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Validation of a new model for aerobic organic solids decomposition: simulations with substrate specific kinetics

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Abstract

This study is a synthesis of substrate specific kinetics and a mass and energy model to predict the process dynamics of the aerobic degradation of synthetic food waste (SFW). The model is validated against pilot scale experimental data obtained from two previous studies. In all the observations the model tended to over predict values of the state variables. The maximum rates of oxygen uptake, cumulative oxygen uptake, and the maximum process temperature were all over predicted. The sensitivity of the model to two key parameters, the specific O_2 uptake, γ_{O_2}, and the respiration quotient, β_r, was also investigated. It was noted that the smaller values of respiration quotient produced better estimates later in the process. The maximum rate of O_2 uptake was insensitive to changes in specific oxygen uptake rate at low aeration rates and more sensitive at high aeration rates. Discrepancies between the model predictions and actual data are explained by the violations of basic assumptions of homogeneous bed conditions. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Aerobic; Composting; Model; Kinetics; Simulation; Validation; High-solids

1. Introduction

Composting is a microbial process that decomposes organic wastes into a stable humic product. It is a complex process that involves a highly variable, heterogeneous substrate, and the metabolic activity of a diverse microbial population. In aerobic composting, air is forced through a high-solids organic matrix to support aerobic metabolic activities. The products of the metabolic activities are water, carbon dioxide, ammonia, and heat. Thus, composting is a complex bioprocess that involves many coupled physical and biological mechanisms. These coupled, and often nonlinear, mechanisms yield a broad spectrum of process behaviours that are challenging to analyze both empirically and theoretically. Mathematical modeling provides one approach for understanding the dynamic interactions between these coupled mechanisms, and provides a framework for rational process design.

The basic approach used to model composting processes is to couple empirically derived substrate degradation kinetics with mass and energy balances for the salient physical state variable such as temperature (T), moisture content (M), oxygen mass fraction (X_{O_2}), and humidity (H) [1–10]. Rates of substrate degradation, oxygen (O_2) uptake, or carbon dioxide (CO_2) evolution have been correlated with T, M and X_{O_2} to obtain empirical substrate degradation kinetics [1,6,11–13]. Richard et al. [13] evaluated the four most common models used to simulate the effect of temperature on microbial growth and found that the parameters obtained from the CTMI model were more consistent over the duration of the degradation process [1,6,14,15].

Mass and energy balances have been developed for the compost process and translated into a number of mathematical models [1–10]. All of these models assume that substrate degradation kinetics is a first order process where the rate constants are a function of the physical state variables. The major differences in these models are the assumptions regarding heat and mass transport mechanisms, and whether the process is modeled as a lumped parameter system (system of ordinary

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Table 1
Model parameters

Model parameter and units	Value	References
T_{max} (°C)	71.6	[20]
T_{min} (°C)	5	[20]
T_{opt} (°C)	58.6	[20]
$(R_{CO_2 opt})_{max}$ (CO_2/kg VS per day)	178	[20]
$R_{CO_2 slow}$ (CO_2/kg VS per day)	22	[20]
β_r (gO_2/gCO_2)	1	[20]
ΔH_{rxn} (kJ/kg)	16 000	[6]
γ_{O_2} (kg O_2/kg BVS oxidized)	1.5	[20]
h_{fg} (kJ/kg)	2250	[6]
c_v (kJ/kg per K)	1.8673	[6]
c_w (kJ/kg per K)	4.1868	[6]
c_a (kJ/kg per K)	1.0132	[6]
c_b (kJ/kg per K)	1.8	[6]
ρ_b (kg/l)	0.301	[6]
ε	0.5	[21]

differential equations) or distributed parameter system (system of partial differential equations). Several researchers modeled composting as a distributed parameter problem assuming either bulk or conductive

transport mechanisms coupled with a heat generation term [2,7–9], while others have modeled the process using a lumped parameter energy balance with evaporative cooling as the major heat transport mechanism [1,4,6,10].

The objective of this study is to combine the new process kinetics developed by Richard et al. [13] with the mass and energy equations developed by Oppenheimer [10] to create a model of food waste decomposition. This model was validated using the pilot scale data of VanderGheynst et al. [16] and Walker et al. [17] to determine its effectiveness in predicting process dynamics.

