

## Modeling composting kinetics: A review of approaches

H.V.M. Hamelers

*Wageningen University, Agrotechnology and Food Sciences, Sub-department of Environmental Technology, P.O. Box 8129, 6700 EV Wageningen, The Netherlands (phone: +31 (317) 483447; fax: +31 (317) 485883; e-mail: bert.hamelers@wur.nl)*

### Abstract

Composting kinetics modeling is necessary to design and operate composting facilities that comply with strict market demands and tight environmental legislation. Current composting kinetics modeling can be characterized as inductive, i.e. the data are the starting point of the modeling process and determine the type of model used. It is argued that the inductive empirical approach has been developed to its limit of practicality. Further progress is not expected because of limits in measurement techniques and the resources needed to perform all experiments needed. Contrary to the inductive, the deductive modeling approach uses the existing theory as its starting point for model development. Deductive models of realistic situations contain many basic parameters representing the theoretical basis. These basic parameters however tend to be non-identifiable, limiting practical application.

To overcome this problem, it is proposed that the basic parameters in the deductive model must be combined to a smaller number of so-called combined parameter that are identifiable. In this way a model is developed that can incorporate both the theoretical knowledge introduced via the basic parameter and the information of data as represented by the identifiable combined parameters.

As an example of how information of both theory and data can be used, the case of the temperature effect on the composting rate is analyzed. The temperature effect is quantified as the activation energy  $E$ , a parameter derived from the well-known Arrhenius equation. The theoretical analysis shows that the  $E$ -value changes strongly during the process, which is very remarkable, as the  $E$  value of basic parameter remains constant. These results are in accordance with literature findings. The results suggest that the multiplicative approach used in first-order modeling should be reconsidered, as both the literature findings as well as the theoretical analysis of the model predict a shift in  $E$ -value. Missing a shift in the  $E$ -value could lead for instance to instability in temperature control algorithms.

### 1. Introduction

Proper design and operation of the composting reactor is necessary to guarantee a good compost quality and reduced emissions (Keener et al. 1992). As composting is primary a microbial process, the main function of the composting reactor will be the realization of optimal environmental conditions for the microbial population (Finstein 1980). To define these optimal conditions the dependence of the composting rate on environmental conditions, i.e. composting kinetics should be known.

Knowledge of only the optimum conditions is not sufficient. Optimal composting temperature

can be as low as 45 °C (Finstein & Hogen 1992). For pathogen reduction an elevated temperature well above 45 °C is necessary (Bollen 1992; Farrel 1992). These demands for the operational composting temperature obviously conflict, and a temperature level has to be chosen such that pathogen reduction is assured while the composting process rate is not too much hampered. In composting engineering a trade-off always has to be made between different conflicting objectives. Knowledge of the optimum alone is therefore not sufficient and the explicit dependence of the composting rate in a broad range of the environmental factors should be known. This allows better optimization through calculation. The best way to

achieve this is via mathematical modeling of the kinetics of the process. Although for design purposes there is a pressing need for a composing kinetics model, at present there is no standard model.

Topic of this review is the mathematical modeling of composting kinetics. The topic is treated from a more general perspective of systems science. Models described in literature will be categorized according to their model building strategies. Two main strategies can be distinguished, the inductive strategy that is data based and the deductive strategy that is theory based. It will be argued that both strategies can not succeed in delivering a validated general kinetic model. A modified deductive strategy is proposed that might avoid the shortcomings of the currently used strategies. This strategy is exemplified by handling the temperature effect on composting.

## 2. Model building strategies

Aris (1978) defines a mathematical model concisely as “any set of equations that under certain conditions and for a certain purpose provide an adequate description of a physical system.” A physical system is an outlined part of reality whose properties one seeks to understand, in this paper the composting rate of a waste sample. A model contains basically two types of quantities, parameters that are constant in time and variables that vary in time. An input variable is a variable that is not affected by other quantities within the model and that can be freely chosen (to some extent) or is imposed by the outside world. The output is a variable that is observed.

A model building strategy describes the steps needed to build an adequate model for a given process. A model building strategy is no strict methodology, it is more a set of guidelines that have proven useful. In literature many different sets of guidelines can be found. (Eykhoff 1974; Beck 1980; Spriet & Vansteenkiste 1982; Heij & Williams 1989; Keesman 1989; Beck 1993; Ljung & Glad 1994a; Reichert & Omlin 1997). Figure 1 gives a schematic representation of the model building process based on the work of Heij and Williams (1989) and Eykhoff (1974). The figure is structured around the starting points and outcomes that are printed in *italic* in the text.

The starting point of the strategy lies in the phenomenon or process of interest, the theory about the process and the objectives of the modeling exercise. *Modeling objectives* influence modeling process during all phases. Typical modeling objectives are understanding, describing, predicting, controlling or optimising the process. For instance, in modelling a composting process it is important to know whether one wants to have a model that just describes the rate of a specific waste or one wants to understand the processes that are occurring. In the case of describing the rate one might use an empirical model, while for understanding how various factors affect the rate one uses a mechanistic model. Objectives are especially important when evaluating the resulting model.

*The process* of interest in this paper is composting kinetics. Associated with this process is a body of more or less well developed *theory* that describes and explains the phenomenon. Theory if available leads to a set of a priori concepts about the process. For instance, realising that composting is a microbial process leads to inclusion of the concept “microbial biomass” into the model. The choice for concepts is also influenced by the model objective. Based on the a priori concepts a *model structure* is defined, i.e. a collection of feasible models is constructed. The strategy of deriving a model structure from theory is called the deductive strategy (classical modeling, white box modeling), where the theory takes a central place. However theory is not always available, or theory is deemed less relevant, in such a case a so-called inductive strategy (black box modeling) is followed. Instead of deducting a model from first

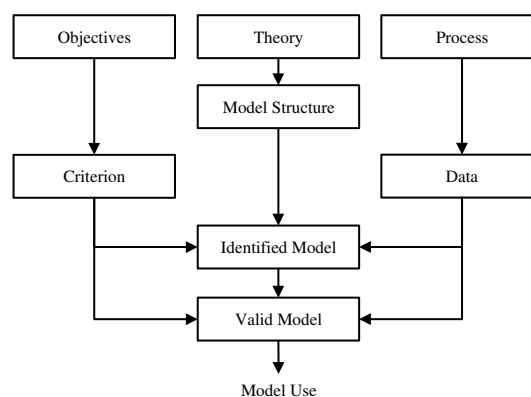


Figure 1. Schematic flow scheme of the model building process.

principles, a flexible model family (e.g. linear regression, difference equations with flexible order, etc.) is chosen as the model structure. The inductive approach tries to find the relationship between output and input.

