Review

Mathematical modelling of the composting process: A review

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Abstract

In this paper mathematical models of the composting process are examined and their performance evaluated. Mathematical models of the composting process have been derived from both energy and mass balance considerations, with solutions typically derived in time, and in some cases, spatially. Both lumped and distributed parameter models have been reported, with lumped parameter models presently predominating in the literature. Biological energy production functions within the models included first-order, Monod-type or empirical expressions, and these have predicted volatile solids degradation, oxygen consumption or carbon dioxide production, with heat generation derived using heat quotient factors. Rate coefficient correction functions for temperature, moisture, oxygen and/or free air space have been incorporated in a number of the first-order and Monod-type expressions. The most successful models in predicting temperature profiles were those which incorporated either empirical kinetic expressions for volatile solids degradation or CO_2 production, or which utilised a first-order model for volatile solids degradation, with empirical corrections for temperature and moisture variations. Models incorporating Monod-type kinetic expressions were less successful. No models were able to predict maximum, average and peak temperatures to within criteria of 5, 2 and 2 °C, respectively, or to predict the times to reach peak temperatures to within 8 h. Limitations included the modelling of forced aeration systems only and the generation of temperature validation data for relatively short time periods in relation to those used in full-scale composting practice. Moisture and solids profiles were well predicted by two models, but oxygen and carbon dioxide profiles were generally poorly modelled. Further research to obtain more extensive substrate degradation data, develop improved first-order biological heat production models, investigate mechanistically-based moisture correction factors, explore the role of moisture tension, investigate model performance over thermophilic composting time periods, provide more information on model sensitivity and incorporate natural ventilation aeration expressions into composting process models, is suggested.
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1. Introduction

Mathematical modelling has been widely utilised in science and engineering in order to improve understanding of the behaviour of systems, explore new theoretical concepts, predict system performance and, in an increasing number of cases, aid in the solution of practical design problems. In the latter context, mathematical models offer the potential to reduce, or even replace, the need for physical experimentation when exploring new material and/or process options. Given the challenges and costs involved in conducting appropriate laboratory and pilot scale investigations, increased ability to assess new process options through such modelling is to be welcomed.

Mathematical models of the composting process have appeared in the literature since 1976, with more than 30 papers addressing this topic published through to December 2003. In addition, contributions from studies on liquid-phase aerobic digestion, and the broader field of high solids aerobic degradation, have provided models with potential relevance to the understanding and prediction of composting system behaviour.

This review will examine composting process models, their structure, kinetic foundations, simulation

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Nomenclature

A	heat transfer area (m^2); OM loss model saturation constant (%) (Bernal et al., 1996; Paredes et al., 2000, 2001, 2002)
A, B	BOD model saturation constants (kg or g/m^3) (Haug, 1993)
$\acute{A}$	Arrhenius constant (cm/h) (Finger et al., 1976)
β	respiratory quotient (kg-O_2/kg-CO_2) (Kaiser, 1996); maintenance coefficient (kg-substrate/kg-cell mass h) (Stombaugh and Nokes, 1996)
β, β_r	respiratory quotient (kg-O_2/kg-CO_2) (Kaiser, 1996; Higgins and Walker, 2001)
BOD	biochemical oxygen demand (kg or g/m^3)
BVS	biodegradable volatile solids (kg)
c	specific heat of compost mixture (kJ/kg °C)
c^*, c	oxygen concentration (g/m^3) (Finger et al., 1976)
c_c	mass fraction of carbon (dimensionless) (Kaiser, 1996)
DM	dry matter (kg)
ε	porosity (dimensionless)
E_a	activation energy (cal/mole)
E_b	biological heat (kJ or cal)
F	aeration rate (kg-dry air/h) (Kishimoto et al., 1987)
FAS	free air space (dimensionless) (Haug, 1993)
FS	solids fraction (dimensionless) (Smith and Eilers, 1980)
G	mass flow dry air (kg/s)
G_o	molar flow rate dry air (mole/h or mole/d) (Bach et al., 1987)
h_c	heat of combustion (MJ/kg) (Keener et al., 1993)
H, H_c	heat of combustion (kJ/kg-BVS removed)
ΔH^0	heat of combustion for cellulose (van Lier et al., 1994)
$H_{i,o}$	enthalpy of inlet (i) and outlet (o) air (kJ/kg)
H_R, H_{rx}	heat of reaction (kJ/g-TS or kJ/g-VS)
H_s	saturated humidity (kg-H_2O/kg-dry air)
HCOMB	heat of combustion (cal/g-VS) (Smith and Eilers, 1980)
k	first-order rate coefficient (d^{-1})
m	moisture (kg/kg wet basis) (Stombaugh and Nokes, 1996)
$m_{t,e}, m_{DS,R}$	mass of composting materials (kg) (Scholwin and Bidlingmaier, 2003)
M	moisture (kg), or mass of composting material (kg) (Kaiser, 1996)
M_b	moisture content (kg-H_2O/kg-dry solids) (Higgins and Walker, 2001)

M_c	moisture content (kg/kg; wet basis)
M_c(opt)	optimum moisture content (kg/kg; wet basis)
MM	molecular mass (Kaiser, 1996)
$[O_2]$	oxygen concentration in the exit gas (%v/v)
OM	organic matter (%) (Bernal et al., 1996; Paredes et al., 2000, 2001, 2002)
q_r	rate of heat generation (kcal/h) (Kishimoto et al., 1987)
Q	heat generation factor (kJ/kg-O_2) (VanderGheynst et al., 1997)
Q_o	heat generation factor (kcal/mole-O_2) (Bach et al., 1987; Nakasaki et al., 1987)
ρ_{db}	dry bulk density (kg/m^3)
R	universal gas constant (cal/K mole)
rO_2, RO_2	oxygen consumption rate (mole-O_2/h g-VS) (Nakasaki et al., 1987) or (kg-O_2/m^3 h) (VanderGheynst et al., 1997)
RCO_2	carbon dioxide evolution rate (g-CO_2/kg-VS d) (Higgins and Walker, 2001)
s	substrate concentration (g/m^3)
SMOUT	solids content of the mixture output (Haug, 1993)
t	time (s, h or d)
T	temperature (°C)
T_{max}	maximum temperature for microbial growth (°C)
T_{min}	minimum temperature for microbial growth (°C)
T_{opt}	optimum temperature for microbial growth (°C)
U	overall heat transfer coefficient (kW/m^2 °C)
V	volume (m^3)
VOLPO2	volume percentage oxygen in exhaust gas (Haug, 1993)
w_c	water content (%) (Kishimoto et al., 1987)
W	watt; density (g/cm^3) (Smith and Eilers, 1980)
W_s	weight dry solids (g) (Nakasaki et al., 1987)
X	cell mass (kg/m^3)
X_{O_2}	concentration of oxygen (kg-O_2/kg-dry air) (Higgins and Walker, 2001)
$y_{O_2,DS,R}$	specific oxygen consumption rate (kg-O_2/kg-DS time) (Scholwin and Bidlingmaier, 2003)
y, Y	yield (kg/kg)
$Y_{H_2O/BVS}$	stoichiometric yield of moisture (kg-H_2O/kg-BVS)
$Y_{O_2/BVS}$	stoichiometric consumption of oxygen (kg-O_2/kg-BVS); (Bari et al., 2000a)
Z_o	molar fraction oxygen in inlet and exit air (dimensionless) (Bach et al., 1987)

abilities and validation performance. The discussion will provide a basis for an assessment of the present status of composting process modelling, and has potential implications for developing new and improved models for the future.

2. Conceptual frameworks

2.1. Overview

The solution of coupled heat and mass balance equations in time, and in some cases, spatially has provided the basis for most composting process models. The general form adopted for analysis has been as follows:

$$\text{accumulation} = \text{input} - \text{output} \pm \text{transformation}. \quad (1)$$

A deterministic approach has been adopted for all published models (Table 1). However, stochastic elements have been incorporated into two of these models which have appeared within the past few years (Seki, 2000; Scholwin and Bidlingmaier, 2003). Modellers have typically looked at the composting system on a macroscale, in which the focus of analytical attention has been on the reactor as a whole; however, several authors have approached the problem by starting from a microbiological point of view (Kaiser, 1996; Stombaugh and Nokes, 1996; Seki, 2000). Adopting a different perspective, Hamelers (1993) used the composting particle as the basis for analysis.

Model parameters have either been lumped over the complete reactor (Kishimoto et al., 1987; Nakasaki

et al., 1987; Haug, 1993; Kaiser, 1996; VanderGheynst et al., 1997; Mohee et al., 1998; Ndegwa et al., 2000; Seki, 2000; Higgins and Walker, 2001), or distributed, over horizontal layers (Finger et al., 1976; Keener et al., 1993; van Lier et al., 1994; Stombaugh and Nokes, 1996; Das and Keener, 1997), rectangular and triangular shaped elements (Smith and Eilers, 1980), or regions based on temperature homogeneity (Scholwin and Bidlingmaier, 2003). The finite element approach has allowed mixture compressibility and other spatially distributed factors to be taken into account (Das and Keener, 1997). Finite elements were also used by Bari et al. (2000b) in a layer-wise analysis of BVS degradation.

A number of the models have been further investigated, typically by different groups of authors. The model of Haug (1993) was used as the basis for subsequent studies reported by Bertoni et al. (1997), Kim et al. (2000) and Ndegwa et al. (2000), whilst Das and Keener (1997) and Mohee et al. (1998) utilised elements of the model originally proposed by Keener et al. (1993). The model of VanderGheynst et al. (1997) was further developed by Higgins and Walker (2001).