2. Modeling and simulation methods

In the composting process several factors influence the rate of biological volatile solids (BVS) oxidation. Through mass and energy balance, process chemistry, transport processes, and thermodynamics, a set of equations describing a well-mixed composting process were derived. BVS oxidation was modeled as a function

Table 2
Comparison of measured and predicted $T_{b,max}$s for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min per kg)	$T_{b,max}$ (°C)				Difference (%)
		Measured [16]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	0.06	64	71.2	71.1	71.3	11.3
	0.15	63	70.9	70.7	71.1	12.5
	0.31	61	70.3	69.9	70.7	15.2
	0.63	58	68.9	67.9	69.8	18.8
55	0.06	74	71.1	70.9	71.2	−3.9
	0.15	69	70.8	70.5	71.0	2.6
	0.31	65	70.0	69.4	70.5	7.7
	0.63	59	68.2	66.7	69.4	15.6

Table 3
Comparison of measured and predicted $RO_{2,max}$s measured over 0–30 cm above plenum for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min per kg)	$RO_{2,max}$ (g/h per kg VS)				Difference (%)
		Measured [16]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	0.06	1.8	1.03	1.02	1.03	−42.8
	0.15	1.9	2.51	2.46	2.54	32.1
	0.31	2	4.64	4.23	4.97	132
	0.63	3.3	6.51	4.99	8.44	97.3
55	0.06	1.6	1.00	0.99	1.02	−37.5
	0.15	2.2	2.39	2.29	2.47	8.6
	0.31	2.7	4.15	3.68	4.70	53.7
	0.63	3.6	5.49	4.30	6.84	52.5

Table 4
Comparison of measured and predicted COCs at 100 h for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min per kg)	COC after 50 h (g/kg VS)				Difference (%)
		Measured [16]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	0.06	20	12.5	11.9	13.0	−37.5
	0.15	26	27.6	23.9	30.9	6.2
	0.31	21	41.9	34.5	45.5	99.5
	0.63	27	49.4	37.7	59.7	83.0
55	0.06	17	11.5	10.5	12.4	−32.4
	0.15	25	22.4	17.7	27.3	−10.4
	0.31	25	32.3	21.5	46.1	29.2
	0.63	32	37.1	22.0	58.7	15.9

Table 5
Comparison of measured and predicted COCs at 100 h for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min per kg)	COC (g/kg VS)				Difference (%)
		Measured [16]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	0.06	48	48.1	47.9	48.3	0.2
	0.15	54	79.3	77.5	81.9	46.9
	0.31	58	128	121.3	135	120
	0.63	77	201	181	225	161
55	0.06	33	55.7	55.0	56.2	68.8
	0.15	56	85.1	81.9	88.0	52.0
	0.31	60	129	119	138	115
	0.63	73	192	166	219	163

Table 6
Comparison of measured and predicted $RO_{2,max}$s for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min)	$RO_{2,max}$ (g/h per kg VS)				Difference (%)
		Measured [17]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	25	1.5	1.82	1.81	1.84	19.7
	50	1.9	3.51	3.40	3.60	83.8
	100	1.5	5.78	5.17	6.59	285.3
55	25	1.7	1.76	1.73	1.80	3.5
	50	3.0	3.26	3.08	3.45	8.3
	100	3.1	4.95	4.19	5.90	60.7

of temperature, moisture content, and oxygen mass fraction. These state variables are the most important for representing the compost process dynamics.

2.1. Moisture content

It was assumed that the only inflow of moisture to the reactor volume was water vapour in the saturated air used for aeration. This saturation assumption for the influent air need not be strictly satisfied because humidity ratio at the higher temperature of the compost process is much greater than the humidity ratio at ambient temperature. However, experiments conducted by VanderGheynst et al. [16] and Walker et al. [17] were done for a fixed aeration rate at a constant temperature with saturated air. Because of the low aeration, and the relatively high moisture content of the organic matrix, it was assumed that there was no

resistance to the transport of moisture from the organic matrix to the air. Thus, the air is assumed saturated across the reactor bed. The saturated air assumption is often made when formulating compost models [19], and has been shown to be a good assumption for moisture rates above 45% wet basis (w.b.) [6,18]. It was also assumed that water is gener-

ated only in the process of BVS oxidation, and is related to this oxidation with process stoichiometry by a constant yield coefficient $y_{H_2O/BVS}$. If the dry bulk density, ρ_{db}, of the matrix is assumed constant, and changes in the working volume of the reactor are negligible, the storage of water in the organic matrix is modeled as follows:

Table 7
Comparison of measured and predicted COCs at 100 h in mixed reactors for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min)	COC (g/kg VS)				Difference (%)
		Measured [17]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	25	65.7	65.4	64.4	66.0	-0.5
	50	82.5	101	97.5	104	22.4
	100	82.2	159	150	170	93.4
55	25	51.3	71.8	70.4	73.4	40.0
	50	47.3	104	100	109	119.9
	100	80.5	156	145	172	93.8

Table 8
Comparison of measured and predicted COCs between 100 and 200 h in mixed reactors for a range of β_rs, aeration rates, and initial moisture contents

Initial moisture (%)	Aeration rate (l/min)	COC (g/kg VS)				Difference (%)
		Measured [17]	Predicted			
			$\beta_r = 1$	$\beta_r = 0.84$	$\beta_r = 1.36$	$\beta_r = 1$
45	25	79.7	60.2	58.9	62.1	−24.5
	50	162	108	103	115	−33.3
	100	129.2	168	151	193	30.0
55	25	107.5	59.2	57.7	61.2	−44.9
	50	101.8	105	99.4	112	3.1
	100	167.8	157	140	184	−6.4

Table 9
Comparison of measured and predicted $RO_{2,max}$s with and without f_m for $\beta_r = 1$ and a range of aeration rates and initial moisture contents

Initial moisture (%w.b.)	Aeration rate (l/min per kg)	$RO_{2,max}$ (g/h per kg VS)		
		Measured [16]	Predicted without f_m	Prediction with f_m
45	0.06	1.8	1.0	1.0
	0.15	1.9	2.5	2.4
	0.31	2.0	4.6	4.0
	0.63	3.3	6.5	4.3
55	0.06	1.6	1.0	1.0
	0.15	2.2	2.4	2.4
	0.31	2.7	4.2	4.1
	0.63	3.6	5.5	5.1
	Aeration rate (l/min)	Measured [17]	Predicted without f_m	Predicted with f_m
45	25	1.5	1.8	1.8
	50	1.9	3.5	3.2
	100	1.5	5.8	4.3
55	25	1.7	1.8	1.8
	50	3.0	3.3	3.2
	100	3.1	5.0	4.7

Table 10
Comparison of $RO_{2,max}$s for various deviation in γ_{O_2}, a range of aeration rates, and an initial moisture content of 55% w.b.

Deviation in γ_{O_2} (%)	$RO_{2,max}$ (g/h per kg VS)		
	25 (l/min)	50 (l/min)	100 (l/min)
−25	1.799	3.3728	5.8978
−10	1.7787	3.3385	5.2609
−5	1.7721	3.3025	5.1973
0	1.7629	3.2564	4.9537
5	1.7548	3.1955	4.6849
10	1.7467	3.1679	4.6275
25	1.718	3.0012	4.095

Table 11
Comparison of COCs at 100 h for various deviation in γ_{O_2}, a range of aeration rates, and an initial moisture content of 55% w.b.

Deviation in γ_{O_2} (%)	COC (g/kg VS)		
	25 (l/min)	50 (l/min)	100 (l/min)
−25	73.3899	107.7464	170.7837
−10	72.4542	106.2846	162.2218
−5	72.1637	105.2866	159.2783
0	71.842	104.3117	156.2897
5	71.493	103.2151	153.2112
10	71.1199	102.0977	150.1423
25	69.9885	98.7227	140.9098

Fig. 1. Sensitivity of temperature profile to changes in γ_{O_2} at an aeration rate of 25 l/min and initial moisture content of 55%.

$$\frac{dM_b}{dt} = \frac{G_a(H_s(T_a) - H_s(T)) - y_{H_2O/BVS}(d(BVS)/dt)}{\rho_{db}V_r} \quad (1)$$

where G_a is the mass flow rate of dry air (kg dry air/day); $H_s(T_a)$, the saturated humidity of the ambient air (kg H$_2$O/kg dry air); $H_s(T)$, the saturated humidity of the air at reactor temperature (kg H$_2$O/kg dry air); $y_{H_2O/BVS}$, the yield coefficient for water (kg H$_2$O/kg

Fig. 2. Sensitivity of temperature profile to changes in γ_{O_2} at an aeration rate of 100 l/min and initial moisture content of 55%.