From studying the phenomenon through experimentation data are obtained. These data are used to identify the model that best describes the data. From the theory it is sometimes possible to partly specify the parameter values. However parameter values for the specific process are often not sufficiently accurately known and parameter estimation is necessary from data. The parameter values are estimated by selecting those parameter values that give the best correspondence between the model outcome and data. To evaluate the correspondence between data and prediction a criterion is needed, that ideally is based on the modeling objective. In the inductive strategy model identification is broader in the sense that also changes in the model structure can be investigated. Based on the data decisions are made on what terms to retain in, add to, or remove from the model. The distinction between parameter estimation and model identification in a broader sense is not so clear cut, if parameter estimation yields zero for a certain parameter value, this might induce a change in the model structure. As a result of the model identification an *identified model* results.

After having identified the model the validity of the result should be assessed. Model validation might be loosely defined as assessing the quality of the model i.e. determining whether the model will be adequate for its intended use. As validity is not a clearly defined property, it is not surprising there are no universal tools to measure validity. However, a number of elements may be distinguished (Spriet & Vansteenkiste 1982).

Before validating the model first the extent to which the model can describe the data is evaluated. This is not an element of model validation, as during model development the parameter values have been chosen such that the data and model prediction correspond best. If this correspondence is poor the model validity may be doubted, but if there is a good correspondence this does not necessarily mean that the model is good. A faulty model containing sufficient parameters may well be able to describe the data very well.

A first element of model validation is to compare the model prediction with new data, i.e. data that have not been used for parameter estimation. Although this test is better than using the data used for parameter estimation it still does not tell whether the model represents the underlying structure of the process (van Straten 1998).

A second element is to investigate to what extent the model structure corresponds to what is known about the process. Elements of this step are comparing parameter values and the output development to what is known or expected. This is not a step that can be put rigorously in a statistical framework like the first element. However it does give information on how good the model represents the underlying structure of the process. This latter step makes sense only for the deductive modeling strategy.

Iteration (not shown in figure) is an important step in modeling process. If at some stage of the modeling process the outcome is not satisfactory, this stage or some previous stage has to be repeated.

The inductive and deductive strategy can be viewed as the extremes of a continuum of modeling strategies. Intermediate strategies, using both theoretical elements and empirical functions are sometimes called grey box modeling. These grey-box modeling strategies are commonly used, however this concept needs the concepts of inductive and deductive modeling for definition and tools.

### 3. Inductive composting kinetics modeling

Composting kinetics is defined in this paper as a comprehensive set of equations (mathematical model) that describe the dependence of the composting rate on environmental factors over a range of practical interest. The kinetic model to be developed should be able to predict the process rate in relation to the (actual) composition of the waste and (actual) conditions to which this waste is exposed in the reactor. Starting point of any inductive kinetic model is the degradation of organic matter as this supplies the free energy to drive the process (Waksman et al. 1939; Godden et al. 1983; Finstein et al. 1985; Godden & Peninckx 1987). The other factors influencing the process rate are generally referred to as environmental factors. The most important environmental

factors distinguished are: temperature (Gray et al. 1971; Suler & Einstein 1977; Finstein 1980; Nakasaki et al. 1985b; Cathcart et al. 1986; Golueke & Diaz 1987; Richard & Walker 1998), biomass (Nakasaki et al. 1985a; Nakasaki & Akiyama 1988), moisture (Schulze 1961; Jeris & Regan 1973b; Suler & Finstein 1977; Bakshi et al. 1987), oxygen (Suler & Finstein 1977; Nakasaki et al. 1987; Richard et al. 1999), porosity (Jeris & Regan 1973b), particle size (Gray et al. 1971) and C/N ratio (Morisaki et al. 1989).

### 3.1. Organic matter degradation modeling

The process rate is preferably expressed on the basis of a unit amount of waste and not of the total amount of the waste. Keener (1992) discusses this matter in more detail and proposes the following first order model:

$$\frac{dm}{dt} = -k(x_1, x_2, \dots, x_n) \cdot [m - m_e] \quad (1)$$

where  $m$  (kg) is the composting mass;  $k$  ( $\text{h}^{-1}$ ) the composting process rate constant;  $x_i$  the environmental factor e.g. temperature, oxygen, moisture, etc;  $t$  (h) the time; and  $m_e$  (kg) is the equilibrium mass, i.e. the residual mass after infinite composting time.

The model above is a state space model with  $m$  as a state variable. The output of the model is also  $m$  as this is the observation. The model has two parameters  $m_e$  and  $k$ . The latter parameter is the function of a number of exogenous variables or inputs. If the environmental factors remain constant in time, integration of the above equation directly leads to:

$$R = \frac{m - m_e}{m_0 - m_e} = e^{-k(x_1, x_2, \dots, x_n) \cdot t} \quad (2)$$

where  $R$  (dimensionless) is the compost mass ratio.

The compost mass ratio changes from 1 at  $t = 0$  to 0 at  $t = \infty$  and is a useful measure for the process progress and consequently compost stability. The value of the compost process rate constant  $k$  depends on the type of waste. In case of chicken manure the data of Keener (Keener et al. 1992) show that this model is applicable over a short time period (approx. 3 days), after such a

period the  $k$ -value had to be updated, to reflect the changes in waste composition. In the case of yard waste the model is applicable over a much longer period once the peak activity has been reached (Marugg et al. 1993).

### 3.2. Environmental factor modeling

A number of kinetic models have been published in the literature about the dependence of the compost process rate constant  $k$  on environmental factors (Schulze 1961; Jeris & Regan 1973b; Jeris & Regan 1973a; Finger et al. 1976; Haug 1980; Whang & Meenaghan 1980; Cathcart et al. 1986; Nakasaki et al. 1987; Stombaugh & Noke 1996; Richard 1997). These models share the following multiplicative structure:

$$k(x_1, x_2, \dots, x_n) = k_S \cdot f_1(x_1) \cdot f_2(x_2) \dots f_n(x_n) \quad (3)$$

where  $k_S$  ( $\text{h}^{-1}$ ) is the composting process rate constant under standard environmental conditions;  $n$  the number of environmental factors; and  $f_1, f_2$  the Environmental factor effect function.