2.2. Heat balance considerations

Heat balance components in composting models have included sensible heating of the system contents, sensible heat of input and output streams (input air, water vapour and any supplementary water, exit gases and vapours), conductive/convective losses, radiative inputs and losses, latent heat of evaporation of water and biological heat production (Table 2). Biological heat production and

Table 1
General overview of composting models

References	Deterministic	Stochastic	Parameters		Terms in energy balance (see Table 2 for key)	Comments
			Lumped	Distributed		
Finger et al. (1976)	Y	–	–	Y	1, 8[a],11	[a]Thermal diffusion only
Smith and Eilers (1980)	Y	–	–	Y	1, 2, 3, 5, 6, 7, 8, 10, 11	Radiation input only
Bach et al. (1987)	Y	–	na	na	1, 2, 3, 6, 7, 8, 10, 11	Heat balance only
Kishimoto et al. (1987)	Y	–	Y	–	1, 2, 3, 6, 7, 8, 10, 11	–
Nakasaki et al. (1987)	Y	–	Y	–	1, 2, 3, 6, 7, 8, 10, 11	–
Hamelers (1993)	Y	–	Y	–	none	–
Haug (1993)	Y	–	Y	–	1, 2, 3, 6, 7, 8, 10, 11	–
Keener et al. (1993)	Y	–	–	Y	1, 2, 3, 6, 7, 10, 11	No conduction or radiation losses
van Lier et al. (1994)	Y	–	–	Y	1, 2, 3, 6, 7, 8, 10, 11	–
Kaiser (1996)	Y	–			1, 2, 3, 6, 7, 8, 10, 11	–
Stombaugh and Nokes (1996)	Y	–	–	Y	1, 2, 3, 6, 7, 8, 10, 11	Conduction constant
Das and Keener (1997)	Y	–	–	Y	1, 2, 3, 6, 7, 8, 10, 11	–
VanderGheynst et al. (1997)	Y	–	Y	–	1, 2, 3, 6, 7, 10, 11	No radial conduction
Mohee et al. (1998)	Y	–	Y	–	1, 2, 3, 6, 7, 8, 10, 11	–
Seki (2000)	Y	Y	Y	–	1, 2, 3, 6, 7, 8, 10, 11	–
Higgins and Walker (2001)	Y	–	Y	–	1, 2, 3, 6, 7, 10, 11	No radial conduction
Robinzon et al. (2000)	Y	–	na	na	1, 2, 3, 5, 6, 7, 8, 9, 10, 11	Radiation included; heat balance only
Scholwin and Bidlingmaier (2003)	Y	Y	–	Y	1, 2, 3, 6, 7, 8, 10, 11	–

Table 2
Energy balance components in composting models

Accumulation terms	Input terms	Output terms	Transformation terms
Sensible heating of reactor contents (1)	Sensible heat of inlet dry air (2) Sensible and latent heat of inlet water vapour (3) Sensible heat of supplementary water (4) Radiation (5)	Sensible heat of dry exit gas (6) Sensible heat of exit water vapour (7) Conductive/convective losses (8) Radiation losses (9) Latent heat of evaporation (10)	Biologically generated heat (11)

latent heat of evaporation of water have been shown to be the most significant terms in the heat balance for full-scale systems (Bach et al., 1987; Harper et al., 1992; Weppen, 2001) and these have been incorporated in nearly all reported models (Table 1). In the majority of cases, latent heat of evaporation of water has been accounted for by the enthalpy term for exit gas water vapour, appearing within an advective gas transport expression. Heat loss through reactor walls has generally been incorporated (Bach et al., 1987; Kishimoto et al., 1987; Nakasaki et al., 1987; Haug, 1993; van Lier et al., 1994; Kaiser, 1996; Stombaugh and Nokes, 1996; Das and Keener, 1997; Mohee et al., 1998; Seki, 2000; Scholwin and Bidlingmaier, 2003), whilst convective boundary losses were included in the models of Smith and Eilers (1980) and Ndegwa et al. (2000). The overall heat transfer coefficient (U), which incorporates the combined roles of convection, conduction and radiation at system boundaries, has typically been employed, although the term conduction is frequently used in this context. Radiation as a separate term has typically been ignored, although it was explicitly included as an input in the aerated static pile focused model of Smith and Eilers (1980), and was found to be important for open windrows in the heat balance of Robinzon et al. (2000), with a net radiation gain indicated. However, in the model of Hamelers (1993), which predicted oxygen concentration, oxygen uptake rate, substrate utilisation and biomass growth patterns, temperature gradients at the particle level were considered negligible and were neglected. Wall losses were ignored by VanderGheynst et al. (1997) who modelled heat transport as a one-dimensional problem along a vertical axis, and were likewise not incorporated in the models of Keener et al. (1993) and Higgins and Walker (2001). Where wall losses comprise only a small proportion of the overall heat budget, it may be argued that this simplification is acceptable. However, wall losses can be significant in small-scale systems, even with substantial insulation present (Mason and Milke, in press-a). Finger et al. (1976) modelled heat transport by thermal diffusion only, with no explicit reference to advective, or other, transport mechanisms. However, advective heat transport is known to play a major role in most composting systems. Heat balance analyses, without predictive equations, were presented by Bach et al. (1987), Harper et al. (1992), Koenig and Tao

(1996) and Bari et al. (2000a) and, along with a mass balance evaluation, by Robinzon et al. (2000). Useful mass balance analyses have also been reported by Batista et al. (1995) and Straatsma et al. (2000).

A generalised heat balance model, configured for sensible heat accumulation as the dependent variable, is presented below:

$$\frac{d(mcT)}{dt} = GH_i - GH_o - UA(T - T_a) + \frac{d(BVS)}{dt}H_c. \quad (2)$$

Here m is the mass of the composting material (kg), c is the specific heat of the composting material (kJ/kg °C), T is the temperature of the composting material (°C), t is the time (s), G is the mass flow rate of air (kg/s), H_i and H_o are the inlet and exit gas enthalpies (kJ/kg), BVS is the mass of biodegradable volatile solids (kg), H_c is the heat of combustion of the substrate (kJ/kg), U is the overall heat transfer coefficient (kW/m² °C), A is the reactor surface area (m²), and T_a is the ambient temperature (°C). Eq. (2) has units of kW.

In order to solve this expression without simplification, advective, conductive/convective/radiative (CCR) and biological heat energy terms, plus associated rates of moisture and solids change must be known. Solutions to the enthalpy containing terms have typically been obtained in conjunction with psychometric models, commonly assuming 100% relatively humidity in the exit gas (e.g. Haug, 1993; VanderGheynst et al., 1997), plus representative values for relative humidity and temperature of the inlet air. Haug (1993) predicted saturation exit gas water vapour levels as a function of temperature, and applied an adjustment at low mixture moisture levels, when saturated conditions could not reasonably be assumed. This model also allowed for supplementary water addition and prediction of ammonia levels. To date, all models have simulated forced aeration systems, using fixed aeration rates. Given the widespread use of naturally ventilated systems, future research aimed at the incorporation of natural ventilation sub-models into composting process models would be valuable. Diffusive transport of moisture and gases was incorporated into the distributed parameter models of Finger et al. (1976), Smith and Eilers (1980) and van Lier et al. (1994) and was also modelled by VanderGheynst et al. (1997). Oxygen limitation was assumed as the rate controlling

factor by Finger et al. (1976). However, as pointed out by Agnew and Leonard (2003) in their review paper, oxygen diffusion is unlikely to be significant in the composting process, except at the particle level (Hamelers, 1993). The CCR heat loss term may be readily solved using either commonly available heat transfer information (e.g. Mills, 1995) or experimental heat transfer data (e.g. Bach et al., 1987).

A number of authors have treated 'mc' in Eq. (2) as a constant term (van Lier et al., 1994; Stombaugh and Nokes, 1996; Das and Keener, 1997; VanderGheynst et al., 1997; Mohee et al., 1998; Higgins and Walker, 2001) resulting in expressions of the following form:

$$mc\frac{\mathrm{d}T}{\mathrm{d}t} = GH_{\mathrm{i}} + \frac{\mathrm{d(BVS)}}{\mathrm{d}t}H_{\mathrm{c}} - GH_{\mathrm{o}} - UA(T - T_{\mathrm{a}}) \qquad (3)$$

from which the expression for the rate of temperature change is:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{GH_{\mathrm{i}} + \frac{\mathrm{d(BVS)}}{\mathrm{d}t}H_{\mathrm{c}} - GH_{\mathrm{o}} - UA(T - T_{\mathrm{a}})}{mc}. \qquad (4)$$

Nakasaki et al. (1987) assumed constant specific heat only. Since the accumulation term will likely account for a relatively small proportion of the heat balance (see Weppen, 2001), this simplification may introduce relatively little error into model performance.

VanderGheynst et al. (1997) assumed a constant moisture content in the composting material over the period of their study, and validated this supposition experimentally. Additional assumptions discussed and implemented by VanderGheynst et al. (1997) included those of constant mass air flux, minimal diffusion of mass and energy (since forced aeration was used), and equilibrium between solid and gas phases (homogenous assumption). These authors also used simplified equations for calculating the enthalpy of dry air and assumed that both influent and effluent air were saturated and at constant total pressure. Both air mass and water vapour mass were assumed constant by Keener et al. (1993).

Models for the degradation of BVS, from which the generation of biological heat, release of biological water and oxygen consumption are predicted, are of key importance in the heat balance expression and will be examined in detail later.

