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Application of validated mathematical model of composting process for study the effect of air flow rate on process performance

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Abstract

The objectives of this study were to develop and validate the mathematical model (kinetic and reactor model) of composting process, as well to used validated model in order investigate the effects of the air flow rate on organic matter conversion, carbon dioxide concentration and mixture temperature. The mathematical model incorporated two microbial populations that metabolized composting material which was split into two different fractions according to its degradability (easily-degradable and hardly-degradable). Comparisons of simulation and experimental results for five dynamic state variables demonstrated that the model has very good predictions of the composting process. Simulations with validated model showed that among three dynamic state variables (organic matter conversion, carbon dioxide concentration, mixture temperature), carbon dioxide concentration is the most sensitive while organic matter conversion is the least sensitive to the change of air flow rate.

1. INTRODUCTION

Composting can be defined as the aerobic microbiological decomposition of organic matter, to produce a stable, pasteurized product that is beneficial to apply to soil and plants [1]. During the composting process, the biodegradable organic compounds are broken down whereas part of the remaining organic material is converted into humic-like substances [2]. This process consumes oxygen and emits carbon dioxide, water vapor and heat resulting in a volume reduction of the waste and pathogen destruction when a good control is performed [3].

Growth of biomass is described as complex kinetics, usually Monod type, in regard to substrate [4-7] and oxygen [4]. Oxygen is necessary for microbial activity because the composting is aerobic process. Ventilation and supplying compost mass with oxygen can be carried out inverting the mass, convection air flow and mechanical ventilation. Passive ventilation convection is highly dependent on the porosity of the compost mass. A lack of oxygen results in the decay process. Oxygen consumption during composting depends on the humidity, which significantly affects the microbial activity.

The main influencing factors for composting process are pH, moisture content, C/N ratio, oxygen, temperature, etc. The mathematical formulation of the physical and biological laws that govern the composting process was described in the reference [8]. This model of the composting ecosystem includes mass transfer, heat transfer, and organic matter conversion into CO_2 and humic substances. There is a lack of uniformity among current models for composting process [11]. Only a few composting models are based on microbial kinetics. Some models consider only one substrate and only one microbial population [5, 9], while the other models consider several substrates and several microbial populations [8, 10]. Taking into account the disadvantages of these models, there is a need to develop a new model that can help to improve prediction and optimization of the process performance.

The first objective of this study is to develop the mathematical model (kinetic model and reactor model) of the composting process based on microbial kinetics. The case study is the mixture of poultry manure and wheat straw. The model will be validated by comparisons of the simulation data and experimental data obtained in the laboratory reactor. Comparison of simulation and experimental results will show if model is efficient for further analysis and optimization of process. The second objective of this study is to use the validated model in order to investigate the effects of the air flow rate on organic matter conversion, carbon dioxide concentration and mixture temperature. Based on the maximum values of these variables, the optimum air flow rate can be determined.

2. MATERIALS AND METHODS

2.1. Mathematical model, constants/parameters and solution method

The growth rate of microbial population is described by [10]:

$$\frac{dm_{x,i}}{dt} = \mu_i \cdot m_{x,i} - k_{d,i} \cdot m_{x,i} \tag{1}$$

where: mx,i - mass of microbial population i (kg), μi - specific growth rate of microbial population i (h^{-1}), - specific death rate of microbial population i (h^{-1}), t - time (h), i - index for different fraction of substrate (1 = easily degradable fraction, 2 = hardly degradable fraction).

The degradation rate of substrate fraction i is given by [2]:

$$\frac{dm_{S,i}}{dt} = -\frac{1}{Y_{X_i/S_i}} \cdot \left(\frac{dm_{x,i}}{dt}\right) + \beta_i \cdot m_{x,i} \tag{2}$$

where: - yield coefficient, cells produced/fraction consumed (kg kg^{-1}), βi - microbial maintenance coefficient of microbial population i (kg $kg^{-1}h^{-1}$).