The functions  $f$  describe the effect of a specific rate determining factor on the process rate constant. If the process rate is measured under standard conditions all functions have the value 1. The most extensive model is still the kinetic model proposed by Haug (Haug 1980). This model takes into account the effect of temperature [ $T$ ,  $^{\circ}\text{C}$ ], the gas phase oxygen content [ $\text{O}_2$ , % vol.], the moisture content of the waste  $M$ , [ $\text{kg water} \cdot (\text{kg waste})^{-1}$ ] and the free air space FAS, [ $\text{m}^3 \text{ air} \cdot (\text{m}^3 \text{ bulk waste})^{-1}$ ]

An important assumption underlying the multiplicative model is the independence of the effects of the different environmental factors involved. However, Richard and Walker (1998) and Richard et al. (1999) have shown that depending on moisture content, oxygen content and material, the optimal temperature varied from 52 to 64  $^{\circ}\text{C}$ . The effect also depends on the extent of organic matter degradation, thus not only do environmental factors influence each other but also the changing composition of the waste influences the effect. Compared to the factors oxygen, moisture and temperature, the dependence of the rate on the waste composition has received little attention.

### 3.3. Inductive modeling approach limitations

A distinct feature of the models used to date is that they are inductive models i.e. they try to relate directly the input (e.g. temperature) to the output, the composting rate. Although these models give a good description of the observed kinetic dependencies, it is expected that the data-oriented approach will not yield a comprehensive kinetic model i.e. a model that embraces all major environmental factors including waste composition. The following justification is given to substantiate this statement.

1. To investigate all environmental factors and their possible interactions a big experimental effort is needed. This is especially so because the heterogeneity of the waste calls for numerous replications. For instance to determine the effect of oxygen and moisture on the optimal temperature Richard (1997) performed the experiments at three moisture levels, three oxygen levels and four temperatures. To achieve sufficient accuracy each combination was measured three times, yielding a total of 108 experiments. Trying to include two additional factors like pH and porosity in this scheme would give  $3 \times 3 \times 108$  experiments, which gives a total of 972 experiments.
2. A number of factors (biomass, particle size) are expected to be important but can not be measured. For instance biomass can not be measured as no techniques are available for quantitative measurement in an organic waste matrix (Mitchell & Lonsane 1992). This makes it impossible to come up with an inductive model for these factors. As these factors tend to be variable, they constitute a source of variability when measuring the effect of other factors.

None of the aforementioned objections is of a principal nature, i.e. with sufficient effort and smart measurement techniques they could be overcome. Nevertheless taking into account the current measurement standards in composting the inductive approach seems to have reached its practical limit.

The lack of a theoretical framework for composting kinetics thus seems to be the main obstacle for further development of kinetics and hence a deductive model approach is needed to achieve further progress.

## 4. Deductive Composting Kinetics Modeling

### 4.1. Inductive modeling approach limitations

Current kinetic models are nearly all inductive models thus primary based on measurements. In contrast, mechanistic models exploit not only the data but also a priori information from the laws of physics, chemistry, etc. The deductive strategy is expected to lead to models with fewer parameters, as no parameters are needed to describe what is already known. As a mechanistic model reflects the structure of the process it is expected to yield better extrapolations (Ljung et al. 1994b). Because deductive modeling is able to exploit both the information from theory and measurements it might be fruitful to exploit this strategy in the compost kinetics.

However to date only two deductive models have been developed (Hamelers 1992; Kaiser 1996). The reason that there are only few deductive models compared to inductive models might be the complexity of the resulting models. This is a phenomenon not uncommon to ecological models. It has been experienced that in the field of environmental and ecological modeling the deductive methodology does not always yield adequate models (Beck 1993; Beck 1994; Hauhs et al. 1996; Reichert & Omlein 1997; Harremoes & Madsen 1999; Schulze et al. 1999), in particular the predictive power is sometimes low (van Straten 1998). As the composting process can be considered as a microbial ecological process, the problems encountered in the field of ecological modeling may be expected for composting kinetics modeling.

If the deductive model is made more complex by incorporating more (state) variables, the number of (unknown) initial values and the number of parameters of the constitutive relationships generally increase. Upon making a model more complex, at a certain point a lack of parameter identifiability will occur. This means that the available data set is insufficient to determine with sufficient accuracy all parameter values. Parameter non-identifiability can occur already in relatively simple models (Schulze et al. 1999).

This is also true for composting models as can be easily seen by considering a simple composting model that goes one step beyond the first order inductive model described by Keener et al. (1992). This first order inductive model for organic

matter degradation does not take explicitly into account the presence of the microbial population. To introduce the biomass into the model the conventional Monod kinetics may serve as a starting point. For solid materials the so-called half-rate constant  $K_s$  is high compared to the substrate concentration  $S$ , i.e.  $S \ll K_s$  (Whang & Meenaghan 1980). Under these conditions one may set up the model as follows (Heijnen 1999):

$$\begin{aligned} \frac{dS}{dt} &= q_s^{\max} \cdot \frac{S}{K_s} \cdot X \\ \frac{dX}{dt} &= -Y_s \cdot \frac{dS}{dt} \\ \text{OUR} &= -\frac{Y_s}{Y_{O_2}} \cdot \frac{dS}{dt} \\ t = 0 &\begin{cases} X = X_0 \\ S = S_0 \end{cases} \end{aligned} \quad (4)$$

in which:  $S$  ( $\text{mol m}^{-3}$ ) is the organic substrate concentration;  $X$  ( $\text{mol m}^{-3}$ ) the biomass concentration;  $t$  the time;  $q_s^{\max}$  ( $\text{mol mol}^{-1} \text{s}^{-1}$ ) the specific maximum substrate consumption;  $K_s$  ( $\text{mol m}^{-3}$ ) the substrate half-rate constant;  $Y_s$  ( $\text{mol mol}^{-1}$ ) microbial yield on substrate; OUR ( $\text{mol m}^{-3} \text{s}^{-1}$ ) the oxygen uptake rate; and  $Y_{O_2}$  ( $\text{mol mol}^{-1}$ ) the microbial yield on oxygen.

where State variables are  $X$ ,  $S$ ; Parameters are  $q_s^{\max}$ ,  $Y_s$ ,  $Y_{O_2}$ ,  $K_s$ ,  $X_0$ ,  $S_0$ ; and Output is OUR.