2.3. Mass balance considerations

Approaches to moisture prediction based on an analysis of inlet air content, exit gas content and biologically produced water, have typically been used, with the latter term estimated from yield factors (y or Y) based on BVS degradation (Keener et al., 1993; Kaiser, 1996; Stombaugh and Nokes, 1996; Das and Keener, 1997; Mohee et al., 1998; Higgins and Walker, 2001). A similar approach has been used to estimate oxygen consumption or carbon dioxide evolution. The following expressions from Higgins and Walker (2001) typify these models:

$$\frac{\mathrm{d}M_{\mathrm{b}}}{\mathrm{d}t} = \frac{G_{\mathrm{a}}(H_{\mathrm{s}}(T_{\mathrm{a}}) - H_{\mathrm{s}}(T)) - y_{\mathrm{H_2O/BVS}}\frac{\mathrm{d(BVS)}}{\mathrm{d}t}}{\rho_{\mathrm{db}}V_{\mathrm{r}}}, \qquad (5)$$

$$\frac{\mathrm{d}X_{\mathrm{O_2}}}{\mathrm{d}t} = \frac{G_{\mathrm{a}}(X_{\mathrm{O_2,a}} - X_{\mathrm{O_2,exit}}) - y_{\mathrm{O_2/BVS}}\frac{\mathrm{d(BVS)}}{\mathrm{d}t}}{V_{\mathrm{r}}\varepsilon\rho_{\mathrm{a}}(T)}, \qquad (6)$$

where M_{b} is the moisture content (kg-H$_2$O/kg-dry solids), t is the time (d), G_{a} is the mass flow rate of dry air (kg-dry air/d), H_{s} is the saturated humidity (kg-H$_2$O/kg-dry air), T is the temperature of the composting material (°C), T_{a} is the ambient temperature (°C), y is the metabolic yield of water (kg-H$_2$O/kg-BVS removed) (Eq. (5)), or metabolic consumption of oxygen (kg-O$_2$/kg-BVS removed) (Eq. (6)), BVS is the mass of biodegradable volatile solids (kg), V_{r} is the working volume of the reactor (l), ρ_{db} is the dry bulk density of the composting material (kg/m^3), $X_{\mathrm{O_2}}$ is the concentration of oxygen (kg-O$_2$/kg-dry air), ε is the porosity of the composting material (dimensionless), and ρ_{a} is the density of dry air (kg/l). In the solution of these equations the volume of the composting material and the descriptive parameters were held constant.

2.4. Prediction of state variables

The state variables of primary interest in composting are temperature, moisture content and oxygen concentration. Temperature has been predicted by all models, excepting that of Hamelers (1993). In the model of Haug (1993), temperatures were determined iteratively for a series of discrete steady state heat and mass balances, rather than predicted for non-steady state conditions. Moisture content has been predicted by several authors (Kishimoto et al., 1987; Nakasaki et al., 1987; Ndegwa et al., 2000), and oxygen concentration by Finger et al. (1976), van Lier et al. (1994) and Mohee et al. (1998). Other variables predicted have included oxygen uptake rate (Hamelers, 1993; Stombaugh and Nokes, 1996; Higgins and Walker, 2001), carbon dioxide evolution rate (Kishimoto et al., 1987; Nakasaki et al., 1987; van Lier et al., 1994), dry exit gas mass and exit gas water vapour (Haug, 1993), bulk weight (van Lier et al., 1994; Ndegwa et al., 2000), biomass (Hamelers, 1993; Kaiser, 1996; Stombaugh and Nokes, 1996), total solids (Kishimoto et al., 1987; Hamelers, 1993; Stombaugh and Nokes, 1996; Mohee et al., 1998; Ndegwa et al., 2000) and product solids composition (Haug, 1993; Kaiser, 1996). Given the importance of moisture tension in soil processes, the absence of this term as a state variable is worthy of consideration and may be an important factor at low moisture levels. Miller (1989) has discussed the application of matric potential to composting systems, and has reported an empirical relationship between matric potential and gravimetric water content.

2.5. Related models

Related models include those describing the thermophilic aerobic digestion of waste activated sludge and ground garbage (Andrews and Kambhu, 1973), and cassava fermentation by *Aspergillus* spp (Saucedo-Castaneda et al., 1990; Rodriguez Leon et al., 1991). In common with the composting models, analytical approaches were based around the solution of heat and mass balance expressions, with biological heat and latent heat of evaporation of water identified by Andrews and Kambhu (1973) as the most important items in the heat balance. Temperature was predicted in all cases, although the solution presented by Andrews and Kambhu (1973) was for steady state conditions only. The Saucedo-Castaneda et al. (1990) model also predicted substrate, biomass and carbon dioxide production. One of the features of the latter model was the use of the Peclet (Pe), Biot (Bi) and Damkohler (Da_m) dimensionless numbers, plus dimensionless geometric reactor ratios, in modelling heat transport. The Peclet number also was employed by van Lier et al. (1994), as a guide to which finite difference method to utilise in their model discretisation procedure. The use of dimensionless numbers in future composting process models would be beneficial for scale-up purposes and may offer advantages in helping to explain variations in reactor performance.

3. Substrate degradation and biological energy expressions

3.1. Introduction

The general approach to modelling biological energy production in composting energy balances has been to describe solids degradation, either explicitly using BVS, or implicitly using oxygen consumption or carbon dioxide generation, and then to apply appropriate heat yield factors in order to obtain an energy expression.

3.2. Kinetic foundations

Modellers have used first-order substrate degradation kinetics, Monod-type expressions or empirical substrate degradation equations in modelling biological energy production (Tables 3, 5, 6). Alternatively, Kishimoto et al. (1987) used an empirical expression (without a substrate term), whilst Rodriguez Leon et al. (1991) employed an electron balance technique, in conjunction with an exponential growth function, for biological heat estimation.

The first-order kinetic relationships have been based on either oxygen utilisation (Finger et al., 1976) or volatile solids degradation (Smith and Eilers, 1980; Haug, 1993; Keener et al., 1993; Das and Keener, 1997; Mohee et al., 1998; Higgins and Walker, 2001; Scholwin and Bidlingmaier, 2003) (Table 3). It should be noted that the expression used by Haug (1993), although written in terms of biodegradable volatile solids (BVS), was based on BOD data. First-order rate coefficient values ranging between 0.002 and 0.15 d^{-1}, depending on substrate type and temperature, have been reported (Table 4). Additionally, high temperature values, ranging from 0.025 to 0.190 d^{-1} at 50–60 °C, were tabulated by Keener et al. (1993). Corrections to first-order rate coefficients have been made for temperature, moisture content, oxygen concentration and free air space. The models used for these correction factors are discussed later.

The Monod-type expressions have proceeded from cell growth (first-order) and/or substrate utilisation considerations, and have been used to predict either oxygen uptake rates (Kaiser, 1996) or solids production rates (Stombaugh and Nokes, 1996; Seki, 2000) (Table 5). Kaiser (1996) separately modelled the degradation of four different substrates (sugars and starches, hemicellulose, cellulose and lignin) by four microbial groups (bacteria, actinomycetes, brown-rot fungi, white rot fungi). In two models, temperature corrections to the rate coefficients were made using empirical expressions related to microbial growth (Kaiser, 1996; Stombaugh and Nokes, 1996). Substrate limitation was accounted for in all models and adjustments for moisture level and oxygen concentration made by Stombaugh and Nokes (1996).

Monod-type kinetics, with temperature correction using an Arrhenius-type expression, were also used by Saucedo-Castaneda et al. (1990). In a related approach, a Michaelis–Menten-type kinetic expression for carbon disappearance in a composting system, based on the formation of an intermediate enzyme/substrate complex, was derived by Whang and Meenaghan (1980) and rate constants were evaluated using a Lineweaver–Burke analysis. However, the kinetic model was not utilised for the prediction of biological heat production. An exponential microbial growth expression was used to model biological heat production by Rodriguez Leon et al. (1991).

Empirical kinetic relationships have utilised either oxygen consumption data (Bach et al., 1987; VanderGheynst et al., 1997), carbon dioxide generation data (Nakasaki et al., 1987) or total solids degradation data (van Lier et al., 1994) (Table 6). The data used by Nakasaki et al. (1987) were obtained from the work of Bach et al. (1984). A polynomial relationship describing total solids degradation over a 7-d period in a forced aeration system composting a horse manure and straw mixture, was fitted to experimental results by van Lier et al. (1994). The model used by VanderGheynst et al. (1997) incorporated a power law relationship, and was fitted to O_2 consumption rates from the composting of

Table 3
First-order biological energy (E_b) rate expressions used in composting models

Biological energy rate equation	Rate coefficient corrections used	References
$\frac{dE_b}{dt} = A' \, e^{-\frac{E_a}{RT}} a(c^* - c_1)H_R$	Temperature	Finger et al. (1976)
$\frac{dE}{dt} = [RO_2(\max) \times e^{-\frac{(T-57)^2}{254}} \times e^{-10.973(FS-0.3)^2}] \frac{[HCOMB \times W \times BVS]}{1200}$	Temperature, moisture	after Smith and Eilers (1980)
$\frac{dE_b}{dt} = -[k_{T(fast)} \, BVS_{(fast)} + k_{T(slow)} \, BVS_{(slow)}]H$	Temperature, oxygen, moisture, FAS	Haug (1993)
$\frac{dE_b}{dt} = -k(m_t - m_e)\Delta h_c$	Temperature	Keener et al. (1993), Das and Keener (1997)
$\frac{dE_b}{dt} = -k(m_t - m_e)h_c$	Temperature, moisture	Mohee et al. (1998)
$\frac{dE_b}{dt} = -[k_{BVS} \, BVS]H_{rx}$	Temperature, oxygen	Higgins and Walker (2001)
$\frac{dE_b}{dt} = -9760 y_{O_2,DS,R} m_{DS,R}$	–	Scholwin and Bidlingmaier (2003)

a dog food substrate over a period of 35 h. As previously mentioned, Kishimoto et al. (1987) used an empirical relationship in which biological heat generation was expressed in terms of temperature, moisture content, cumulative energy and airflow rate. The relationship described data from seven previous runs in the same apparatus and using the same substrate.

3.3. Temperature correction functions

Models of the effect of temperature on composting reaction rates have been developed from Arrhenius functions (Finger et al., 1976; Haug, 1993; Bari et al., 2000a; Neilsen and Berthelsen, 2002), empirically from composting data (Schulze, 1962; Smith and Eilers, 1980; VanderGheynst et al., 1997; Mohee et al., 1998), empirically from microbial growth data (Kaiser, 1996; Stombaugh and Nokes, 1996) or based on cardinal (minimum, maximum and optimum) temperatures for microbial growth (Rosso et al., 1993) (Tables 7 and 8).

