



Particle-scale modeling of oxygen uptake rate during pig manure–wheat straw composting: A new approach that considers surface convection



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ABSTRACT

A new oxygen uptake rate (*OUR*) model that considers surface convection between composting materials and gas (Q_{surf}) has been developed for the composting of pig manure and wheat straw. This was found to provide a more precise simulation of maximum *OUR*, which was especially true for the thermophilic phase due to a significant increase in the temperature difference between the composting materials and gas in the bottom part of reactor. Heat contribution analyses indicated that Q_{surf} heat loss represents 8.86% of the total, implying that Q_{surf} needs only be quantified for large-scale composting systems, and so can be omitted with systems in which there is a small exchange-surface of composting materials. Sensitivity analyses suggested that expanding the exchange-surface could protect microorganisms from overheating and be beneficial to degradation. These findings provide a theoretical basis for improving simulation precision, while also further elucidating the heat transfer mechanism during composting.

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1. Introduction

Composting is an example of a sustainable biodegradation practice that is capable of converting solid waste into humified end-products that are free of pathogens [1]. However, low intensity aeration during this process can impair microbial activity, leading to incomplete degradation of organic matter and the emission of environmentally hazardous gases such as methane and nitrous oxide. In contrast, high intensity aeration increases energy costs and can overcool the composting materials, which is detrimental to the killing of pathogens [2]. Designing a strategy to more accurately meet the oxygen (O_2) demand of microorganisms therefore has the potential to increase degradation efficiency and compost quality, while also reducing greenhouse gas emissions and operating costs [3].

Oxygen uptake rate (*OUR*) is a fundamental indicator of the actual O_2 demand of microorganisms and the overall degree of degradation [4–6]. Mathematical modeling and simulation of *OUR* can therefore provide practical insight into the mechanism of composting and theoretical guidance for optimization. One particle-scale *OUR* model has attracted particular attention, as it considers the specific microbial kinetics of different substrate conditions [7–10]. This model divides the composting mixture into

two particle groups (large and small), and then applies the Monod equation and first-order hydrolysis kinetics to each; the *OUR* of the overall composting mixture being determined from an integration of the two groups. Using this model, satisfactory results have been achieved in the simulation of composting chicken manure [7,8], horticultural waste [9] and pig manure–wheat straw [10].

When using the Monod equation there is a need to assess the influence of temperature on the microbial kinetics, as these are easily affected by the composting temperature (T) [11]. Lin et al. [9] have used a regression of experimental T data to describe this dependence during the composting of horticultural wastes, but their empirical equations lack a theoretical rationale. The Arrhenius equation has also been used for temperature correction of microbial kinetic parameters [11,12], but as this equation is mainly used for correcting the rate constants of chemical reactions the results are not always satisfactory. The cardinal temperature equation has also been widely used recently to calculate the temperature dependence of Monod parameters by considering the influence of three cardinal temperatures on the growth of microorganisms [10,13,14]. As there is a clear physical meaning to these parameters, it provides a sound theoretical basis for temperature correction.

Ge et al. [10] have previously incorporated the cardinal temperature equation into a particle-scale *OUR* model, with an energy balance being constructed to acquire simulated values of T to feed into the temperature correction equation. Heat fluxes in this energy balance included heat generation from bio-oxidation

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(Q_{bio}), the sensible heat of the input and output streams (Q_{sens}), the latent heat of evaporation (Q_{evap}), and heat loss through the reactor wall (Q_{wall}). However, research into the composting of poultry manure and wood shavings [15], chicken manure and vegetable wastes [16], and pig slaughterhouse sludge [17] have suggested that in addition to these heat fluxes one must also consider the surface convection between composting materials and gas in the bottom/upper parts of the reactor (Q_{surf}). The value of Q_{surf} and Q_{wall} are often combined into one heat flux, which can be calculated from the constant overall heat transfer coefficient through regression of experimental data. Nevertheless, Mudhoo and Mohee [16] have shown that the overall heat transfer coefficient changes extensively during composting, and therefore cannot be considered a constant. This finding demonstrates the necessity of determining Q_{surf} separately, with de Guardia et al. [17] finding that Q_{surf} heat loss accounts for about 50% of the total heat generation. The development of a particle-scale OUR model that characterizes Q_{surf} would therefore greatly assist in improving simulation precision and serve to further our understanding of the microbial kinetics and heat transfer mechanism of composting.