This example shows that this (already oversimplified) mechanistic model contains a much larger number of parameters (6) compared to the first-order organic matter degradation model that contains basically two parameters. The output of the model is the OUR, this is often the only measure that can be measured in a composting system. The solid nature of the material and the variability of waste make measurement on the organic material or biomass costly, difficult and uncertain.

An identifiability analysis would show that none of the aforementioned parameters would be identifiable, if only OUR is measured. This can be seen directly from the equation 4, describing the substrate depletion. Any combination of  $q_s^{\max}$  and  $K_s$  with the same ratio is able to describe a similar output. In such a situation the advantage of a good predictability attributed to deductive mod-

eling is lost, as numerous sets of parameters are able to describe the same data set. In this way an increase in the number of parameters may lead to an increase in the uncertainty of the prediction. The crux of the problem is that what one assumes about the system is much more complex than what one observes from the system. (Beck 1993).

#### 4.2. A modified deductive strategy

Previous analysis might lead to the conclusion that neither strategy is able to deliver a validated model and that a valid general model is out of reach anyhow. However, the problems of inadequate theory and incomplete measurements are related. If sufficient measurements were available, probably more complete and well accepted theory would be available. Incomplete measurements are thus a problem both in inductive and deductive modeling. Either strategy tends to obscure the problem. The inductive strategy discards the theory and thus has no way of knowing that measurements might be lacking. The deductive modeling often tacitly assumed that there exists a well-established quantitative theory of the phenomenon of interest. This is however not always the case. Neglecting the status of the a priori concepts would lead to overconfidence in the predictive power of the model (Reichert & Omlein 1997).

To handle this problem, recently a modified deductive strategy has been explored for composting kinetics. The strategy aims at reducing the model such that a model with only identifiable parameters is left. One starts with the conceptual model that includes parameters that are derived from more general principles. These parameters are called the basic parameters. In case of the example  $q_s^{\max}$ ,  $Y_s$ ,  $Y_{O_2}$ ,  $K_s$ ,  $X_0$ ,  $S_0$  are the basic parameters, they that have a solid grounding in biotechnological principles.

By solving the model for the output, i.e. an analytical model is sought that describes the measurement, i.e. the output variables. This analytical model will contain in general less parameter than the conceptual model. The parameters in the analytical model are less in number and consist of combinations of (functions of) general parameters. The combined parameters are chosen such that they are identifiable, while the basic parameters are in most cases not. For the example a solution for the OUR can be found with three identifiable

combined parameters  $\alpha$ ,  $\delta$ ,  $v$ . The solution and the identifiable combined parameters are given by:

$$\begin{aligned} \text{OUR} &= \delta \cdot (1 + v) \cdot \frac{e^{-\alpha t}}{(1 + v \cdot e^{-\alpha t})^2} \\ \alpha &= q_s^{\max} \cdot \frac{X_0 + Y_s \cdot S_0}{K_S} \\ \delta &= \frac{Y_s}{Y_{O_2}} \cdot q_s^{\max} \cdot \frac{S_0}{K_S} \cdot X_0 \\ v &= \frac{Y_s \cdot S_0}{X_0} \end{aligned} \quad (5)$$

The parameter  $\alpha$  is a time constant and is the inverse of the time needed for the maximum biomass concentration to deplete a substrate concentration equal to  $K_S$ . The parameter  $\delta$  equals the initial OUR, the parameter  $v$  is the ratio of the maximally produced biomass and the initial biomass. It is interesting to note that this relationship approaches a first order description if  $v$  becomes small.

As there are less combined parameters (3) than basic parameters (6), it is not possible to extract all basic parameters from knowledge of the combined parameters. However the opposite is not true, knowledge of the complete set of basic parameters leads to knowledge of the combined parameter. This also applies to the dependence of the basic parameters on the environmental factors. If this dependence is known for a basic parameter it can be translated to an effect on the combined parameter. For instance of all general parameters, temperature influences mainly the basic parameter  $q_s^{\max}$ . This means that if one knows that the parameter  $q_s^{\max}$  will double over a certain temperature range, one directly can predict that the values of  $\alpha$  and  $\delta$  will double while the other combined parameter  $v$  remains constant upon a temperature change. This prediction can be made independent of the knowledge of the exact value of the parameter  $q_s^{\max}$ .

Thus if at a certain temperature the values of  $\alpha$ ,  $\delta$  and  $v$  are determined experimentally, the prediction for a different temperature can be directly made by multiplying  $\alpha$  and  $\delta$  by a suitable factor. This example shows a big advantage of deductive modeling, general knowledge about the process can be used. This is not true for the inductive strategy when investigating the effect of temperature. Experiments must then be performed at other temperatures to understand the effect of temperature.

## 5. Application to composting kinetics

### 5.1. The deductive composting kinetic model

The deductive kinetic model is based on a conceptual description of the structure of waste particle. The waste particle is considered to be composed of small solid particles consisting of either degradable organic matter or non-degradable matter. The small degradable particles are degraded in a two-step process. First microbial mediated hydrolysis occurs that transforms the insoluble material into soluble substrate. Second the soluble substrate is aerobically degraded. These small particles are connected via the water phase that serves as a medium for microbial growth and mass transport of oxygen and soluble substrate. The small particles together with the connecting water phase constitute form a bigger macroscopic lump, the waste particle. Starting from this conceptual model of a waste particle (both composition and size distribution), a set of biotechnological principles describing microbial transformations and mass transport a mathematical model has been set up (Hamelers 2001). This model contains the basic parameters as listed in Table 1. Except for the parameter  $\gamma$  all parameters are standard parameters used in biotechnology as described in standard texts (Bailey & Ollis 1986). The parameter  $\gamma$  describes the spread of the particle size distribution, a large value of  $\gamma$  indicates a small particle size stretch, a small  $\gamma$  value a large stretch. From this mathematical model the following analytical model with identifiable combined parameters has been derived (Hamelers 2001).