Experimental composting data has shown that as temperature is increased from about 20 °C, biological activity tends to first increase slowly, then rise moderately to a peak value, following which a rapid decline in activity occurs, typically over a small temperature range. Thus a right-hand skewed curve results, with

Table 4
Rate coefficients and goodness of fit for first-order models of substrate degradation

Model	Rate coefficient (d^{-1})	Goodness of fit[a]	Time (d)	Substrate	References
$BOD_t = A[1 - e^{-k_1 t}] + B[1 - e^{-k_2 t}]$	0.15/0.05[b]	–	60	Raw sludge	Haug (1993)
	0.015/0.004[b]	–	242	Raw sludge	
	–/0.0095[b]	–	200	Pulp mill sludge	
	0.15/0.02[b]	–	90	Softwood sawdust	
	–/0.0081[b]	–	368	Hardwood sawdust	
$\frac{m(\theta)-m_e}{m_o-m_e} = e^{-kt}$	0.048	–	3	Poultry manure, corn cobs	Keener et al. (1993)
OM loss $= A[1 - e^{kt}]$	0.0665	RMS = 67.94	>70	Sorghum bagasse, pig manure, poultry manure	Bernal et al. (1996)
	0.0279	RMS = 29.76	>70	Sorghum bagasse, sewage sludge	Bernal et al. (1996)
$\frac{\Delta BVS}{BVS_0} = 1 - (1 - k'_1 \Delta t) \cdots x(1 - k'_n \Delta t)$	0.002–0.013[c] 0.018–0.051[d]	R^2 = 0.450–0.844	28	Food waste, paper, sawdust	Bari et al. (2000a)
OM loss $= A[1 - e^{-kt}]$	0.0598	RMS = 4.031 d	>84	Poultry manure, cotton waste, olive mill ww[e]	Paredes et al. (2000)
	0.0226	RMS = 32.34	>84	Sewage sludge, cotton waste, olive mill ww	Paredes et al. (2000)
	0.0594	RMS = 13.48	>84	Sewage sludge, cotton waste[e]	Paredes et al. (2001)
OM loss $= a[1 - e^{-kt}]$	0.0749	RMS = 12.20	>84	Sewage sludge, cotton waste	Paredes et al. (2001)
	0.0377	RMS = 12.72	>84	Orange waste, cotton waste[e]	Paredes et al. (2001)
	0.0203	RMS = 33.50	>84	Orange waste, cotton waste	Paredes et al. (2001)
OM loss $= a[1 - e^{-kt}]$	0.0181	RMS = 23.55	>168	Olive mill sludge, cotton gin waste	Paredes et al. (2002)

[a] R^2 = correlation coefficient; RMS = residual mean square.
[b] Data obtained from constant temperature and pressure respirometry, with substrates present in solution. The data is tabulated as fast coefficient (k_1)/slow coefficient (k_2).
[c] At 25 °C.
[d] At 50 °C.
[e] Watered with olive mill wastewater (ww).

Table 5
Monod-type biological energy (E_b) rate expressions used in composting models

Biological energy rate equation	Rate coefficient corrections	References
$\frac{dE_b}{dt} = c_c \frac{MM_{CO_2}}{MM_c}(Y-1) \times \left(\frac{ds_1}{dt} + \frac{ds_2}{dt} + \frac{ds_3}{dt} + \frac{ds_4}{dt}\right) \times M\beta 14{,}000$	Temperature, substrate type	Kaiser (1996) (β and 14,000 (kJ/kg O_2) terms added)
$\frac{dE_b}{dt} = \left[\frac{1}{Y_{X/S}}\frac{dX}{dt} + \beta X\right] Y_{H/S}$	Temperature, substrate type, moisture, oxygen	Stombaugh and Nokes (1996)
$\frac{dE_b}{dt} = V\left\{\frac{dS}{dt} + \frac{dX}{dt}\right\}\Delta h_s$	Temperature, substrate type	Seki (2000)

Table 6
Empirical biological energy (E_b) rate expressions used in composting models

Basis	Biological energy rate equation	Rate coefficient corrections used	References
–	$\frac{dE_b}{dt} = G_o(Z_0 - Z_e')Q_0$	None	Bach et al. (1987)
Regression	$\frac{dE}{dt} = e_0 + e_1 T + e_2 w_c + e_3 \int q_r \, dt + e_4 F$	na	Kishimoto et al. (1987)
Linear	$\frac{dE_b}{dt} = -r_{O_2} W_s Q_0$	None	Nakasaki et al. (1987)
Polynomial model of substrate degradation data	$\frac{dE_b}{dt} = f(\Delta DM)\Delta H^0$	None	van Lier et al. (1994) ($f(\Delta DM)$ is a fitted polynomial)
Exponential model of oxygen consumption data	$\frac{dE_b}{dt} = [RO_{2,0} + a(1 - e^{-C(T-T_0)})]Q$	Temperature: $(a[1 - e^{-C(T-T_0)}])$	VanderGheynst et al. (1997)

Table 7
Temperature correction functions used in conjunction with first-order biological energy rate expressions

Temperature correction function	References
$k_g = A' e^{-\frac{E_q}{RT}}$	Finger et al. (1976)
$e^{-\frac{(T-57)^2}{254}}$	Smith and Eilers (1980)
$k_T = k_{20}[1.066^{(T-20)} - 1.21^{(T-60)}]$	Haug (1993)
$k = \{-8e^{-6} \times T^3 + 0.008 \times T^2 - 0.0238 \times T + 0.2643\}$	Mohee et al. (1998)
$k_{BVS(T)} = k_{BVS}(f_T)$	Higgins and Walker (2001)
$k_{BVS} = \frac{\beta_r R_{CO_2 opt}}{10^3 \gamma_{O_2}(BVS)}(f_T)(f_{O_2})$	
$f_T = \frac{(T-T_{max})(T-T_{min})^2}{(T_{opt}-T_{min})(T_{opt}-T_{min})(T-T_{opt})-(T_{opt}-T_{max})(T_{opt}+T_{min}-2T)}$	(Model of Rosso et al. (1993))

the optimum and maximum temperatures generally very close together. Similar behaviour has been described for other microbial growth studies. A number of models have generated profiles which reflect this phenomenon well (Haug, 1993; Rosso et al., 1993) or are relatively close to it (Smith and Eilers, 1980). However, in other cases this pattern has been less well represented. For example, the temperature correction functions used by

Table 8
Temperature correction functions used with Monod-type biological energy (E_b) rate expressions

Temperature correction	References
$f_1^{temp} = \frac{T(80-T)}{1600} \ldots 0 < 80\,°C$	Kaiser (1996)
$f_{2\ldots4}^{temp} = \frac{T(60-T)}{20(80-T)} \ldots 0 < 60\,°C$	
$k_{temp} = \frac{T}{T_2 - T_1} \qquad T_1 < T < T_2$	Stombaugh and Nokes (1996)
$k_{temp} = 1.0 \qquad T_2 < T T_3$	
$k_{temp} = 3.75 - \left[\frac{T}{T_2 - 10}\right] \qquad T_3 < T$	
$T_1 = 0\,°C$	
$T_2 = 30\,°C$	
$T_3 = 55\,°C$	

Kaiser (1996) showed parabolically shaped curves, with a high degree of activity indicated at 20 °C, peak temperatures of 40 °C for all substrates and organisms, and a relatively slow decline above the optimum temperature. A simpler approach was used by Stombaugh and Nokes (1996), who adopted three linear temperature correction functions over the ranges 0–30, 30–55 and >55 °C, with a constant value for peak activity from 30 to 55 °C.

The temperature correction model of Neilsen and Berthelsen (2002) was based on an enzyme/substrate mechanism in combination with an Arrhenius type expression. It was developed to overcome problems with negative values at high temperature (i.e., above 80 °C) occurring with the Haug (1993) model. Whilst it is unlikely that many composting systems would operate at or above 80 °C, the model may be useful for related solid-state processes. No validation data was presented.

In contrast to the models showing a peak, followed by a decrease, in activity, the Arrhenius model utilised by Finger et al. (1976) increased exponentially. The empirical model developed by VanderGheynst et al.

(1997) tended to a plateau at a temperature differential of about 30 °C, which is equivalent to 50 °C given a starting temperature of 20 °C. However, given the high degree of scatter in the experimental data and evidence of a declining trend in the rate at higher temperatures, a model of the skewed form described above might also be fitted in this case. A polynomial expression for the rate coefficient k, with a form similar to the skewed models in their sub-optimal temperature range, was used for temperature correction by Mohee et al. (1998). However, a peak and subsequent decrease within the biologically active range was not indicated and the function continued to increase beyond 80 °C.

Three models used to correct for the effect of temperature on the microbial growth rate (Andrews and Kambhu, 1973; Ratkowsky et al., 1983; Rosso et al., 1993) were evaluated in detail by Richard and Walker (1998), using new experimental data. Whilst all models showed an acceptable fit, it was concluded that the model of Rosso et al. (1993) provided the best description of the rate coefficient temperature dependence, since it involved the fewest parameters, all of which were easily measurable and each of which had a physical meaning in terms of the composting process.

3.4. Moisture, oxygen and FAS correction functions

Published moisture correction functions employed in composting process models (Table 9) have all been derived empirically. An exponential expression indicating maximum activity at 70% moisture content was used by Smith and Eilers (1980). A similar model, reportedly based on data of Smith and Eilers (1980), was employed by Mohee et al. (1998), although in the form presented in the literature, this produces an unrealistic curve. However, following adjustment to ensure that a negative exponent is always present and the moisture content is expressed as a fraction, a curve with a peak at 0.56 moisture content may be produced. However, the modified function is negative at fractional moisture levels of

<0.17 and >0.97 and has a different profile to the model of Smith and Eilers (1980). In contrast, a function with a plateau above 70% was proposed by Haug (1993). As noted by Haug, a decreasing trend in data at higher moisture levels, which was not described by the model, was probably attributable to diminishing free air space. In order to correct for this, Haug (1993) also presented a free air space correction function of similar mathematical form to that used for moisture dependence. When the moisture and free air space correction functions are combined, a model of similar form to that of Smith and Eilers (1980) is produced, illustrating the interdependence of these two factors in terms of their influence on reaction rates. As noted by Haug (1993), it can be difficult to separate out the effects of moisture, free air space and also bulk weight. More recently, a mechanistic model relating moisture content and respiration rate has been proposed by Hamelers and Richard (2001). This model predicts a relationship of similar form to that generated by the temperature correction model of Rosso et al. (1993) and has shown a promising fit to experimental data as reported by Richard et al. (2002).