Fig. 3. Sensitivity of oxygen mass fraction in reactor effluent to changes in γ_{O_2} at an aeration rate of 25 l/min and initial moisture content of 55%.
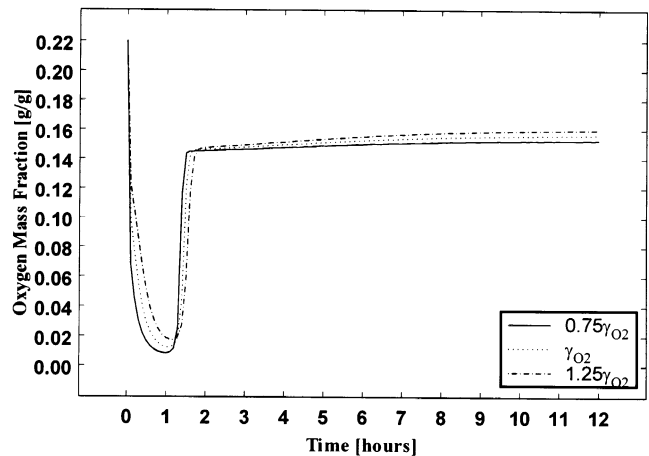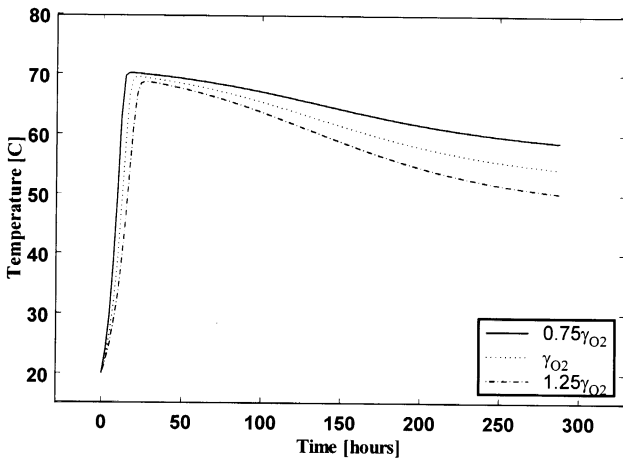

Fig. 4. Sensitivity of oxygen mass fraction in reactor effluent to changes in γ_{O_2} at an aeration rate of 100 l/min and initial moisture content of 55%.

BVS oxidized); ρ_{db}, the dry bulk density of the solids (kg dry solids/l); V_r, reactor working volume (l), T_a, the ambient air temperature (°C) and T is the reactor air temperature (°C).

Eq. (1) has units of dry basis moisture content per day or kgH$_2$O/kg dry solids per day.

2.2. Oxygen mass fraction

Oxygen inflow was modeled by assuming that oxygen only enters the compost matrix through the forced aeration with ambient air; that air exits the reactor at the same concentration as the homogeneous reactor concentration, and that O$_2$ can only be consumed by the oxidation of BVS. The oxygen stored within the organic matrix is measured by the oxygen mass fraction within the pore space of the organic matrix. Changes in porosity, and reactor working volume were assumed to be negligible. The change in the oxygen mass fraction in the matrix, X_{O_2}, was model by:

$$\frac{dX_{O_2}}{dt} = \frac{G_a(X_{O_2, a} - X_{O_2, exit}) + y_{O_2/BVS}(d(BVS)/dt)}{V_r \varepsilon \rho_a(T)} \quad (2)$$

where $X_{O_2, a}$ is the concentration of oxygen in ambient air (kg O$_2$/kg dry air); $X_{O_2, exit}$, the concentration of oxygen in the exit flow (kg O$_2$/kg dry air) ε, the porosity; $y_{O_2/BVS}$, the yield coefficient of O$_2$ (kg O$_2$/kg BVS oxidized); V_r, the working volume of the reactor (l); G_a, the mass flow rate of dry air (kg dry air/day); $\rho_a(T)$, the dry air density (kg/l).

Eq. (2) has units of kg O$_2$/kg dry air per day.

2.3. Temperature

Energy is generated during the process of BVS oxidation in the form of heat. It was assumed that BVS oxidation is the sole source of energy, and that this production of energy is related to BVS oxidation kinetics through the heat of reaction H_{rx} which is assumed to be constant over the course of the simulation. Latent heat transfer due to the vaporization of water dominates heat loss, and sensible heat loss to the air is neglected [9,10].