The specific growth of microbial population i can be calculated as follows:

$$\mu_i = \mu_{\max,i} \cdot \left(\frac{m_{OM,i}}{K_{S,i} + m_{OM,i}}\right) \cdot k_{O_2} \cdot k_T \cdot k_{H_2O} \tag{3}$$

where: - maximum specific growth of microbial population i (h^{-1}), - saturation constant of microbial population i (kg kg^{-1}), $m_{OM,i}$ - organic matter content in fraction i (-), - correction factor for oxygen (-), kT - correction factor for temperature (-), - correction factor for moisture content.

The microbial maintenance coefficient of microbial population i can be written as [5]:

$$\beta_i = \beta_{\max,i} \cdot \left(\frac{m_{OM,i}}{K_{S,i} + m_{OM,i}}\right) \cdot k_{O_2} \cdot k_T \cdot k_{H_2O} \tag{4}$$

where: $\beta_{max,i}$ - maximum microbial maintenance coefficient of microbial population i (kg kg^{-1}).

The mass fraction of organic matter content i (wt %) is calculated as follows:

$$w_i = \frac{m_{S,i}}{m_{S,1} + m_{S,2} + m_{IM}} \cdot 100 \tag{5}$$

where: m_{IM} - mass of inorganic matter (kg).

Correction factor for oxygen is described by the following equation [6]:

$$k_{O_2} = \frac{c_{O_2}}{k_{O_2(0)} \cdot (K_{O_2} + c_{O_2})} \tag{6}$$

where: - correction factor for oxygen concentration in atmospheric air (20.95 vol %), - half velocity constant for oxygen (vol %), - volume fraction of oxygen in exhaust air (vol %).

The volume fraction of oxygen in exhaust air (vol %) can be calculated as follows [12]:

$$\phi_{O_2} = \frac{m_{O_2}}{\rho_{O_2} \cdot V} \cdot 100 \tag{7}$$

where: V - volume of composting mixture (m^3), - mass of oxygen (kg), - oxygen density (kg m^{-3}). The volume of mixture is given by:

$$V = 0.85 \cdot V_R \cdot \varepsilon \tag{8}$$

where: is VR - reactor volume (m^3), - porosity (-).

The oxygen density is calculated by the following equation (based on data [13]):

$$\rho_{O_2} = 1.4012 - 0.0041 \cdot T \tag{9}$$

The equation (9) is valid in the range between 0-70°C. Correction factor for temperature is described by the following equation [12]:

$$k_T = \frac{T \cdot (80 - T)}{1600} \qquad 0 < T < 80°C$$
$$k_T = \frac{T \cdot (60 - T)}{20 \cdot (80 - T)} \qquad 60°C < T < 80°C \tag{10}$$

Correction factor for moisture content is described by the following equation [14]:

$$k_{H_2O} = \frac{1}{e^{(-17.684 \cdot w_w + 7.0622)} + 1} \tag{11}$$

where: ww - mass fraction of water in the mixture (-).

The mass fraction of water in the mixture (wt %) is calculated as follows:

$$w_w = \frac{m_w}{m_{S,1} + m_{S,2} + m_{IM} + m_w} \cdot 100 \tag{12}$$

where: mw - mass of water in composting mixture (kg).

Mass balance of oxygen is derived as follows:

$$\frac{dm_{O_2}}{dt} = -Y_{O_2/S} \cdot \left(\frac{dm_{S,1}}{dt} + \frac{dm_{S,2}}{dt}\right) + \frac{q_{air}}{V} \cdot \left(m_{O_2,,in} - m_{O_2,out}\right) \tag{13}$$

where: $Y_{O_2/S}$ - oxygen yield coefficient, O_2 consumed / substrate consumed (kg kg^{-1}), q_{air} - air flow rate (m^3 h^{-1}), $m_{O_2,,in}$ - inlet oxygen mass (kg), $m_{O_2,,out}$ - outlet oxygen mass (kg).