The effect of oxygen concentration has been modelled using Monod-type and exponential, expressions (Haug, 1993; Richard et al., 1999). A simple one-parameter model was used by Haug (1993), with a half saturation constant value of 2%. More recently, Richard et al. (1999) compared the performance of one-parameter, modified one-parameter and two-parameter Monod-type models, plus an exponential model, using an extensive data set. It was concluded that the Monod-type models gave the best performance over the complete temperature range, and suggested that the simple one-parameter model was best suited to windrow composting applications where low oxygen levels may be encountered, whilst the modified one-parameter model may be preferable for forced aeration systems operating at relatively high oxygen concentrations. The simple one-parameter model, with the half saturation constant expressed as an empirical function of temperature and

Table 9
Moisture, oxygen and free air space rate coefficient adjustment expressions used in composting models

Moisture correction	Oxygen correction	FAS correction	References
$F_1(I) = \frac{1}{e^{[-17.684(1-SMOUT)+7.0622]}+1}$	$F_{O_2}(I) = \frac{VOLPO2(I)}{VOLPO2(I)+2}$	$F_1(I) = \frac{1}{e^{[-23.675FAS(I)+3.4945]}+1}$	Haug (1993)
$e^{-10.973(FS-0.3)^2}$	None	None	Smith and Eilers (1980)
$f(m_c) = -56.97 + 57.98\, e^{((-0.5(m_c-0.56)/1.52)^2)}$	None	None	Mohee et al. (1998)
None	$f_{O_2} = \frac{O_2}{k_{O_2}(T.X_{H_2O})+O_2}$ $k_{O_2} = 0.79 - 0.041T + 0.040X_{H_2O}$	None	Higgins and Walker (2001)
$kH_2O = 0.0 \quad m_1 < m < m_2$ $kH_2O = \frac{m}{m_2} - 1.0 \quad m_2 < m \leqslant m_3$ $kH_2O = 1.0 \quad m_3 < m$ $m_1 = 0$ kg/kg(wb) $m_2 = 0.2$ kg/kg(wb) $m_3 = 0.4$ kg/kg(wb)	Monod	None (Note: moisture factor = 1, when $m > 0.4$)	Stombaugh and Nokes (1996)

moisture concentration, was subsequently used in the composting model validation study of Higgins and Walker (2001).

3.5. Heat conversion factors

Most modellers have utilised simple heat conversion factors, based on volatile solids degradation or oxygen consumption, to obtain energy, or power, values from substrate degradation models. Values have been obtained from calorimetric measurements, calculated from COD data (Haug, 1993), or determined using an electron balance method (Rodriguez Leon et al., 1991). The reported available energy from organic substrates has ranged from 17.8 to 24.7 kJ/g-TS removed (sometimes expressed as kJ/g-volatile solids (VS) removed) (Haug, 1993; Keener et al., 1993; van Ginkel, 1996), or, on an oxygen basis, been reported as 9760 kJ/kg-O_2 consumed (Harper et al., 1992) and 14,000 kJ/kg-O_2 consumed (Kaiser, 1996). Given the range of values reported and the importance of biologically generated heat in composting process models, it is suggested that the sensitivity of models to variations in this parameter would be worthy of further investigation.

3.6. Model parameters

The number of model parameters required, and the ease by which their values may be obtained, will influence the utility of mathematical models, and to some extent determine whether they are employed as operational or research tools. Furthermore, whether the parameters are obtained independently, or fitted by the model, will impact on the usefulness of the model. Whilst fitted parameters may facilitate the demonstration of general trends, they do not enable the model to be properly validated.

Parameters may be considered under three major categories: (a) those describing fundamental properties of air, water and insulating materials (e.g., specific heat of water, density of air, thermal conductivity); (b) those describing the raw composting material characteristics (e.g., bulk density, porosity); and (c) those relating to substrate degradation rates and microbial growth. The total number of parameters (not including reactor dimensions or fitted mathematical constants) specified in composting process models have ranged from approximately 6, for a model comprised largely of empirical expressions (Nakasaki et al., 1987), to 20–30 for models where extensive heat and mass related calculations, or Monod-type expressions, are incorporated (Kaiser, 1996; Stombaugh and Nokes, 1996; Scholwin and Bidlingmaier, 2003). Fundamental parameter values for air, water and insulation materials used in composting process models have generally been independently measured and/or previously reported elsewhere in the literature, and may comprise a large proportion of the total number of parameters utilised (e.g., Scholwin and Bidlingmaier, 2003). Likewise, compost material, reaction rate and microbial growth parameters have typically been measured independently. First-order rate models require a single rate coefficient, plus parameters for temperature, moisture and oxygen correction factors, whereas the Monod-type models require four, or more, reaction rate related parameters, including maximum specific growth rate (μ_{max}), decay coefficient (λ), half-saturation coefficient (k_s) and maintenance coefficient (β). In the model of Seki (2000) initial values for μ_{max} and λ were adjusted in order to obtain a good simulation. Monod-type models also require an estimate of initial microbial mass (X_i) (Kaiser, 1996; Stombaugh and Nokes, 1996; Seki, 2000). Up to five yield factors, based on BVS removal (moisture, O_2, CO_2, heat, cell mass), may be employed. In several models mathematical constants have been fitted from experimental data (e.g., VanderGheynst et al., 1997; Seki, 2000).

Other fitted parameters have included a thermal diffusion coefficient value of 6.86×10^{-12} ft^2/h (1.77×10^{-16} m^2/s) (Finger et al., 1976) and a heat coefficient of 9500 kJ/kg-O_2 obtained by VanderGheynst et al. (1997). Whilst the heat coefficient compared closely to the value reported by Harper et al. (1992), the thermal diffusivity coefficient value of was low compared to expected values (e.g., Iwabuchi et al., 1999).

4. Simulation

4.1. Temperature

Temperature profile simulations have been reported by Kishimoto et al. (1987), Kaiser (1996), Stombaugh and Nokes (1996), Bertoni et al. (1997), Das and Keener (1997) and Mohee et al. (1998). The profiles presented by Stombaugh and Nokes (1996) showed patterns similar to those reported for full-scale systems, whilst those of Das and Keener (1997) showed general similarities over 7 d. In contrast, the profile predicted by the model of Kaiser (1996) showed a typical lag phase and rapid rise at early time, but subsequently an apparently linear relationship of low slope. The latter was similar to data and predictions reported by van Lier et al. (1994). The model simulations of Mohee et al. (1998) suggested a relatively flat temperature rise compared to typical rapid temperature increases at early time in response to variations in airflow rate. A simulation to determine the optimum aeration regime for composting waste activated sludge was reported by Kishimoto et al. (1987). This produced a schedule of aeration rates, with the objective of reaching a

temperature of 65 °C in 16.7 h, rather than the 40 h achieved experimentally. A temperature versus time simulation for a biosolids/woodchips mixture at constant airflow (Haug, 1993), showed a realistic profile over a 10 d period. Additional simulations, in which temperature set points were used, and airflow rates varied, showed an eventual decline in temperature, following initially flat profiles.

4.2. Moisture, oxygen and solids

Other simulations have included moisture profiles (Kishimoto et al., 1987; Kaiser, 1996; Stombaugh and Nokes, 1996; Bertoni et al., 1997; Das and Keener, 1997; Ndegwa et al., 2000), oxygen concentrations (Hamelers, 1993; van Lier et al., 1994; Bertoni et al., 1997; Mohee et al., 1998) and solids levels (Hamelers, 1993; Kaiser, 1996; Stombaugh and Nokes, 1996; Das and Keener, 1997; Mohee et al., 1998; Ndegwa et al., 2000; Seki, 2000). Profiles of oxygen, substrate and biomass concentration with time, plus oxygen uptake rates for four different substrates were reported by Hamelers (1993), whilst effects of pad insulation, pile height, mixture density, external temperature and external oxygen, on compost uniformity, were explored by Finger et al. (1976). Haug (1993) presented a range of simulations as a function of time, airflow rate and other variables.

The simulations described have provided valuable insights into the response of models to a range of operating parameter variations. However, their value is limited when validation against experimental data is not included.

4.3. Model sensitivity

The sensitivity of a Monod-type model to variations in key microbial parameters was investigated by Stombaugh and Nokes (1996). It was reported that variations in μ_{max} and λ had the greatest effect on biomass, substrate and maximum temperature values, whilst the model was relatively insensitive to changes in k_s, X_i, the decay coefficient (k_d), the cell yield ($Y_{X/S}$) and the oxygen half saturation coefficient (k_{O_2}). VanderGheynst et al. (1997) explored the effect of assumptions of saturation, constant dry mass air flux and constant moisture on their model, and concluded that these were not significant enough to account for the observed discrepancies between the model and the data. They noted however that their rate equation was expressed as a function of temperature only, and not of time, and suggested that the differences were most likely due to an error in the heat generation equation.

Analyses of the sensitivity of models to changes in fundamental parameters have been relatively limited, and further investigation in this area is suggested.

5. Validation

5.1. Temperature

In comparing model performance to experimental data, quantitative measures of performance may be provided by differences in maximum, average and peak temperatures, relative times to reach peak temperatures, the relative areas beneath the curves and a specified baseline, and times for which specified temperatures are maintained. Profile shape characteristics may also be compared to typical curves for a qualitative assessment. In the following analysis, parameters used were areas bounded by the profiles and a 40 °C baseline (A_{40}), the times for which thermophilic temperatures were equalled or exceeded (t_{40}), the times to reach peak temperatures and the general shape characteristics compared to those of a generic profile. Details of the methods used to determine A_{40} and t_{40}, plus a description of the generic profile characteristics, are given in Mason and Milke (in press-b). Summaries of model performance on the above bases are presented in Tables 10 and 11 and example temperature profiles presented in Figs. 1–4.