Since there is little or no resistance to heat transfer from the compost matrix to the air in the compost vessel, it was assumed that the temperature of the air in the reactor was in equilibrium with the organic matrix. The reactor temperature is a good measure of the total stored energy, where the total heat energy is the sum of the energy contained in the organic matrix, the dry air, and in the water vapor. Specific heat and density of these constituents were held constant. The time rate of the change of temperature within the reactor is given by:

$$\frac{dT}{dt} = \frac{-H_{rx}(d(BVS)/dt) - h_{fg}G_a(H_s(T) - H_s(T_a))}{V_r(\varepsilon\rho_a(T)c_a + \rho_{db}(c_b + M_b c_w) + \rho_a(T)H_s(T)c_v)} \quad (3)$$

where H_{rx} is the heat of reaction (kJ/kg BVS oxidized); h_{fg}, the heat of vaporization of water (kJ/kg water); G_a, the mass flow rate of dry air through reactor (kg dry air per day); $H_s(T)$, the saturated humidity at reactor temperature (kg H$_2$O/kg dry air); $H_s(T_a)$, the saturated humidity at ambient temperature (kg H$_2$O/kg dry air); V_r, the working volume of the reactor (l); ε, the porosity; $\rho_a(T)$, the density of dry air at reactor temperature (kg dry air per l); c_a, the specific heat of dry air (kJ/kg per K); ρ_{db}, the dry bulk density of the solids (kg dry solids per l); c_b, the specific heat of the dry solids (kJ/kg per K); M_b, the moisture content dry basis (kg water/kg dry solids); c_w, the specific heat of water (kJ/kg per K); c_v, the specific heat of water vapor (kJ/kg per K);

The units of the above equation are K per day.

2.4. First-order-reaction kinetics

It has been shown that the Cardinal Temperature Model with Inflection (CTMI) of Rosso et al. [15] provided parameters that were more consistent over the composting temperature range, and, more importantly, variability in parameters could be attributed to the microbial processes. Richard et al. [19] used the CTM model to develop the following model for the rate of carbon dioxide evolution R_{CO_2} from a synthetic food waste reactor:

$$R_{CO_2} = R_{CO_2 opt}(f_T)(f_{O_2})\left[\frac{CO_2}{kg\ Vs\ per\ day}\right] \quad (4)$$

where

$$f_T = \frac{(T - T_{max})(T - T_{min})^2}{(T_{opt} - T_{min})\{(T_{opt} - T_{min})(T - T_{opt}) - (T_{opt} - T_{max})(T_{opt} + T_{min} - 2T)\}} \quad (5)$$

$$f_{O_2} = \frac{O_2}{k_{O_2}(T, X_{H_2O}) + O_2} \quad (6)$$

$$k_{O_2}(T, X_{H_2O}) = 0.79 - 0.041(T) + 0.040(X_{H_2O}) \quad (7)$$

$R_{CO_2 opt}$ is the optimal CO$_2$ evolution rate (g CO$_2$/kg VS per day); T_{min}, the minimum temperature for system bioactivity (°C); T_{max}, the maximum temperature for system bioactivity (°C); T_{opt}, the optimum temperature (°C); T, temperature (°C); X_{H_2O}, moisture content (%w.b.); O$_2$, the oxygen concentration (%)

The optimal rate of CO$_2$ evolution, $R_{CO_2 opt}$, was calculated as follows:

$$R_{CO_2 opt} = [(R_{CO_2 opt})_{max} - R_{CO_2 slow}]e^{[-k(t-\tau)]} + R_{CO_2 slow} \quad (8)$$

where $R_{CO_2 slow}$, is the steady long term degradation (g CO_2/kg VS per day); τ, the lag time (day); $(R_{CO_2 opt})_{max}$, the magnitude of peak degradation rate (g CO_2/kg VS per day); k, first order decay constant (per day). Eq. (4) was used to define the kinetic framework for BVS oxidation in a similar way that Haug [6] used a model for oxygen uptake to define reaction kinetics. First it was assumed that CO_2 evolution and O_2 uptake are related through the process stoichiometry by a respiration quotient β_r (gO_2/gCO_2). Then, a specific oxygen uptake rate, γ_{O_2} (kg O_2 consumed/kg BVS oxidized), was assumed. Lastly, a fraction of total BVS included in the total VS measurement was assumed. This measure has units of (total BVS/total VS). From this conversion, the final kinetic parameter, k_{BVS}, emerged.