Mass balance of carbon dioxide is derived as follows:

$$\frac{dm_{CO_2}}{dt} = Y_{CO_2/S} \cdot \left(\frac{dm_{S,1}}{dt} + \frac{dm_{S,2}}{dt}\right) + \frac{q_{air}}{V} \cdot \left(m_{CO_2,,in} - m_{CO_2,,out}\right) \tag{14}$$

where: - carbon dioxide yield coefficient, CO_2 produced/substrate consumed (kg kg^{-1}), - inlet carbon dioxide (kg), - outlet carbon dioxide mass (kg).

The volume fraction of carbon dioxide in exhaust air (vol %) can be calculated as follows:

$$\phi_{CO_2} = \frac{m_{CO_2}}{\rho_{CO_2} \cdot V} \cdot 100 \tag{15}$$

The carbon dioxide density is calculated by the following equation (based on data [13]):

$$\rho_{CO_2} = 1.9376 - 0.0057 \cdot T \tag{16}$$

Mass balance of water is derived as follows:

$$\frac{dm_w}{dt} = -Y_{W/S} \cdot \left(\frac{dm_{S,1}}{dt} + \frac{dm_{S,2}}{dt}\right) - q_{air} \cdot \rho_a \cdot \left(r_{air,in} - r_{air,out}\right) \tag{17}$$

where: - water yield coefficient, H_2O produced/substrate consumed (kg kg^{-1}), - density of dry air (kg m^{-3}), rair,in - humidity ratio of inlet air (kg kg^{-1}), rair,out - humidity ratio of outlet air (kg kg^{-1}).

The density of dry air is calculated by the following equation (based on data [13]):

$$\rho_a = 1.271 - 0.0035 \cdot T \tag{18}$$

The humidity ratios of inlet and outlet air are calculated by the following equation (based on data [13]):

$$r_{air} = 0.1158 - 0.0072 \cdot T + 0.0001 \cdot T^2 \tag{19}$$

The equations (18-19) are valid in the range between 20-70°C. Heat balance is derived as follows:

$$\frac{dT}{dt} = \frac{H_{R,1} \cdot \frac{dm_{S,1}}{dt} + H_{R,1} \cdot \frac{dm_{S,2}}{dt} - q_{air} \cdot \rho_a \cdot (h_{in} - h_{out}) - \dot{Q}}{c_{P,w} \cdot m_w + c_{P,IM} \cdot m_{IM} + c_{P,S1} \cdot m_{S,1} + c_{P,S2} m_{S,2}} \tag{20}$$

where: T - temperature of composting mixture (°C), HR - heat of reaction, heat produced/substrate consumed (J kg^{-1}), - enthalpy of inlet air (J kg^{-1}), - enthalpy of outlet air (J kg^{-1}), - heat loss by conduction through the reactor wall (J h^{-1}), $c_{P,w}$ - specific heat capacity of water (J kg^{-1}°$C^{-1)}$, $c_{P,IM}$ - specific heat capacity of inorganic matter (J kg^{-1}°C^{-1}), $c_{P,S}$ - specific heat capacity of substrate (J kg^{-1} °C^{-1}). The enthalpies of inlet and outlet air are calculated by the following equation (based on data [13]):

$$h = 17844 + 1007.2 \cdot T \tag{21}$$

The equation (21) is valid in the range between 20-70°C. The heat loss by conduction through the reactor wall is given as:

$$\dot{Q} = U \cdot A \cdot (T - T_a) \tag{22}$$

where: U - overall heat transfer coefficient (J $h^{-1}m^{-2}$°C^{-1}), A - heat transfer area (m^2), Ta - ambient temperature.
The specific heat capacities are calculated by the following equation [15]:

$$c_p = 1.48 - 0.64 \cdot w_{IM} + 4.18 \cdot w_w \tag{23}$$

where: w_{IM} - inorganic matter content (-), ww - dry-basis moisture content (-).
With the assumption about known initial elementary composition of the substrate, the degradation of organic part of the substrate is presented by the equation [14]:

$$C_aH_bO_cN_d + \left(\frac{4a+b-2c-3d}{4}\right)O_2 \rightarrow aCO_2 + \frac{b-3d}{2}H_2O + dNH_3 \tag{24}$$

where: a, b, c and d are indices which describe the molar fraction of carbon, hydrogen, oxygen and nitrogen, respectively. The values in the equation (24) are calculated using the known molecular formula of the substrate. Physical, thermodynamic and stoichiometric constants/parameters were measured from the experiment, calculated from literature data and/or taken original or adjusted data from available literature [5,7,12,14-18]: $m_{X,1(0)}$ = 0.01 kg, $m_{X,2(0)}$ = 0.0006 kg, $\mu_{max,1}$ = 0.260 h^{-1}, $\mu_{max,2}$ = 0.13 $^{h-1}$, $k_{d,1}$ = 0.03 h^{-1}, $k_{d,2}$ = 0.05 h^{-1}, $\beta_{max,1}$ = 0.48 kg $kg^{-1}h^{-1}$, $\beta_{max,2}$ = 0.38 kg $kg^{-1}h^{-1}$, Y_{X_1/S_1} = 0.35 kg $kg^{-1}h^{-1}$, Y_{X_2/S_2} = 0.35 kg_{X_2} $kg_{S_2}^{-1}$, $K_{S,1}$ = 0.5 kg kg^{-1}, $K_{S,2}$ = 0.5 kg kg^{-1}, $k_{O_2(0)}$ = 0.96189, K_{O_2} = 0.75 %, Y_{O_2/S_1} = 1.228 kg kg^{-1}, Y_{O_2/S_2} = 1.296 kg kg^{-1}, Y_{CO_2/S_1} = 1.743 kg kg^{-1}, Y_{CO_2/S_2} = 1.793 kg kg^{-1}, Y_{H_2O/S_1} = 0.400 kg kg^{-1}, Y_{H_2O/S_2} = 0.495 kg kg^{-1}, $H_{R,1}$ = 15244 J kg^{-1}, $H_{R,2}$ = 16722 J kg^{-1}, V_R = 0.032 m^3, ϕ = 0.85, ε = 0.4, q_{air} = 0.18 m^3h^{-1}, T_a = 21.4°C, $c_{P,w}$ = 4200 J kg^{-1} °C^{-1}, $c_{P,IM}$ = 840 J kg^{-1} °C^{-1}, $c_{P,S1}$ = 1340 J kg^{-1} °C^{-1}, $c_{P,S2}$ = 1403 J kg^{-1} °C^{-1}, UA = 4546.8 J h^{-1} °C^{-1}.
The mathematical model consists of eight ordinary differential equations of the first order and corresponding equations. The Runge-Kutta-Fehlberg method was applied in order to obtain a numerical solution of the model. The model was implemented in the numerical software package POLYMATH 6.0 [19].

2.2. Experimental materials and experimental methods

Moisture content, organic matter content (dry basis), pH and electrical conductivity for poultry manure are 72.59 %, 78.07 %, 8.17 and 3.34 dS m^{-1}, respectively. Moisture content, organic matter content, pH and electrical conductivity for wheat straw are 10.87 %, 87.91%, 7.18 and 1.91 dS m^{-1}, respectively. Moisture content, organic matter content, pH and electrical conductivity for composting mixture (poultry 83%, straw 27%, on dry basis) are 69.11 %, 80.22 %, 7.40 and 3.10 dS m^{-1}, respectively. The experiment was conducted using a composting reactor made of polyethylene, insulated with a layer of polyethylene foam. Other details about the composting reactor can be found in literature [15]. The reactor was aerated using an air compressor with air flow rate of 0.9 L min^{-1} kg^{-1} (measured by air flow meter). Temperature was measured at 15-min intervals using the thermocouple type T and the acquisition module. Mixing of composting mixtures was performed several times per day. The samples were taken from the top, middle and bottom of the mixture in order to obtain representative samples. The moisture content and the organic matter content of the sample were analyzed by standard methods [20]. The following equation [21] was used to calculate the organic matter conversion, X_{OM} (%):

$$X_{OM} = \frac{\left\{\left[w_{OM,m} - w_{OM,p}\right] \cdot 100\right\}}{w_{OM,m} \cdot \left[100 - w_{OM,p}\right]} \cdot 100 \tag{25}$$

where: $w_{OM,m}$ – mass fraction of organic matter content at the beginning of the process (mass %) and $w_{OM,p}$ – mass fraction of organic matter content at each sampling (mass %). Oxygen and carbon dioxide concentration were determined by an Orsat analyzer.