$$\begin{aligned} \text{OUR}_a(t) &= \sqrt{\frac{1}{1 + e^{-\mu_{\text{eff}}(t-\Omega)}}} \cdot \frac{\text{OUR}_{m,\lambda}}{\gamma_c - 1} \\ &\times \int_{\zeta_s(t)}^{\infty} \zeta^{\gamma-2} \cdot e^{-\zeta} d\zeta + k_n \cdot S_{i,0} \cdot e^{-k_n t} \\ &\times \int_0^{\zeta_s(t)} \zeta^{\gamma-1} \cdot e^{-\zeta} d\zeta \end{aligned} \quad (6)$$

$\text{OUR}_a(t)$  (mol  $\text{O}_2$   $\text{m}^{-3}$   $\text{h}^{-1}$ ) is the oxygen uptake rate at time  $t$  for a matrix with variably sized particles;  $\mu_{\text{eff}}$  ( $\text{h}^{-1}$ ) the effective maximal biomass growth rate;  $\gamma$  is the distribution parameter;  $\text{OUR}_{m,\lambda}$  (mol  $\text{O}_2$   $\text{m}^{-3}$   $\text{h}^{-1}$ ) is the scaled maximum OUR of the mean sized particle;  $\Omega$  (h) the lag time;

Table 1. The deductive model basic parameters; symbol, name, value at 55 °C, value at 35 °C, units and apparent  $E$ -value

Symbol	Name	55 °C	35 °C	Unit	$E$
$\mu_n$	Maximal net growth rate constant	$7 \times 10^{-5}$	$3.4 \times 10^{-5}$	[s <sup>-1</sup> ]	30
$X_m$	Maximal biomass density	6000	6000	[mole $X$ m <sup>-3</sup> ]	0.0
$L_c$	Particle size	$1.5 \times 10^{-3}$	$1.5 \times 10^{-3}$	[m]	0.0
$D_{O_2}$	Effective diffusion coefficient of oxygen	$1.9 \times 10^{-9}$	$1.5 \times 10^{-9}$	[m <sup>2</sup> s <sup>-1</sup> ]	9.9
$k_h$	Hydrolysis rate constant	$4.9 \times 10^{-7}$	$1.9 \times 10^{-7}$	[s <sup>-1</sup> ]	40
$O_{2,i}$	Oxygen content at gas side interface	0.11	0.2	[mole $O_2$ m <sup>-3</sup> ]	-25.1
$S_{i,0}$	Initial insoluble substrate concentration	5000	5000	[mole $S$ m <sup>-3</sup> ]	0.0
$S_{s,0}$	Initial soluble substrate concentration	3600	3600	[mole $S$ m <sup>-3</sup> ]	0.0
$X_0$	Initial biomass concentration	0.1	100	[mole $X$ m <sup>-3</sup> ]	-290
$Y_{O_2}$	Biomass yield on oxygen	0.82	1.19	[mole $X$ mole $O_2^{-1}$ ]	-15.6
$Y_{S_i}$	Biomass yield on polymeric substrate	1.0	1.0	[mole $X$ mole $S_i^{-1}$ ]	0.0
$Y_{S_s}$	Biomass yield on soluble substrate	0.44	0.53	[mole $X$ mole $O_2^{-1}$ ]	-7.8
$\gamma$	Gamma distribution coefficient	3	3	[-]	0.0

$\zeta$  is the scaled particle size;  $\zeta_s$  is the scaled switch particle size;  $\gamma_c$  is the characteristic shape factor;  $k_n$  (h<sup>-1</sup>) the hydrolysis rate constant; and  $S_{i,0}$  (mol  $O_2$  m<sup>-3</sup>) is the initial insoluble substrate expressed in oxygen equivalents.

The scaled switch particle size  $\zeta_s$  is given by:

$$\zeta_s(t) = \frac{\text{OUR}_{m,\lambda} \int_0^t \sqrt{\frac{1}{1+e^{-\mu_{\text{eff}}(\tau-\Omega)}}} d\tau}{S_{s,0} + S_{i,0} \cdot (1 - e^{-k_n t})} \quad (7)$$

where  $S_{s,0}$  (mol  $O_2$  m<sup>-3</sup>) is the Initial soluble substrate in oxygen equivalents.

The relationship between the combined parameters in this model and the basic biotechnological parameters is described the first two columns of Table 2. The background and prop-

erties of this model are extensively discussed in (Hamelers 2001).

## 5.2. Parameter temperature effect

The deductive model as described before, only incorporates oxygen and substrate as state variables. At first sight it might seem odd to set up a deductive model without taking important kinetic factors like FAS, moisture content and temperature into account. However it should be remembered that the kinetic model is based on a description at the micro-level, i.e. at the particle level. At the particle level moisture and temperature can be expected to have negligible gradient, i.e. the gradient does not influence the rate. Therefore these factors can be described as input

Table 2. The deductive model basic parameters; symbol, definition in terms of basic parameters, name, value at 55 °C, value at 35 °C, unit and apparent  $E$ -value

Symbol	Definition	Name	55 °C	35 °C	Units	$E_a$
$\mu_n$	$\mu_n$	Maximal net growth rate constant	$7 \times 10^{-5}$	$3.4 \times 10^{-5}$	[s <sup>-1</sup> ]	30
$\text{OUR}_{m,\lambda}$	$\frac{\gamma_c}{L_c} \cdot \sqrt{2 \cdot D_{O_2} \cdot O_{2,i} \cdot \frac{X_m \mu_n}{Y_{O_2}}}$	Maximum oxygen uptake rate	0.029	0.020	[mole $O_2$ m <sup>-3</sup> s <sup>-1</sup> ]	15.6
$k_n$	$k_h \cdot (1 - \frac{Y_{S_i}}{Y_{S_s}})$	Net hydrolysis rate constant	$2.7 \times 10^{-7}$	$8.9 \times 10^{-8}$	[s <sup>-1</sup> ]	46.6
$S_{i,0}$	$\frac{Y_{S_i}}{Y_{S_i} - Y_{S_s}} \cdot \frac{Y_{S_s}}{Y_{O_2}} \cdot (S_{i,0} + S_{s,0} \cdot \frac{Y_{S_s}}{Y_{S_i}})$	Initial insoluble substrate concentration	6605	6905	[mole $O_2$ m <sup>-3</sup> ]	-1.9
$S_{s,0}$	$\frac{Y_{S_s}}{Y_{O_2}} \cdot S_{s,0}$	Initial soluble substrate concentration	1976	1696	[mole $O_2$ m <sup>-3</sup> ]	6.4
$\Omega$	$\ln\left(\frac{X_0}{X_m - X_0}\right)$	Lag time	$1.58 \times 10^5$	$1.19 \times 10^5$	[s]	11.9
$\gamma$	$\frac{\mu_n}{\gamma}$	Gamma distribution coefficient	3	3	[-]	0.00