$$k_{BVS} = \frac{\beta_r R_{CO_2 opt}}{10^3 \gamma_{O_2}(BVS)}(f_T)(f_{O_2}) \qquad (9)$$

Eq. (9) is then used to define the first order reaction kinetics of the system by the following relationship:

$$\frac{d(BVS)}{dt} = -k_{BVS}(BVS) \qquad (10)$$

Several parameters in the model were held constant during the model simulations. A table of these parameters and their values are presented in Table 1. The kinetic parameters obtained by Richard [20] were used to simulate the experiments performed by Vander-Gheynst et al., [16] and Walker et al. [17]. The heat of reaction, ΔH_{rxn}, and the specific oxygen uptake γ_{O_2} were taken from Haug [6]. Specific heat of water and water vapor, and the heat of vaporization of water were taken from steam tables. Oppenheimer et al. [21] calculated the dry bulk density, the dry specific heat, and the porosity of the organic matrix; while VanderGheynst et al. [16] reported the ash content of the organic matrix.

2.5. Numerical solution of equation set

Numerical solutions to Eqs. (1)–(3) and (10) were implemented using the integration Runge Kutta method. A fourth and fifth order approximation was used in the adaptive step size algorithm provided with the software package Matlab (MathWorks Inc.) The algorithm performs both fourth and fifth order approximations simultaneously to compare the two results for error analysis.

3. Results and discussion

3.1. Model validation

To validate the model, simulations were run using the operating conditions of VanderGheynst et al. [16] and Walker et al. [17]. Comparisons of temperature and

oxygen concentrations between the simulations and experimental results were performed for the first 100 and 200 h for the experiments of VanderGheynst et al. [16] and Walker et al., [17] respectively. Since the model does not include a microbial growth mechanism, it cannot simulate the lag in temperature and oxygen uptake rate during the process. Thus, the simulation results were shifted 36 h to coincide with the onset of temperature ramping in experimental data.

Comparisons of maximum bed temperatures, $T_{b,max}$, with those observed by VanderGheynst et al. [16] are presented in Table 2. $T_{b,max}$s were calculated for three values of β_r. β_r is directly proportional to the kinetic expressions, and Richard [20] observed that β_r decreased as decomposition continued. Therefore, simulations were performed with the maximum, average, and minimum values of β_r. From Table 2 it is clear that the model over predicted $T_{b,max}$ except at the lowest aeration rate. Under high aeration conditions the largest difference between the model and the experimental $T_{b,max}$ was 10.9°C. The best prediction of $T_{b,max}$ was observed for the 0.15 l/min per kg flow rate at 55% w.b. moisture content where the difference between predicted and measured temperature was 1.8°C. Varying β_r had little effect on the model's prediction of $T_{b,max}$ as shown in Table 2. The over prediction is greatest at high aeration rates and low initial moisture contents. This over prediction at high aeration rates and low moisture is likely due to the lower rates of substrate degradation due to reduced moisture content. Haug [6] noted that the rate of decomposition dropped rapidly when the moisture content of the organic matrix was below 45% w.b. VanderGheynst et al. [16] reported axial moisture gradients as high as 21–38% w.b., and the moisture content of the organic matrix dropped below 45% w.b. at 80 h for the initial moisture content of 55% w.b. and the highest aeration rate.

Table 3 shows comparisons of maximum oxygen uptake rates, $RO_{2,max}$, measured by VanderGheynst et al. [16] and those predicted by the model. Simulation results for β_r equal 0.84 yielded the best agreement with experimental results 40% average error, while the $\beta_r = 1$ simulations resulted in an average error of 59%. The model under predicted $RO_{2,max}$ for the lowest aeration rate, and over predicted for higher aeration rates.

Tables 4 and 5 present comparisons of the cumulative oxygen consumption, COC, measurements of VanderGheynst et al. [16] with model predictions. For $\beta_r = 1$ and the lowest aeration rate, the model under predicted COC at 50 h by 37.5%, and over predicted by 83% at the highest aeration rate. Note that the largest differences between experimental and simulation results occur in the 45% moisture data and that the error was never greater than 32.4% for the 55% moisture data. This over prediction is another indication that drying is influencing the rate of substrate decomposition. Van-

derGheynst et al. [16] presented moisture profiles for the two extreme cases of aeration. VanderGheynst et al. [16] noted that moisture did not limit decomposition for the lowest aeration rate, but could have been limiting to microbial activity 50 h into the process at the highest aeration rate. During the first 50 h of the process, the model predicts COC best with the average value of β_r.