3. RESULTS AND DISCUSSION

The comparisons between the model and experimental data are shown in Figures 1-5. The deviations between the model and experimental results for temperature occurred mostly during the cooling phase of the process (Figure 1). Mature compost and poultry manure added to the composting mixture made the process begin within a few hours because microorganisms adapted quickly to a new environment. The maximum simulated temperature was 66.9°C, whereas the maximum experimental temperature was 64.8°C. After reaching a thermophilic peak, cooling of the substrate started and the simulation results showed faster cooling in comparison to the experimental data. This is because each of the reactions (which normally occur during the biodegradation process) was not taken into account during the modeling. The limited precision of the thermodynamic parameters might have also contributed to the deviations. As commonly done in other studies, a single heat yield coefficient was used. A slight increase in temperature after the tenth day of the process indicates the beginning of the second phase with degradation of hardly degradable organic fractions. It seems that the model is particularly sensitive to the value of overall heat transfer coefficient, so it should be measured experimentally (not calculated). The agreement between the model predictions and experimental data for carbon dioxide concentration is shown in Figure 2. The deviations that occurred between 72nd and 120th hour can be explained by decreased microbial activity during this time interval as well as by daily opening of the reactor for sampling. The maximum and mean difference between the model and experimental results for carbon dioxide concentration are similar to the results in the reference [8]. The agreement between the model and experimental data for oxygen concentration is shown in Figure 3. Oxygen concentration has declined sharply in the first 72 h. The fluctuation of oxygen concentration is related to microbial activities during the composting process. The results in Figure 3 showed that the minimum of simulated oxygen concentration (12.96%) is close to the experimental value (12.30%). Oxygen concentrations obtained by the model and experiment showed excellent agreement during the whole process. Some small deviations between the model and experimental data are probably caused by a decomposition of the hardly degradable fraction, by an excessive aeration, and by the fact that oxygen concentration was measured in exhaust air (not in composting material). Oxygen concentration is measured at the exit of reactor and not in the material, and this fact also contributes to deviation between simulated and experimental data. Deviations can be also explained with variations in the rate of mass transfer between liquid and gas phases, due to drying of substrates [10]. Comparison of experimental and simulated data for organic matter content showed very good agreement (Figure 4). Some small deviations were noticed between the third and the ninth day. The simulated organic matter content was lower than the experimental values between the third and the ninth day. Observed deviations can be explained by transition between the first and the second phase of the process where the most of the easily degradable fraction was decomposed due to high process rate, while a small part of the hardly degradable fraction was decomposed due to low process rate.Comparison of model and experimental results for the moisture content showed that the model generally follows the profile of moisture content during the experiment (Figure 5). The deviations that occurred are most likely a result of material mixing. The simulation and experimental results of the final moisture content were 55.89% and 59.43%, respectively. The reason why the experimental results were higher than the simulation results is due to the fact that some amount of water was condensed on the inside of the reactor's lid and returned to composting mass. This agrees with the findings in the reference [6].