to the kinetic model and need not to be taken into account as state variables for the kinetic model. Of course for a reactor model these factors (temperature, moisture and FAS) would serve as state variables. The value of the state variables then serves as input to the kinetic model where they serve to update the several parameter values.

Temperature dependency of microbial processes is often described by the Arrhenius relationship. This relationship can be described as:

$$p(T) = p(T_r) \cdot e^{-\frac{E}{R}(\frac{1}{T} - \frac{1}{T_r})} \quad (8)$$

in which:  $T$  (K) the absolute temperature;  $T_r$  (K) the reference temperature;  $p(T)$  parameter  $p$  value at  $T$ ;  $p(T_r)$  parameter value  $p$  at the reference temperature;  $E$  (kJ mol<sup>-1</sup>) is the activation energy;  $R$  (kJ mol<sup>-1</sup> K<sup>-1</sup>) is the gas constant.

Using this relationship, the temperature dependency is characterized by the value of the activation energy  $E$ .

The temperature effect on the composting kinetics of chicken manure will be studied. For this type of material the deductive model has been shown to be valid. The basic parameters for the model are listed in Table 1. The rationale for the choice of the different parameters at 55 °C is described elsewhere (Hamelers 2001).

The main basic parameters that are influenced by temperature are the growth rate constant (Sonnleitner 1983), diffusion coefficient (Wilke 1950), hydrolysis rate constant (Pfeffer 1974), oxygen content (Wilhelm et al. 1977) and microbial yields (Heijnen 1999). Based on the reported relationships for the temperature dependency of these basic parameters the parameter values are calculated at 35 °C, using the values at 55 °C as reference values. To make the temperature dependency of all parameters comparable an apparent activation energy is calculated for each parameter from its value at 55 °C and 35 °C. These  $E$  values are also listed in Table 1. The various parameters have of course been calculated using the original reported relationships.

Based on the basic parameters the combined parameters as used in the deductive model are calculated for both temperature levels. From these values again for each combined parameter the apparent  $E$ -value is calculated. Results of the calculations are shown in Table 2.

### 5.3. Deductive temperature effect modeling

Using these combined parameters the OUR as a function of time was calculated for both temperatures. The results of these calculations are shown in Figure 2. It is clear that under mesophilic conditions the OUR is initially higher as a result of the higher initial biomass. However at some point of time the thermophilic OUR becomes bigger as the thermophilic OUR increase more rapidly. From this point on, the OUR remains higher throughout the process. From the simulated data OUR versus time a new data set is constructed, OUR versus the Cumulative Oxygen Uptake (COU). The COU is a measure of the amount of organic matter degraded. If two samples of the same wastes have the same COU, the remaining organic matter level is the same in both samples. According to the first order model, the ratio of the process rates of those samples equals the ratio of the first order  $k$ -values, which follows directly from equation 1.

Using the OUR-COU data, the ratio of the OUR values can be calculated for each COU value. From this ratio, the  $E$ -value can be calculated at each COU value. This  $E$ -value describes the effect of temperature on the OUR and will be denoted  $E_{OUR}$ , to distinguish it from the  $E$ -values of the temperature effect on the parameters. Figure 3 shows the  $E_{OUR}$  as a function of the COU. Initially (COU = 0–0.4 mol O<sub>2</sub> kg<sup>-1</sup>) the  $E_{OUR}$  is negative as a result of the fact that mesophilic temperatures are favorable at the start of the process. From COU = 2–4 mol O<sub>2</sub> kg<sup>-1</sup> the  $E_{OUR}$  stabilizes at a value around 20 kJ mol<sup>-1</sup>. After this stable phase the  $E_{OUR}$  starts to rise to a level of 83 kJ mol<sup>-1</sup> until COU = 10 mol O<sub>2</sub> kg<sup>-1</sup>. From this point the

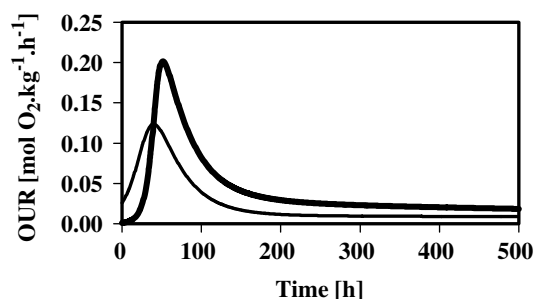


Figure 2. The OUR time course for two temperatures of 35 °C (thin line) and 55 °C (thick line) as calculated with the deductive model using the parameter values listed in Table 2.

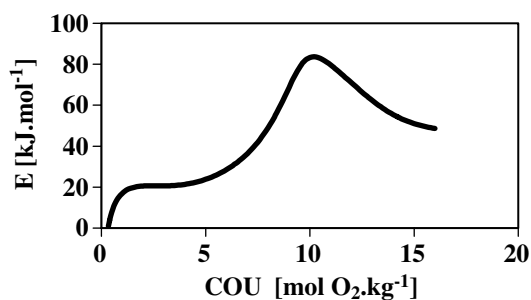


Figure 3. The  $E$ -value as calculated from the simulated OUR curves. The  $E$ -values is determined from the OUR ratio determined at equal COU values.

$E_{OUR}$  decreases again slowly. The most remarkable fact is that the  $E_{OUR}$  seems to change most of the time, while the  $E$ -value of the underlying parameter of course remains constant.