Comparisons of the measured and predicted COCs for the first 100 h of decomposition show that the model consistently over predicted COC (see Table 5). This over prediction is 162% for $\beta_r = 1$ at high aeration rates, and is no greater than 68.8% for the lowest aeration rate. Here, the minimum β_r gives a better estimation of the experimental data. This is consistent with Richard's [20] observation that β_r tends to decrease as the degradation process proceeds. In addition, the increase in total difference for later predictions is partially due to the accumulation of error inherent in the summing O_2 uptake. Also, at these later times, spatial gradients in moisture content and temperature are likely to influence the rate of substrate decomposition. VanderGheynst et al. [16] observed gradients of 25°C at 100 h for the highest aeration rate, and 4°C for the lowest aeration rate at 100 h. Although aeration rate had little influence on the size of the moisture gradients, these gradients were still significant — one of them reaching a 21% w.b. difference before 100 h. Once these spatial gradients form, the homogeneous assumption breaks down (VanderGheynst et al. [9]).

Table 6 shows comparisons of $RO_{2,max}$ measured by Walker et al. [17] and those predicted by the model. The reactors in this study were mixed three times a week. The simulation results for β_r equal 0.84 best agreed with experimental results; 52% average error. While the $\beta_r = 1$ simulations resulted in average errors of 66%, the model over predicted $RO_{2,max}$ at all aeration rates. The percent differences for the 45% w.b. were an order of magnitude higher than those for 55% initial moisture content and for all aeration rates.

Tables 7 and 8 compare the measured and predicted COCs. The measure valued are from the mixing experiments conducted by Walker et al. [17]. Comparisons show that the model still over predicted COC for the first 100 h, but this over prediction is much less when comparing the model with the mixed reactor data. Here again, the minimum β_r gives the best predictions.

Comparison of the model predictions with the data from 100 to 200 h show that the three different values of β_r give a similar error in the overall estimate (the average error in estimates differ by no more than 3.5 percentage points.) But again, lower values of β_r gave slightly better predictions at later times. Over-prediction in COC could be due to the accumulation of error inherent to the summing or RO_2 values. The data presented by Walker et al. [17] is representative of mixed reactors. Here, the model's error at later times is

reduced, a reflection on the basic assumptions that were made in model development, namely that the reactor was well-mixed, and spatial gradients were reduced. However, Walker et al. [17] observed the formation of gradients even in the mixed reactor. Drying could also have an influence on oxygen uptake as the moisture content of the compost bed with 55% w.b. initial moisture content and 100 l/min aeration dropped below 45% w.b. moisture content at 72 h [17]. One hundred hours into the process, the pilot scale reactor with a 45% w.b. initial moisture content and 100 l/min aeration had reached a 35% w.b. moisture content [17].

3.2. Influence of matrix drying

The observation that the model over predicts the value of several state variables at high aeration and low initial moisture suggests that the model needs a stronger component to deal with substrate drying. To investigate the influence of drying, simulations were performed by introducing the following discount factor for non-optimal moisture content into the BVS degradation kinetics [6].

$$f_m = \frac{1}{\exp\left(-17.684\, M_{wb} + 7.0622\right) + 1} \tag{11}$$

The addition of this discount factor brings the effect of moisture on substrate degradation directly into the kinetic expression as follows:

$$\frac{d(BVS)}{dt} = -k_{BVS}\, f_m(BVS) \tag{12}$$

Tabulated in Table 9 are the results obtained from adding f_m into the BVS degradation kinetics. The addition of the moisture discount factor had little effect on $RO_{2,max}$ for the initial moisture content of 55%, while at 45% w.b. initial moisture content and at high aeration rates the effect was largest. This reduction in the differences between model predictions and observations is significant, but cannot be the sole explanation of the discrepancies between model predictions and experimental observations.

In all observations the model tended to over predict values of the state variables. $RO_{2,max}$, total COC, and $T_{b,max}$ were all over predicted. The model's main assumption is that there are no gradients in temperature or oxygen mass fraction in the reactor. Frequent mixing satisfies this assumption; however, it has been shown that mixing has little effect on the elimination of oxygen and temperature gradients [22]. If gradients always exist, even in the presence of mixing, there is always a possibility for part of the reactor to be at sub-optimal conditions. Thus, models that assume minimal spatial gradients will have a tendency to over predict the rate of BVS oxidation in the reactor.