Using a particle-scale OUR model, this study considers Q_{surf} as part of the energy balance equation to simulate the evolution of T and provide the cardinal temperature equation to correct the microbial kinetic parameters of pig manure–wheat straw composting. Heat contribution and sensitivity analyses are used to assess the effectiveness of characterizing Q_{surf} on the model accuracy and the evolution of T and OUR, with the aim of providing future model developers with an insight into whether they should consider Q_{surf} or not.

2. Model description

2.1. Main state variables and assumptions

The main state variables include the aerobic layer thickness (L_p), composting temperature (T), gas temperature in the bottom part of the reactor (T_{bot}), and gas temperature in the upper part of the reactor (T_{up}). The model assumptions are listed as follows. (1) Since the composting system used in this research is laboratory-scale, a uniform temperature in the whole mass was assumed. (2) As straw biodegrades relatively slowly [5,18,19], pig manure was considered to be the major reactant; thus, the chemical properties and particle characteristics of pig manure were investigated. (3) Since heat is mainly released by aerobic microbial metabolism [2,11], Q_{bio} was assumed to be proportional to OUR. (4) The proportion of heat radiation was negligible for the laboratory-scale reactor [15].

2.2. OUR model incorporating Q_{surf}

The composting mixture is first divided into large and small particle groups. The former is defined by a particle radius (L) that lies between the switch radius (L_s) and maximum particle radius (L_{max}), for which soluble substrate (S_s) is considered adequate, the growth rate of aerobic microbes (R_{X_a}) follows the Monod equation, and OUR is considered proportional to R_{X_a} . The small particles ($0 < L < L_s$) are considered depleted of substrate, and so both R_{X_a} and OUR are dependent on the production rate of S_s by hydrolysis [i.e., the hydrolysis rate (R_{S_i})]. The OUR evolution of the composting mixture is simply an integration of the two particle groups [7–10]:

$$\text{OUR} = \int_{L_s}^{L_{\text{max}}} G(L, \lambda, \gamma) \frac{L_p}{L} \cdot \frac{1}{Y_{O_2}} R_{X_a} dL + \int_0^{L_s} G(L, \lambda, \gamma) \frac{1}{Y_{O_2}} Y_{S_s} R_{S_i} dL \quad (1)$$

where $G(L, \lambda, \gamma)$ is the probability density function of the gamma distribution (dimensionless), λ is the scale parameter (m^{-1}), γ is

the shape parameter (dimensionless), Y_{O_2} is the biomass yield on oxygen ($\text{mol C mol}^{-1} O_2$), Y_{S_s} is the biomass yield on soluble substrate ($\text{mol C mol}^{-1} C_{\text{man}}$), and man represents pig manure. According to the previous research of the particle-scale OUR model [7], R_{X_a} is proportional to the concentration of aerobic microbes (X_a):

$$R_{X_a} = \mu(T) \cdot X_a \quad (2)$$

where $\mu(T)$ is the corrected specific growth rate of aerobic microbes (h^{-1}). The relation between X_a and the maximum concentration of aerobic microbes (X_{max}) can be described as follows [7]:

$$X_a = \frac{X_{\text{max}}}{1 + e^{-\mu(T) \cdot (t - \Omega)}} \quad (3)$$

where t is the composting time (h), and Ω is the lag phase (h). The derivation process of Eq. (3) can be found in [Supplementary Material](#). R_{S_i} follows the first order kinetics:

$$R_{S_i} = k_h(T) S_{i,0} e^{-k_h(T)t} \quad (4)$$

where $k_h(T)$ is the corrected hydrolysis rate constant (h^{-1}), $S_{i,0}$ is the initial insoluble substrate concentration ($\text{mol C}_{\text{man}} \text{kg}^{-1}$), and VS represents the initial volatile solids.