The temperature dependency of composting kinetics has been extensively studied in literature. From a number of studies the observed  $E_{OUR}$  in the mesophilic to thermophilic temperature range have been collected and listed in Table 3. For all of these studies the  $E_{OUR}$  was either listed in the original publication or was calculated from listed data or relationships. Only the optimal temperature range has been taken into account, that is temperatures up to 55 °C. In these range generally no adverse effect of temperature has been observed. From the table it is clear there is large spread in the  $E_{OUR}$ , typically in the range of 10–60 kJ . mol<sup>-1</sup> This large variance is often explained in term of variance of material and or microbial population. The large spread found by McKinley (McKinley & Vestat 1984) is especially interesting as they were determined for the same material but at different points in time.

The finding that initially negative  $E_{OUR}$  values are found is in accordance with the finding of

McKinley (McKinley & Vestat 1984) and Richard (Richard 1997), who found initially the highest activity in the mesophilic range. Once the  $E_{OUR}$  value becomes positive there is a clear maximum in the  $E_{OUR}$ . This mean that the observed  $E_{OUR}$  is not constant, but varies according to the extent of degradation. The range observed here in the simulation 20–60 kJ mol<sup>-1</sup> is in the same range as reported in literature as seen in Table 3.

## 6. Conclusions

Current kinetic models are generally inductive models. The inductive approach seems to have reached its practical limit. The deductive approach seems therefore an additional fruitful direction to investigate composting kinetics. Care should however be taken not to develop models with non-identifiable parameters, as deductive models of complex systems like composting contain many parameters. To prevent this situation it is proposed that a model should be constructed with combined parameters, i.e. fewer parameters that are identifiable however still have a clear relationship with the basic parameters.

The advantage of this approach is that it enables to use information from existing knowledge (as represented by the basic parameters) with the information retained in the data (as represented by the identifiable combined parameters).

The effect of temperature on the OUR is an example of this approach. The theoretical analysis showed that  $E_{OUR}$  changes strongly during the process, while the  $E$ -value of the underlying process remains constant. It is interesting to note that the  $E_{OUR}$  value is larger than the  $E$ -values of any single parameter. This shows that the  $E_{OUR}$  is a result of the interplay of a number of processes

Table 3.  $E$ -values as tabulated from different sources, listed are the source, the  $T$ -range of interest and the observed  $E$ -value

Reference	$T$ -Range [°C]	$E$ [kJ mol <sup>-1</sup> ]
(Wiley 1957)	25–55	35.2
(Schulze 1962)	25–55	54.2
(Jeris & Regan 1973c) newsprint	30–50	14.2
(Jeris & Regan 1973c) stable mixture	22–42	16.5
(Jeris & Regan 1973c) mixed refuse	35–55	59.3
(McKinley & Vestal 1984)	30–40	12–51
(Hamoda et al. 1998)	20–40	20.3

each with a fixed  $E$ -value. This means that the observed variability in  $E_{OUR}$  need not to be solely the result of a changing population, but might be an intrinsic property of the process. This would mean that for the interpretation of the variability of  $E_{OUR}$  during the process, the assumption of a changing population is not necessary.

The variation should be further investigated. It is important for the control of the reactor. If for instance  $T$  is controlled, care should be taken if PI-controllers are used. A change in response to a change in  $T$  might destabilize the controllers action. The current use of a multiplicative model for the description of the effect of temperature seems therefore questionable, and should be reevaluated. The deductive model might be an interesting starting point to develop new functions to describe the effect of temperature.

## References

- Bailey JE & Ollis DF (1986) *Biochemical Engineering Fundamentals*. Mc. Graw Hill, New York
- Bakshi MPS & Gupta VK et al. (1987) Effect of moisture level on the chemical composition and nutritive value of fermented straw. *Biol. Wastes* 21: 283–290
- Beck MB (1980) Model Structure Identification From Experimental Data. IASIA, Laxenburg, Austria
- Beck MB (1993) Construction and evaluation of models of environmental systems. In: Jakeman AJ Beck MB & McAleer MJ (Eds), *Modelling Change in Environmental Systems*. John Wiley & Sons
- Beck MB (1994) *Understanding environmental systems. Predictability and Nonlinear Modelling in Natural Sciences and Economics*. Kluwer, Wageningen
- Bollen GJ (1992) Factors involved in inactivation of plant pathogens during composting of crop residues. *Proceedings of the International Composting Research Symposium*, Renaissance Publications, Columbus OH
- Cathcart TP & Wheaton FW et al. (1986) Optimizing variables affecting composting of blue crab scrap. *Agr. Wastes* 15: 269–286
- Eykhoff P (1974) *System Identification*, John Wiley & Sons
- Farrel JB (1992) Fecal pathogen control during composting. *Proceedings of the International Composting Research Symposium*, Renaissance Publications, Columbus OH
- Finger SM & Hatch RT et al. (1976) Aerobic microbial growth in semisolid matrices: heat and mass transfer limitation. *Biotechnol. Bioeng.* 18: 1193–1218
- Finstein MS (1980) Composting microbial ecosystem: implications for process design and control. *Compost Sci./Land Util.* 21: 25–27
- Finstein MS & Hogan JA (1992) Integration of Composting Process Microbiology, Facility Structure and Decision-making. *Proceedings of the International Composting Research Symposium*, Renaissance Publications, Columbus OH
- Finstein MS & Miller FC et al. (Eds) (1985) *Waste Treatment Composting as a Controlled System*. Biotechnology: A Comprehensive Treatise. VCH, Weinheim
- Godden B & Penninckx M et al. (1983) Evolution of enzyme activities and microbial populations during composting of cattle manure. *Eur. J. Appl. Microbiol. Biotechnol.* 17: 306–310.
- Godden B & Penninckx M (1987) Biochemistry of manure composting: lignin biotransformation and humification. *Compost: Production Quality Use*, Pg.
- Golueke CG & Diaz LF (1987) Composting and the limiting factor principle. *Biocycle*: 22–25
- Gray KR & Sherman K et al. (1971) Review of composting part 1. *Process Biochem* 6(6): 32–36
- Hamelers HVM (1992) A Theoretical Model of Composting Kinetics. *Proceedings of the International Composting Research Symposium*, Renaissance Publications, Columbus OH
- Hamelers HVM (2001) A mathematical model for composting kinetics, Wageningen University
- Hamoda MF & Abu Qdais HA et al. (1998) Evaluation of municipal solid waste composting kinetics. *Resou. Conserv. Recy.* 23: 209–223
- Harremoes P & Madsen H (1999) Fiction and reality in the modelling world- balance between simplicity and complexity, calibration and identifiability, verification and falsification. *Water Sci. Technol.* 39(9): 1–8
- Haug RT (1980) *Compost Engineering: Principles and Practice*. Ann Arbor Science, Ann Arbor
- Hauhs M & Neal C et al. (1996). Summary of a workshop on ecosystem modelling: the end of an era? *Sci. Total Environ.* 183(1–2): 1–5
- Heij C & Willems JC (1989) A deterministic approach to approximate modelling. In: Willems JC (Ed) *From Data to Model* Springer, Berlin
- Heijnen JJ (1999) Bioenergetics of microbial growth. In: Flickinger MC & Drew SW *Bioprocess Technology* (pp. 739–763) John Wiley and sons, New York
- Jeris JS & Regan RW (1973a) Controlling environmental parameters for optimum composting I: experimental procedures and temperature. *Compost Sci.* 14(1): 10–15
- Jeris JS & Regan RW (1973b) Controlling environmental parameters for optimum composting II: moisture, free air space and recycle. *Compost Sci.* 14(2): 8–15
- Jeris JS & Regan RW (1973c) Controlling environmental parameters for optimum composting III. *Compost Sci.* 14(3): 16–22
- Kaiser J (1996) Modelling composting as a microbial ecosystem: a simulation approach. *Ecol. Model.* 9: 25–37
- Keener HM & Marugg C et al. (1992) Optimizing the efficiency of the composting process. *Proceedings of the International Composting Research Symposium*, Renaissance Publications, Columbus OH
- Keesman KJ (1989) A set-membership approach to the identification and prediction of ill-defined systems: application to a water quality system, Twente
- Ljung, L s T. Glad (1994a). *Modeling of Dynamic Systems*. Prentice Hall, New Jersey.
- Ljung L & Glad T (1994b) On Global Identifiability for Arbitrary Model Parameterizations. *Automatica* 30(2): 265–276
- Marugg C & Grebus M et al. (1993) A kinetic model of the yard waste composting process. *Compost Sci. Util.* 1(1): 38–51