3.3. Sensitivity analysis

Sensitivity analysis of the key parameters that were held constant during simulation was performed to assess the robustness of the model and to determine where error propagation is likely to occur. One parameter that is kept constant that can have high variability is γ_{O_2}. Taking the derivative of Eq. (9) with respect to γ_{O_2} shows the influence of this parameter on process kinetics.

$$\mathrm{d}k_{\mathrm{BVS}} = -\frac{\beta_r R_{\mathrm{CO2opt}}}{10^3 \gamma_{O_2}^2 (\mathrm{BVS})} (f_T)(f_{O_2}) \mathrm{d}\gamma_{O_2} \qquad (13)$$

To test the influence of a change in γ_{O_2} on the entire model, simulations were performed that varied γ_{O_2} for three aeration rates presented in the studies performed by Walker et al. [17]. Tables 10 and 11 show a general trend in the model's sensitivity to γ_{O_2}. The model seems to be more sensitive to γ_{O_2} at low aeration rates, with a tendency to become more insensitive to changes in this parameter at high aeration rates.

The variation of $RO_{2,\max}$ with changes in γ_{O_2} is presented in Table 10. The sensitivity of model predictions due to changes in γ_{O_2} increased with increasing flow rate. Note that in Tables 3 and 6, the error in $RO_{2,\max}$ increase as flow rate increases. However, a 10% difference in γ_{O_2} yields only a 6% difference in $RO_{2,\max}$ for an aeration rate of 100 l/min.

The variation of COC over the first 100 h with respect to changes in γ_{O_2} is presented in Table 11. For COC, the model is even less sensitive to changes in γ_{O_2}. The decreased sensitivity may result from integration of the oxygen mass fraction profile as integration tends to average out error.

The sensitivity of the predicted $T_{b,\max}$ to changes in γ_{O_2} is illustrated in Figs. 1 and 2 for aeration rates of 25 and 100 l/min, respectively. These results illustrate that the model $T_{\max}$ predictions are more sensitive to changes in γ_{O_2} at the lower aeration rate of 25 l/min. At 100 l/min, a 25% change in γ_{O_2} yields only a 1.3% change in the predicted $T_{\max}$ value. Figs. 3 and 4 illustrate the sensitivity of the predicted oxygen mass fraction to changes in γ_{O_2}. These results illustrate that predicted oxygen mass fractions are also more sensitive to changes in γ_{O_2} at the lower aeration rate of 25 l/min.

4. Conclusions

The model developed in this study combined the specific substrate degradation kinetic model of Richard [20] with the mass and energy equations of Oppenheimer [10]. The data from these simulations was validated against pilot scale data obtained from experiments of VanderGheynst et al. [16] and Walker et al. [17]. Overall, the model captured the shifts in tem-

perature and O_2 consumption, and major errors in these predictions could be explained based on the formation of spatial gradients in pilot scale experiments, the reduction of substrate moisture to a point which limits mass transfer, and the model's sensitivity to constant parameters.

The sensitivity of the model to two key parameters, γ_{O_2}, and β_r, was investigated. Richard [20] noted that β_r tended to decrease as organic degradation progressed. This effect was investigated by varying β_r for each of the comparisons with experimental observation. It was noted that smaller values of β_r produced better estimates later in the process. $RO_{2,\max}$ was insensitive to changes in γ_{O_2} at low aeration rates, and more sensitive to changes in γ_{O_2} at high aeration rates. The model's error in predictions increased as aeration rate increased.

The model predicted the behavior of a mixed system well into the process once the lag time was taken into account. For mixed pilot scale experiments, it predicted COC with average errors of no greater than 27% between 100 and 200 h into the process. This implies that the model was able to predict the general system dynamics eight days into the process. After this time, the model results significantly deviate from the measured results. This is contrasted with the comparison of the model against non-mixed pilot scale experiments. Here the model predicts the system dynamics well for only the first 50 h.

The kinetic expressions used in this investigation were substrate specific, yet there were still some large discrepancies between model predictions and experimental observations. The modeling results illustrate the difficulty in predicting organic solids decomposition. To make further modeling progress, the formation of spatial gradients must be taken into account since mixing has a limited effect on reducing the formation of gradients in temperature, oxygen mass fraction, and moisture content [22].

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