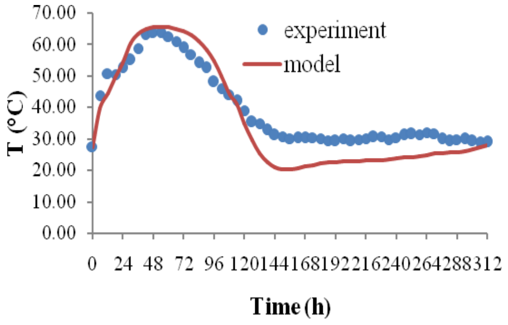

Figure 1. Comparison of model and experimental results for mixture temperature

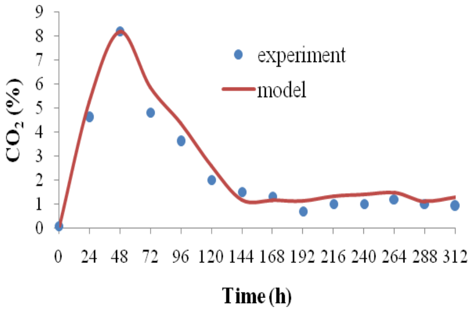

Figure 2. Comparison of model and experimental results for carbon dioxide concentration

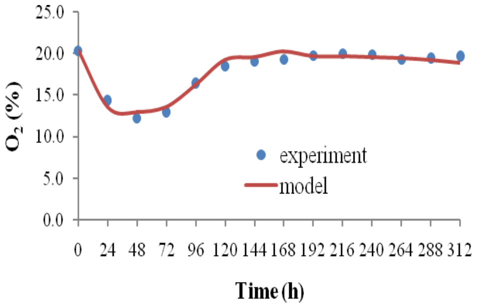

Figure 3. Comparison of model and experimental results for oxygen concentration

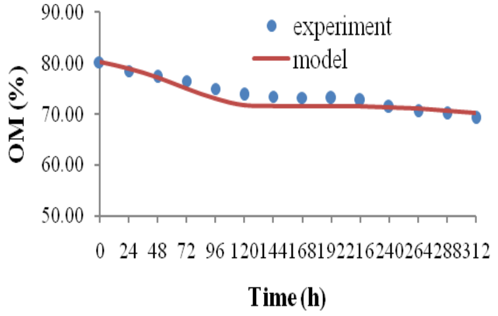

Figure 4. Comparison of model and experimental results for organic matter content

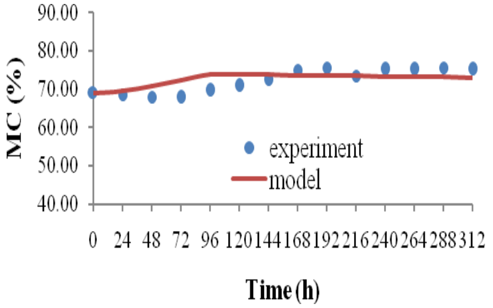

Figure 5. Comparison of model and experimental results for moisture content

Maximum and mean differences between simulation and experimental results for are shown in Table 1. The aeration rate affects microbial activity, substrate degradation rate as well as temperature variation in the composting process. Too little aeration can lead to anaerobic conditions, however, too much aeration can lead to excessive cooling, preventing the thermophilic conditions required for optimum rates of decomposition. Therefore, it is crucial to control the air flow rate. The influence of air flow rate on organic matter conversion, carbon dioxide concentration and mixture temperature are given in Figures 2-4. Among three dynamic state variables, carbon dioxide concentration is the most sensitive while organic matter conversion is the least sensitive to the change of air flow rate.

Table 1. Maximum and mean differences between simulation and experimental results for temperature, CO2 concentration, O2 concentration, organic matter content and moisture content

Reference	Temperature (°C)			CO_2 (%)		O_2 (%)		OM (%)		MC (%)	
	Max.	Mean	Peak	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean
[9]	13.3	4.1	3.3	8.86	1.77	-	-	-	-	-	-
[22]	16.5	4.2	0.5	-	-	0.11	0.02	0.14	0.05	-	-
This paper	14.19	6.03	1.66	1.57	0.43	1.0	0.45	2.61	1.23	6.17	1.78