Maximum differences between modelled and experimental temperature–time profiles varied widely, ranging from 1.2 to 30.4 °C, but with discrepancies >10 °C predominating (Table 10). In several profiles (van Lier et al., 1994; Bertoni et al., 1997; Kim et al., 2000; Scholwin and Bidlingmaier, 2003), these differences occurred during the initial period of rapid temperature rise; however, in most cases they occurred at later time. Average temperature discrepancies also varied considerably, ranging from <0.5 to 17.5 °C, but with most values <10 °C. Peak temperatures tended to be more precisely predicted, with many values within 3 °C of the experimental data. In a majority of cases, times at which peak temperatures occurred were predicted to within 0.5 d of the data, however differences ranged from 0.1 to 4.5 d. In contrast, predicted and experimental A_{40} values were in relatively close agreement. The duration of studies varied widely, but most were conducted over 10 d or less.

In terms of shape characteristics, several models simulated the typical profile closely, although this was not always well correlated with experimental data (e.g., Smith and Eilers, 1980). In several studies (e.g., Kishimoto et al., 1987; Nakasaki et al., 1987) the short time frame precluded presentation of the overall shape of the profile. The model developed by Ndegwa et al. (2000) tracked the overall temperature–time patterns in a semi-continuous system, with bed depths of 0.41 and 0.61 m, relatively well over selected time periods, but was unable to reliably predict peak temperatures arising after mixing.

The ability of models to predict process temperatures to within a specified margin through to the

Table 10
Temperature–time profile validation performance of composting models

System description			Performance						
References	Reactor type	Scale	Temperature difference between model and data (°C)			Times to peak		A_{40} ratio[a]	Duration of study	Comments
			Maximum	Mean	Peak[b]	Model	Data			
Smith and Eilers (1980)	ASP	Full	27.5	17.5	6.6	7.6 d	3.1 d	2.49	29 d	Data for piles A, B, C and D, respectively. Model simulated shape characteristic well, but fit to experimental data was generally poor
			26.5	16.3	6.6	7.6 d	3.5 d	2.30		
			22.4	8.8	1.8	8.4 d	6.1 d	1.07		
			15.3	7.7	1.8	8.4 d	8.1 d	0.82		
Kishimoto et al. (1987)	Column	Lab	4.0	1.7	<0.5	32.8 h	35.9 h	1.09	40 h	Generally close fit between model and data
Nakasaki et al. (1987)	Column	Lab	6.9	1.6	2.8	26.2 h	30.4 h	1.03	90 h	Model over-predicted at later time. Model over-predicted at early and later time
			10.6	1.9	<0.5	71.1 h	78.3 h	1.06	130 h	
van Lier et al. (1994)	Bin	Pilot	1.2	<0.5	1.2	0.4 d	0.5 d	1.04	7 d	Data for top and bottom measuring locations, respectively. Generally close fit between model and data
			4.2	1.0	2.5	0.6 d	0.5 d	1.03		
Kaiser (1996)	Column	Pilot	13.3	4.1	3.3	3.9 d	1.7 d	0.83	10 d	Model under-predicted to about 2 days and from 7.5 days; shape well simulated from 2–7.5 d
Bertoni et al. (1997)	Trench	Full	30.4	8.1	1.5	4.2 d	5.0 d	0.93	33 d	–
Das and Keener (1997)	Bin	Full	17.3–29.9	8.4–13.3	1.7–8.0	0.8 d	0.8–1.0 d	0.87–1.40	7 d	Data range for 5 'slices' in the top layer of the reactor; atypical shape characteristics
Mohee et al. (1998)	Column	Lab	16.5[c]	4.2[c]	0.5[c]	9.4 d	8.9 d	1.66[c]	15 d	Model predicted to within 4.3 °C (average 1.8 °C) to day 11 then over-predicted at later time; atypical shape characteristics
Kim et al. (2000)	Bin	Pilot	9.7	6.1	5.4	2.7 d	5.2 d	0.95	45 d	Model over-predicted peak and at later time
Ndegwa et al. (2000)	Tray	Full	16.5	4.1	14.0	–	–	–	60–120 d	Deep bed system
			24.1	7.5	17.7	–	–	–	120–180 d	Deep bed system
			26.5	4.5	23.6	–	–	–	60–120 d	Shallow bed system
			20.4	4.3	16.8	–	–	–	120–180 d	Shallow bed system
Seki (2000)	Column	Lab	16.5/17.1[d]	5.4/6.5[d]	9.0/10.9[d]	66.1/65.2 h	75.5 h	0.97/1.10[d]	190 h	Both models under-predicted from about 9–59 h and 149–190 h; shape poorly simulated at early time
Higgins and Walker (2001)	Column	Pilot	–	–	1.5–11.8	–	–	–	–	Prediction temperatures varied with initial moisture, airflow and respiration quotient
Scholwin and Bidlingmaier (2003)	Column	Lab	11.4	3.0	1.8	34.7 h	20.8 h	1.00	120 h	Model under-predicted to 35.5 h, then under-predicted by an average 1.9 °C to 120 h; good shape characteristics

[a] A_{40} is the area bounded by the curve and a baseline of 40 °C; ratio is A_{40} (model)/A_{40} (data).
[b] Peak temperatures regardless of time of occurrence.
[c] Top layer data only.
[d] Deterministic model/stochastic model.

Table 11
Temperature–distance profile validation performance of composting models

System description			Performance			
References	Reactor type	Scale	Temperature difference between model and data (°C)		Distance	Comments
			Maximum	Mean		
Finger et al. (1976)	Windrow	Full	2.8	1.0	3.0 ft	Model over-predicted at centre (2.8 °C), otherwise a close fit was shown
VanderGheynst et al. (1997)	Column	Pilot	3.4	1.6	1.8 m	Data at 24 h
			12.1	3.2		Data at 29 h
			10.3	5.2	0.6 m	Data at 29 h

end of the thermophilic phase, and to closely simulate the magnitude and timing of peak temperatures, is important if models are to be used to indicate process

Fig. 1. Temperature–time profile of van Lier et al. (1994) (adapted) (reproduced with permission).

performance. Whilst acceptable margins are open to debate, it is suggested that maximum, average and peak temperature discrepancies of 5, 2 and 2 °C, respectively, with peak times predicted to within about 8 h, would be appropriate for the purposes of discussion. Based on these criteria, no models have shown an acceptable predictive ability, although many have met one or more of the goals. In particular, the models of Kishimoto et al. (1987), Nakasaki et al. (1987) and van Lier et al. (1994) met the average temperature difference goal of <2 °C and predicted the timing of peak temperatures to within 8 h, although some peak temperature differences were slightly >2 °C. The profile presented by van Lier et al. (1994) is shown in Fig. 1. Whilst values of A_{40} agreed to within 3–9%, the studies of Kishimoto et al. (1987), Nakasaki et al. (1987) and van Lier et al. (1994) were all relatively short term, and none was run through to the end of the naturally occurring thermophilic phase.
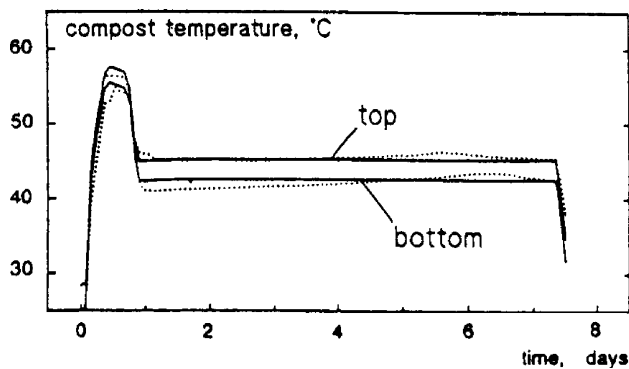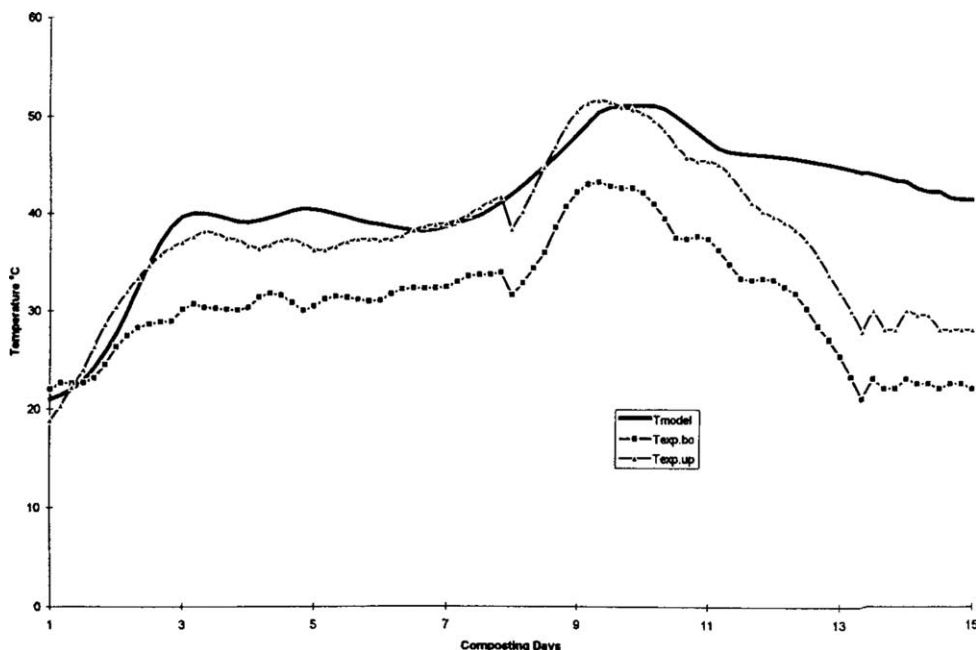

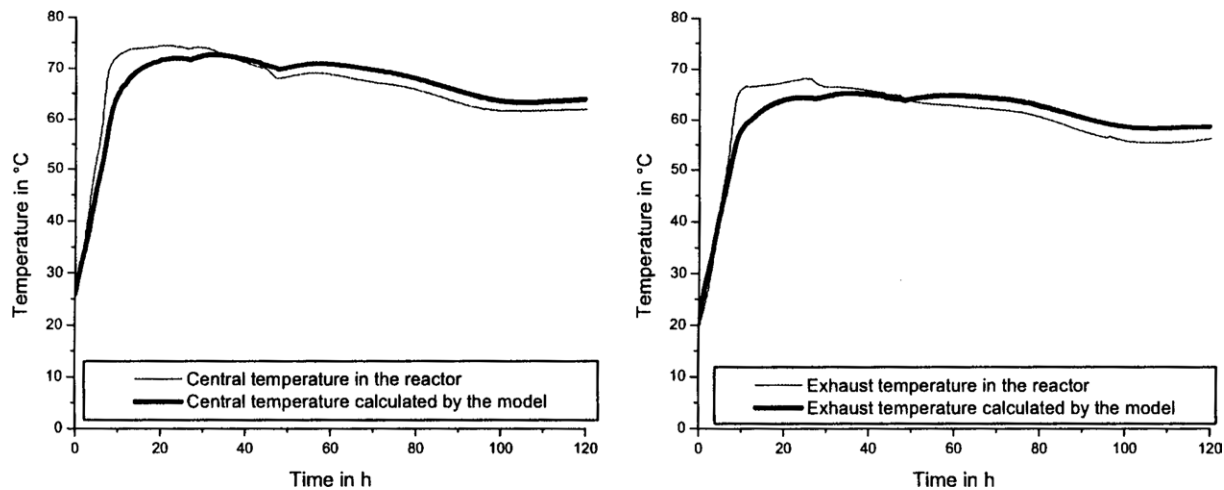Fig. 2. Temperature–time profile of Mohee et al. (1998) (reproduced with permission).