- McKinley VL & Vestal JL (1984) Biokinetic analysis of adaptation and succession: microbial activity in composting municipal sewage sludge. *Appl. Environ. Microbiol.* 47(5): 933–941
- Mitchell DA & Lonsane BK (1992) Definition, characteristics and potential. In: Doelle HW, Mitchell DA & Rolz CE *Solid Substrate Cultivation*. Elsevier Applied Science, London
- Morisaki N & Phae CG et al. (1989) Nitrogen transformation during thermophilic Composting. *J. Ferment. Bioeng.* 67(1): 57–61
- Nakasaka K & Akiyama T (1988) Effects of seeding on thermophilic composting of household organic waste. *J. Ferment. Technol.* 66(1): 37–42
- Nakasaka K & Hakano Y et al. (1987) Oxygen diffusion and microbial activity in the composting of dehydrated sewage sludge cakes. *J. Ferment. Technol.* 56(1): 43–48
- Nakasaka K & Masayuki S et al. (1985a) Effect of seeding during thermophilic composting of sewage sludge. *Appl. Environ. Microbiol.* 49: 724–726
- Nakasaka K & Shoda M et al. (1985b) Effect of temperature on composting of sewage sludge. *Appl. Environ. Microbiol.* 50(6): 1526–1530
- Pfeffer JT (1974) Temperature Effects on anaerobic fermentation of domestic refuse. *Biotechnol. Bioeng.* XVI: 771–787
- Reichert P & Omlin M (1997) On the usefulness of overparameterized ecological models. *Ecol. Model.* 95: 289–299
- Richard TL (1997) *The Kinetics of Solid-State Aerobic Biodegradation*, Cornell University
- Richard TL & Walker LP (1998) Temperature kinetics of aerobic solid-state biodegradation. *Proc. IBE 1*: A10–A30
- Richard TL & Walker LP et al. (1999) The effects of oxygen on solid-state biodegradation kinetics. *Proc. IBE 2*: A22–A39
- Schulze K & Beven K et al. (1999) Equifinality and the problem of robust calibration in nitrogen budget simulations. *Soil Sci. Soc. Am.* 63: 1934–1941
- Schulze KL (1961) Relationship between moisture content and activity of finished compost. *Compost Sci.* 2(2): 32–34
- Schulze KL (1962) Continuous thermophilic composting. *Appl. Environ. Microbiol.* 10(2): 108–122
- Sonnleitner B (1983) *Biotechnology of thermophilic bacteria-growth, products and application.* *Adv. Biochem. Eng./Biotechnol.*
- Spriet JA & Vansteenkiste GC (1982) *Computer-aided Modelling and Simulation.* John Wiley & Sons, London
- Stombaugh & Nokes (1996) Development of a biologically based aerobic composting simulation model. *Trans. ASEA* 39(1): 239–250
- Suler DJ & Finstein MS (1977) Effect of temperature, aeration, and moisture on CO<sub>2</sub> formation in bench-scale, continuously thermophilic composting of solid waste. *Appl. Environ. Microbiol.* 33(2): 345–350
- van Straten G (1998) Models for water quality management: the problem of structural change. *Water Sci. Technol.* 37(3): 103–111
- Waksman SA & Cordon TC et al. (1939) Influence of temperature upon the microbiological population and decomposition processes in composts and stable manure. *Soil Sci.* 47: 37–61
- Whang DS & Meenaghan GF (1980) Kinetic model of composting process. *Compost Sci.* (May/June): 44–46
- Wiley JS (1957) Progress report on high-rate composting studies. 12th Annual Purdue Industrial Waste Conference
- Wilhelm E & Battino R et al. (1977) Low-pressure solubilities of gases in liquid water. *Chem. Rev.* 77(2): 219–262
- Wilke CR (1950) Diffusional properties of multicomponent gases. *Chem. Eng. Prog.* 46(2): 96–104