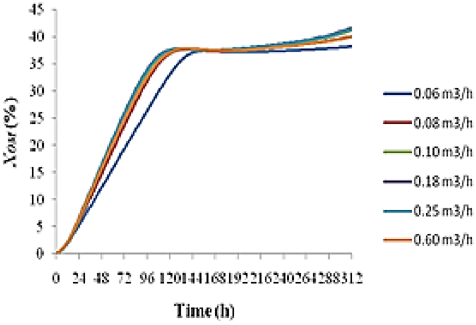

Figure 6. Profiles of organic matter conversion with air flow rates

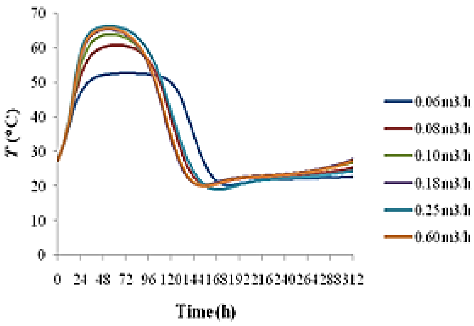

Figure 8. Profiles of temperature of mixture with air flow rates

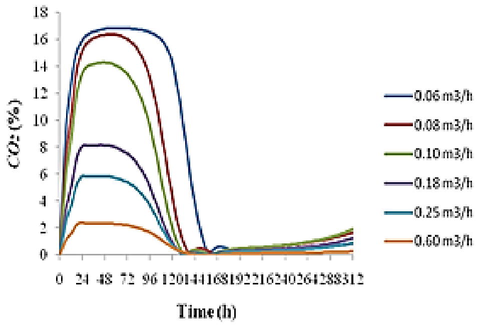

Figure 7. Profiles of carbon dioxide concentration with air flow rates

The values of maximum organic matter conversion, maximum concentration of carbon dioxide and maximum temperature of mixture for different values of air flow rates are given in Table 2.

Table 2. Effects of air flow rates on maximum conversion of organic matter, maximum concentration of carbon dioxide and maximum temperature of mixture

Air flow rate (m^3 h^{-1})	Maximum conversion of organic matter (%)	Maximum concentration of carbon dioxide (%)	Maximum temperature of mixture (°C)
0.06	38.26	16.87	52.77
0.08	40.16	16.39	60.92
0.10	41.24	14.30	64.04
0.18	41.70	8.17	65.51
0.25	41.49	5.86	66.45
0.60	40.04	2.39	65.78

Results showed that air flow rate has strong effects on both organic matter conversion and the mixture temperature up to 0.08-0.10 m^3 h^{-1}. Above these values, changes of organic matter conversion and the mixture temperature are not significant. Maximum value of final organic matter conversion (41.70%) was obtained with air flow rate of 0.18 m^3 h^{-1}. Above this value of air flow rate the maximum value of final organic matter conversion decreases slowly. The maximum mixture temperature of 65.51°C, obtained with air flow rate of 0.18 m^3 h^{-1} is not much lower than mixture temperature of 66.45°C, obtained with air flow rate of 0.25 m^3 h^{-1}. Therefore, air flow rate of 0.18 m^3 h^{-1} (or 0.97 l min^{-1} kg_{OM}^{-1}) should be taken as an optimum, especially if taking into account the economical aspect (i.e. a lower energy costs for aeration). This value of air flow rate is similar to the values in the references [10, 23].

4. CONCLUSIONS

1. Kinetic model (Monod microbial kinetics with correction factors) and reactor model (mass balances, heat balance, stoichiometry) were developed for the composting process of the mixture of poultry manure and wheat straw.
2. Comparison of simulation results and experimental data for five dynamic state variables demonstrated that the model has very good predictions of the composting process.
3. Simulations with validated model showed that among three dynamic state variables (organic matter conversion, carbon dioxide concentration, mixture temperature), carbon dioxide concentration is the most sensitive while organic matter conversion is the least sensitive to the change of air flow rate.
4. According to simulation results, the optimum value for air flow rate is 0.18 m3 h-1 (0.97 l min-1 kgOM-1).
5. Future work will be oriented to model modification as well to application of the model on determination of the optimal values of other inlet process parameters and optimal profiles of dynamic state variables.

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