Fig. 3. Temperature–time profile of Scholwin and Bidlingmaier (2003) (reproduced with permission).
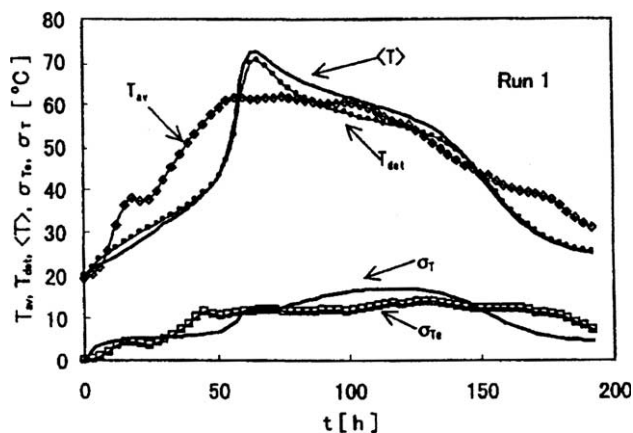

Fig. 4. Temperature–time profile of Seki (2000) (reproduced with permission).

Other models showing good individual predictions include those of Mohee et al. (1998) and Scholwin and Bidlingmaier (2003) (Figs. 2 and 3), where peak temperatures were predicted to within <2 °C, and the model of Das and Keener (1997) which also predicted temperatures to within <2 °C in some cases. It should be noted that whilst the model of Scholwin and Bidlingmaier (2003) showed a large discrepancy during the initial rapid temperature rise phase, it agreed with the experimental data to within 2 °C, from about 36 h onwards.

Steady state spatial temperature predictions in a horizontal plane by Finger et al. (1976) agreed closely with experimental data over most of the profile (Table 11), but as noted above this model used several fitted parameters. Non-steady state spatial predictions in a vertical plane by VanderGheynst et al. (1997) showed varying performance with time. The model predicted temperatures to within <2 °C on average over a depth

of 1.8 m after 24 h, with a peak discrepancy of 3.4 °C, but predictions at 29 h were considerably less precise (Table 11).

Temperature predictions by the cassava fermentation model of Saucedo-Castaneda et al. (1990) showed good agreement with experimental data between 15 and 30 h, with maximum and average discrepancies at the centre of the column of 2.4 and 1.0 °C, respectively. Modelled and experimental temperatures reported by Rodriguez Leon et al. (1991) between 0 and 20 h were particularly close. However, it should be noted that the overall experimental temperature range in this study was very small (<2 °C).

The most successful models in temperature profile prediction have incorporated empirical data into the biological energy rate model (Nakasaki et al., 1987; van Lier et al., 1994; Scholwin and Bidlingmaier, 2003), used a first-order model with empirical correction factors (Mohee et al., 1998), or alternatively, utilised a regression analysis (Kishimoto et al., 1987). Whilst the performance of these models indicated that the basic structure of the heat balance was sound, the use of empirical biological energy expressions limits their application. As already noted, VanderGheynst et al. (1997) considered that the biological heat generation component of their model may have been responsible for the differences between model predictions and experimental data in their work, as the influence of errors in air saturation, dry air mass flux and moisture were found to be insufficient to explain the discrepancies observed. Additionally, CCR losses were omitted from this model, and it would be useful to establish whether this mechanism was significant for the type of experimental system used by these authors. The results presented by Mohee et al. (1998) indicated that a first-order kinetic expression, corrected for temperature and moisture variations, was reasonably appropriate for a bagasse sub-

strate over a period of 0–9 d, even though the temperature profiles showed a large difference between modelled and experimental A_{40} values. The subsequent discrepancy between the model and data is reflected in the solids removal model (Figs. 2 and 7). Given that the typical time frame for thermophilic composting is 20–30 d (Rynk, 1992) any further work should involve the prediction of temperature and other profiles over similar time periods.

In terms of adjustment of first-order rate coefficients, the temperature correction model of Rosso et al. (1993) (Fig. 5) has been shown to work well, whilst saturation-type expressions evaluated by Richard et al. (1999) have given good results for oxygen concentration. However, the moisture correction functions are all empirical and although some may be realistic (e.g., Smith and Eilers, 1980) (Fig. 6), further research in this area, in conjunction with free air space considerations, is suggested.

The models incorporating Monod-type biological energy rate expressions were generally less successful in temperature–time profile prediction. In two cases (Kaiser, 1996; Seki, 2000) the models under-predicted temperature at both early and later time. Whilst soundly based on microbial growth mechanisms, the Monod approach may be difficult to adopt on a broader basis for mixed and variable microbial composting populations, due to difficulties in parameter estimation.

5.2. Solids

Considerable variation in the performance of the first-order models with respect to substrate degradation is evident. Both the single and double exponential BOD expressions used by Haug (1993) as the basis for the BVS model showed reasonably good fit to selected BOD data at constant temperature, over 60–348 d.
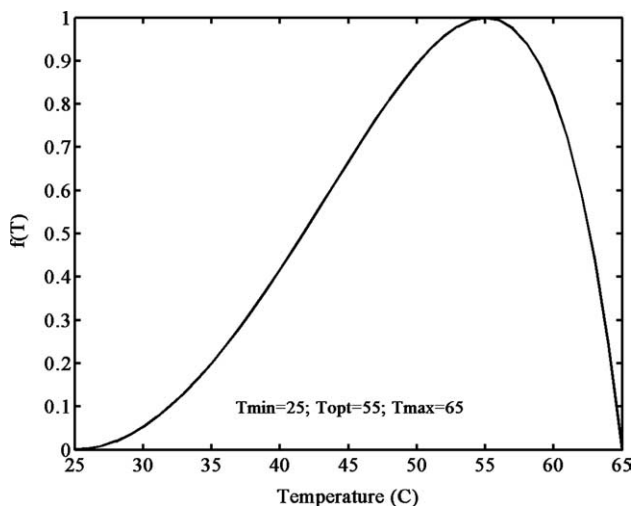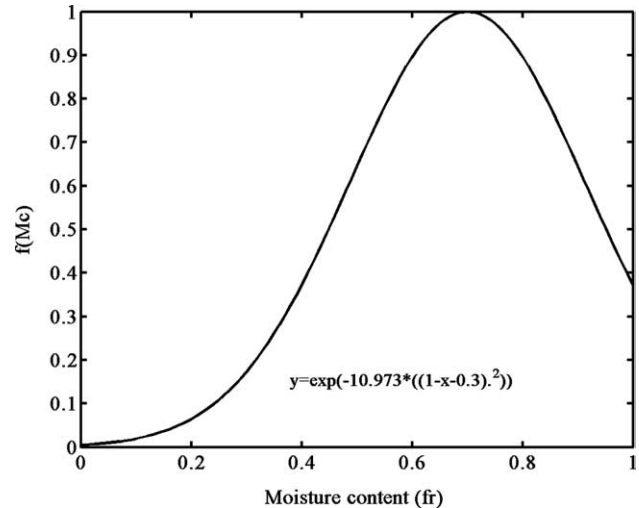

Fig. 6. Moisture correction function of Smith and Eilers (1980).

However, these data were generated from respirometry with the substrate in solution, rather than in a composting environment, and the fit to BVS data under composting conditions was not shown. Solids data from a composting trial presented by Keener et al. (1993) showed that an uncorrected first-order model described substrate removal adequately for two experimental data sets over the first 3 days of composting only. In contrast, when this model was corrected for temperature and moisture (Mohee et al., 1998), it showed relatively close agreement with experimental data over a period 0–8 d, with a subsequent maximum deviation of 2.6% between days 9 and 15 (Fig. 7). More recently, Bari et al. (2000a) have shown evidence of a relatively good fit ($R^2 = 0.844$), using a temperature corrected first-order model (Fig. 8), but have also presented data sets with poorer correlations. It should be noted that volatile solids data in the latter work were calculated from CO_2 data, rather than measured directly. A first-order model without temperature correction has shown evidence of a fairly good fit at later time over periods exceeding 70, 84 and 168 d (Bernal et al., 1993; Paredes et al., 2001, 2002) (Table 4). However, the number of data points at early time was low, and the fit in this region generally poor.

