka, Thermogravimetric analysis of swine manure solids obtained from farrowing, and growing-finisher farms, *J. Sustain. Bioen. Syst.* **4** (1) (2014) 75–86, doi: <https://doi.org/10.4236/jsbs.2014.41008>.
37. D. Kaplan, Teaching Stats for Data Science, *Am. Statistician.* **72** (2018) 89–96, doi: <https://doi.org/10.1080/00031305.2017.1398107>.
38. R. G. Sargent, Verification and validation of simulation models, In *Proceedings of the 2010 winter simulation conference, IEEE*, 2010, 166–183, doi: <https://doi.org/10.1109/WSC.2010.5679166>.
39. P. J. Roache, *Verification and validation in computational science and engineering*, Hermosa Publishers, Albuquerque, 1998.
40. W. L. Oberkampf, T. G. Trucano, Verification and validation benchmarks, *Nucl. Eng. Des.* **238** (3) (2008) 716–743, doi: <https://doi.org/10.1016/j.nucengdes.2007.02.032>.
41. F. Scholwin, W. Bidlingmaier, Fuzzyfying the composting process: a new model based control strategy as a device for achieving a high grade and consistent product quality, In P. Pullammanappallil, A. McComb, L. F. Diaz, W. Bidlingmaier (Eds.): *Proceedings of the Fourth International Conference of ORBIT Association on Biological Processing of Organics: Advances for a Sustainable Society*, 2003 Australia, Orbit Association, Germany, 2003, pp.739–751.
42. J. Denes, A. Tremier, S. Menasseri-Aubry, C. Walter, L. Grateau, S. Barrington, Numerical simulation of organic waste aerobic biodegradation: A new way to correlate respiration kinetics and organic matter fractionation, *J. Waste Manage.* **36** (2015) 44–56, doi: <https://doi.org/10.1016/j.wasman.2014.11.013>.
43. P. Courvoisier, Mathematical modelling of composting processes using finite element method, Doctoral dissertation, McGill University Library, 2011.
44. F. N. Alkoaik, A. M. Abdel-Ghany, M. A. Rashwan, R. B. Fulleros, M. N. Ibrahim, Energy analysis of a rotary drum bioreactor for composting tomato plant residues, *Energies* **11** (2) (2018) 449, doi: <https://doi.org/10.3390/en11020449>.
45. H. B. Zhou, T. B. Chen, D. Gao, G. D. Zheng, J. Chen, T. H. Pan, R. Y. Gu, Simulation of water removal process and optimization of aeration strategy in sewage sludge composting, *Biores. Technol.* **171** (2014) 452–460, doi: <https://doi.org/10.1016/j.biortech.2014.07.006>.
46. D. S. Kim, J. O. Kim, J. J. Lee, Aerobic composting performance and simulation of mixed sludges, *Bioproc. Eng.* **22** (2000) 533–537, doi: <https://doi.org/10.1007/s004499900102>.
47. L. F. Diaz, G. M. Savage, L. L. Eggerth, A. Chiuementi, Systems used in composting, *J. Waste Manage.* **8** (2007) 67–87, doi: [https://doi.org/10.1016/S1478-7482\(07\)80008-X](https://doi.org/10.1016/S1478-7482(07)80008-X).
48. Y. Zhang, G. Lashermes, S. Houot, J. Doublet, J. P. Steyer, Y. G. Zhu, P. Garnier, Modelling of organic matter dynamics during the composting process, *Waste Manage.* **32** (1) (2012) 19–30, doi: <https://doi.org/10.1016/j.wasman.2011.09.008>.
49. R. Kulcu, New kinetic modelling parameters for composting process, *J. Mater. Cycles Waste Manage.* **18** (4) (2016) 734–741, doi: <https://doi.org/10.1007/s10163-015-0376-9>.
50. Z. Li, H. Lu, L. Ren, L. He, Experimental and modeling approaches for food waste composting: A review, *Chemosphere* **93** (7) (2013) 1247–1257, doi: <https://doi.org/10.1016/j.chemosphere.2013.06.064>.
51. J. Zhang, D. Gao, T. B. Chen, G. D. Zheng, J. C. Jun, C. Ma, S. Guo, W. Du, Simulation of substrate degradation in composting of sewage sludge, *Waste Manage.* **30** (2010) 1931–1938, doi: <https://doi.org/10.1016/j.wasman.2010.04.004>.
52. E. Papaćanin, Local and global sensitivity analysis of model parameters for composting process, *Technologica Acta* **11** (2) (2019) 9–16, doi: <https://doi.org/10.5281/zenodo.2563055>.

## SAŽETAK

### Procjena kinetičkih parametara i evaluacija modela procesa kompostiranja organske frakcije miješanog komunalnog otpada

*Edisa Papračanin*

Postupak aerobne biorazgradnje zanimljiv je za numerička istraživanja da bi se postigla bolja učinkovitost postupka, što se odražava u većoj brzini razgradnje organske tvari. Cilj ovog istraživanja bio je procijeniti kinetičke parametre u dinamičkom modelu koji opisuje proces aerobne biorazgradnje organske frakcije komunalnog krutog otpada s različitim dodatcima s inženjerskog aspekta. Predstavljeni matematički model zasnovan na pojavama prijenosa topline i mase dinamički je model sustava plin–tekućina–krutina. U svrhu optimizacije i simulacije postupka izveden je jedan pokus u tri reaktorska sustava sa smjesama različitog početnog sastava. Eksperimentalni podatci dobiveni iz jednog reaktora upotrijebljeni su za procjenu kinetičkih parametara modela, a podatci iz preostala dva reaktora upotrijebljeni su za provjeru i procjenu dinamičkog modela koji izvodi simulaciju. Detaljna statistička analiza pokazala je uske vrijednosti 95 %-tnog intervala pouzdanosti, što ukazuje na odgovarajuću točnost procjene parametara. Bolje slaganje podataka postignuto je u reaktoru s manjim udjelom dodataka, a najpreciznije predviđena varijabla je konverzija organske tvari. Analiza osjetljivosti parametara pokazala je da su najosjetljiviji red reakcije  $n$  i energija aktivacije  $E$ . Sveukupno, primjena ovog modela s procijenjenim kinetičkim parametrima u aerobnom procesu biorazgradnje pruža alat za predviđanje najvažnijih procesnih varijabli ( $SD = 0,3378$ ).

#### Ključne riječi

*Matematičko modeliranje, kinetički parametri, procjena modela, analiza osjetljivosti, aerobna biorazgradnja, OFMSW, otpadni kvasac, kiselgur*

*Katedra za kemijsko inženjerstvo, Tehnološki fakultet, Univerzitet u Tuzli, Urfeta Vejzagića 8, Bosna i Hercegovina*

*Izvorni znanstveni rad  
Prispjelo 6. srpnja 2021.  
Prihvaćeno 15. listopada 2021.*