The cardinal temperature equation used to determine the influence of temperature on $\mu(T)$ can be described as follows:

$$\mu(T) = \frac{\mu(T_r) \cdot (T - T_{\text{max}})(T - T_{\text{min}})^2}{(T_{\text{opt}} - T_{\text{min}})[(T_{\text{opt}} - T_{\text{min}})(T - T_{\text{opt}}) - (T_{\text{opt}} - T_{\text{max}})(T_{\text{opt}} + T_{\text{min}} - 2T)]} \quad (5)$$

where T_r is the reference temperature ($^{\circ}\text{C}$), $\mu(T_r)$ is the specific growth rate of the microorganisms at the reference temperature (h^{-1}), T_{max} is the maximum growth temperature ($^{\circ}\text{C}$), T_{min} is the minimum growth temperature ($^{\circ}\text{C}$), and T_{opt} is the optimal growth temperature ($^{\circ}\text{C}$).

The simulated values of T needed in Eq. (5) can be obtained by solving the energy balance equations for the aeration and non-aeration phases described by Eqs. (6) and (7), respectively:

$$\frac{dT}{dt} = \frac{1}{m_{\text{mix}} \cdot c_{\text{mix}}} (Q_{\text{bio}} - Q_{\text{sens}} - Q_{\text{evap}} - Q_{\text{wall}} - Q_{\text{surf}}) \quad (6)$$

$$\frac{dT}{dt} = \frac{1}{m_{\text{mix}} \cdot c_{\text{mix}}} (Q_{\text{bio}} - Q_{\text{wall}} - Q_{\text{surf}}) \quad (7)$$

where m and c are the mass (kg) and specific heat ($\text{kJ kg}^{-1} \text{ } ^{\circ}\text{C}^{-1}$) of the composting materials, respectively, and Q_{surf} is the sum of the surface convection between the composting materials and gas in the upper part (Q_{up}) and bottom (Q_{bot}) part of the reactor. Q_{bio} was assumed to be proportional to OUR, as heat is mainly released by aerobic microbial metabolism [2,11]:

$$Q_{\text{bio}} = h_{\text{bio}} m_{\text{om_mix}} \text{OUR} \quad (8)$$

where h_{bio} is the heat conversion factor ($\text{kJ mol}^{-1} O_2$), $m_{\text{om_mix}}$ is the initial mass of organic matter in composting materials (kg VS), and VS represents the initial volatile solids. Q_{sens} and Q_{evap} can be expressed as follows [7]:

$$Q_{\text{sens}} + Q_{\text{evap}} = Q m_{\text{om_mix}} \rho (H_{\text{out}} - H_{\text{in}}) \quad (9)$$

where Q is the aeration rate ($\text{m}^3 \text{kg}^{-1} \text{VS h}^{-1}$), ρ is the air density (kg m^{-3}), and H_{out} and H_{in} are the enthalpy of output and input gas, respectively (kJ kg^{-1}). Q_{wall} can be quantified as follows [20]:

$$Q_{\text{wall}} = U_{\text{wall}} A_{\text{wall}} (T - T_a) \quad (10)$$

where U_{wall} is the heat transfer coefficient between the wall of the reactor and the ambient environment ($\text{W m}^{-2} \text{ } ^{\circ}\text{C}^{-1}$), and A_{wall} is the heat transfer area of the reactor wall (m^2). The values of Q_{up} and Q_{bot} can be calculated as below [17,21]:

$$Q_{\text{up}} = U_{\text{surf}} A_{\text{surf}} (T - T_{\text{up}}) \quad (11)$$

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