In the case of Seki (2000) the model predictions for substrate degradation and biomass production fitted experimental data closely (Fig. 9), but the goodness of fit of the other Monod-type models to experimental substrate degradation data was not shown. The success in solids modelling was not always reflected in the temperature profile predictions however (e.g., Seki, 2000) (Figs. 4 and 9), and further investigation of the reasons for this discrepancy is indicated. Predictions of compost mass (Kishimoto et al., 1987; Mohee et al., 1998), volatile solids conversion (Nakasaki et al., 1987) and dry bulk

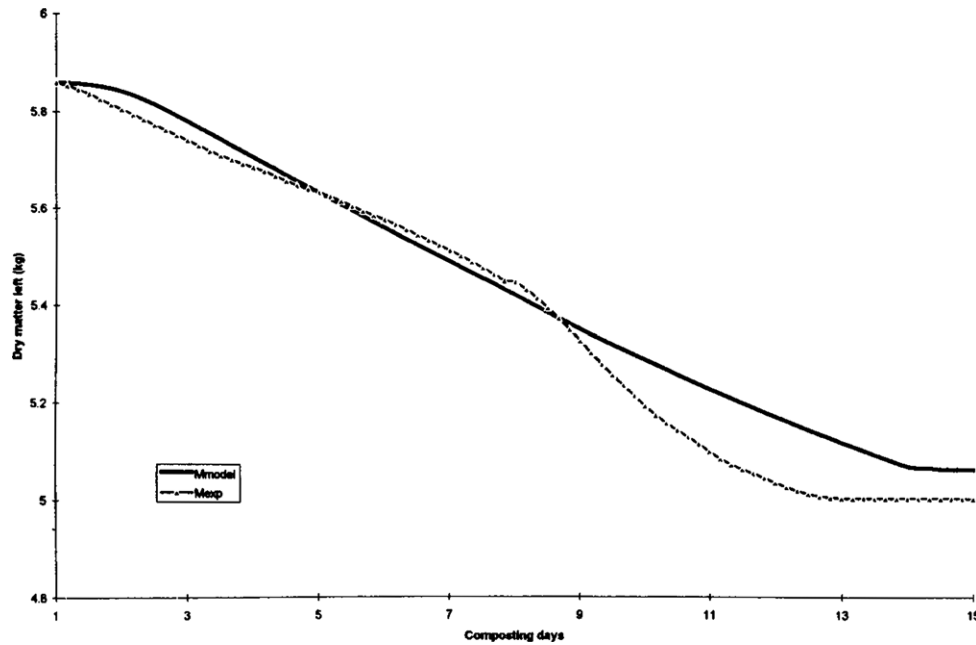Fig. 5. Temperature correction function of Rosso et al. (1993).

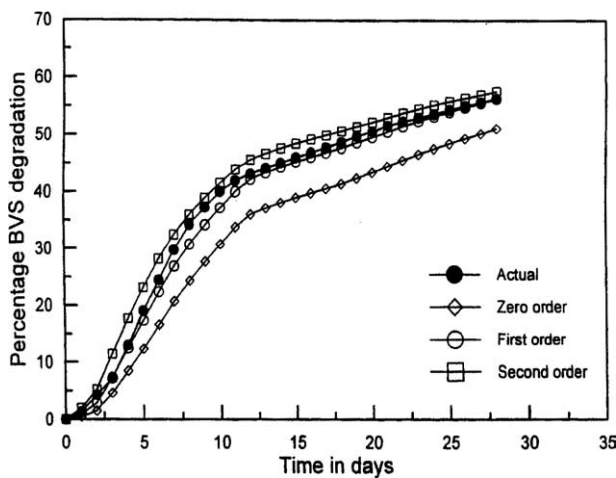Fig. 7. Dry mass vs. time profile of Mohee et al. (1998) (reproduced with permission).

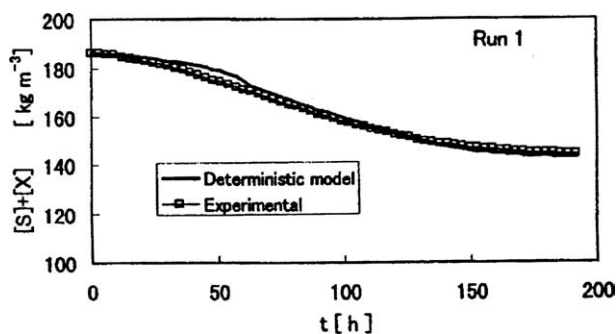Fig. 8. BVS vs. time profile of Bari et al. (2000a) (reproduced with permission).

Fig. 9. Dry matter vs. time profile of Seki (2000) (reproduced with permission).

density (Seki, 2000) all showed close agreement with experimental data (Table 12).

Given the relatively successful fit of a first-order model with temperature correction to BVS degradation data over a 28-d period (Bari et al., 2000a), more research aimed at exploring the development of improved first-order biological heat production models would seem worthwhile. A similar approach, in which the first-order rate coefficient was adjusted using stochastic techniques, has been successfully applied to the modelling of BOD data (Borsuk and Stow, 2000). Alternatively, a double exponential approach, incorporating separate terms for rapidly and slowly degradable substrates (Haug, 1993) along with temperature and moisture correction functions, is suggested for further investigation. Bari et al. (2000a) also showed that BVS degradation could be adequately predicted using exit gas temperatures to adjust the value of the first-order rate coefficient.

5.3. Moisture

Two models have successfully predicted moisture levels over time. Moisture data presented by Kishimoto et al. (1987) showed good agreement with experimental results between 0 and 20 h, after which the model slightly under-predicted the data, whilst mixture moisture content predictions by Nakasaki et al. (1987) showed very close agreement with the experimental data (Table 12). In both cases the discrepancies were small in relation to the moisture levels reported. In contrast, the model of Ndegwa et al. (2000) indicated fair to good agreement only.

Table 12
Moisture, oxygen, carbon dioxide and solids vs. time validation performance of composting models

System description			Performance assessment							
			Differences between model and data							
References	Reactor type	Scale	Moisture		O_2 or CO_2 Concentration		O_2 or CO_2 rate		Solids	
			Maximum	Mean	Maximum	Mean	Maximum	Mean	Maximum	Mean
Kishimoto et al. (1987)	Column	Lab	0.54%	0.23%	–	–	–	–	0.12 kg	0.04 kg
Nakasaki et al. (1987)	Column	Lab	–[a]	–[a]	–	–	4.46[b]	1.33[b]	1.94%[c]	0.75%[c]
			–[a]	–[a]	–	–	2.81[b]	0.81[b]	1.08%[c]	0.31%[c]
Hamelers (1993)	Column	Lab	–	–	–	–	–	–	–[d]	–[d]
Keener et al. (1993)	–	–	–	–	–	–	–	–	0.16[e]	0.07–0.09[e]
Kaiser (1996)	Column	Pilot	–	–	8.86%[f]	1.77%[f]	–	–	–	–
Mohee et al. (1998)	Column	Lab	–	–	0.11%[g]	0.02%[g]	–	–	0.14 kg	0.05 kg
Seki (2000)	Column	Lab	–	–	–	–	–	–	4.19 kg/m^3	1.49 kg/m^3
Higgins and Walker (2001)	Column	Pilot	–	–	–	–	2.23–5.14[h]	0.96–1.95[h]	–	–

[a] Very close fit between model and data.
[b] mol-$CO_2 \times 10^5$/kg-DS h.
[c] % conversion.
[d] Experimental and modelled data were presented separately.
[e] Dry matter ratio (range 0–1).
[f] CO_2.
[g] O_2.
[h] g-O_2/kg-VS h; differences varied with initial moisture, airflow and respiration quotient.

5.4. Oxygen and carbon dioxide

Predictions of CO_2 concentration by Kaiser (1996) followed the data reasonably closely at low concentrations, when aeration was off, but showed large differences immediately following the onset of each aeration cycle (Table 12). Modelled oxygen concentrations reported by Mohee et al. (1998) generally tracked the overall pattern of the data (Table 12), except for a single major downward excursion between days 3 and 5. In both studies, the differences were relatively large in relation to the values reported. Spatial oxygen concentrations predicted by Finger et al. (1976) showed only fair agreement with experimental measurements.

Predicted carbon dioxide production rates reported by Nakasaki et al. (1987) showed moderate agreement with the data, and the differences in proportion to the range of values reported were relatively high. Whilst oxygen uptake rates predicted by the model of Hamelers (1993) were of a similar profile to experimental data curves, these data were not presented on the same plot for closer assessment of validation. Modelled maximum oxygen uptake rates reported by Higgins and Walker (2001), showed average discrepancies ranging from 42% to 98% of the data, with an overall range of 2–285%. Differences varied according to airflow rate, initial moisture content and the adopted values of the respirometric quotient.

Overall, modelled gas consumption or evolution rates showed relatively large errors in relation to the data presented. Further research on the modelling of oxygen consumption and carbon dioxide evolution would be valuable.

6. Conclusions

1. Mathematical models of the composting process have been based on the solution of heat and mass balances in time, and in a limited number of cases, spatially. A deterministic approach has been adopted in all cases, with stochastic elements incorporated into two models, and parameters either lumped over the complete reactor, or distributed over finite reactor elements.

2. Biological energy production has been predicted using either first-order, Monod-type, or empirical expressions, in conjunction with heat conversion factors. Temperature correction functions have been incorporated into most biological energy models, with corrections for moisture, oxygen and free air space also incorporated in some cases.

3. The most successful models in predicting temperature profiles have incorporated either empirical kinetic expressions, or utilised a first-order model, with empirical corrections for temperature and moisture. Models incorporating Monod-type kinetic expressions were less successful. However, no models were able to predict maximum, average and peak temperatures to within 5, 2 and 2 °C, respectively, or to predict the times to reach peak temperatures to within 8 h. Many models were able to successfully predict temperature profile shape characteristics.

4. A number of successful non-empirical rate coefficient temperature and oxygen correction functions suitable for use in composting models are available. Existing functions for moisture correction are all empirically based.

5. Moisture and solids profiles were well predicted by two models, whereas oxygen and carbon dioxide profiles were generally poorly modelled. Limited evidence exists for the applicability of a first-order model to substrate degradation.

6. Further work is suggested to obtain additional substrate degradation data, explore the development of improved first-order biological heat production models, incorporate mechanistically-based moisture correction factors, explore the role of moisture tension, investigate model performance over thermophilic composting time periods, provide further model sensitivity information and incorporate natural ventilation aeration expressions into composting process models.

Acknowledgement

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