

A NEW STRUCTURED MATHEMATICAL MODEL OF THE COMPOSTING PROCESS

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ABSTRACT

A new structured dynamic model has been developed to describe the composting process. The model includes different populations of microorganisms and types of substrates, and heat and mass transfer between the three phases of the system. Computer simulations provided a reliable approach to expected results and sensitivity analysis determined the key parameters of the model.

Key Words: model, composting process, biochemical, mass transfer, sensitivity analysis.

INTRODUCTION

The objectives of modelling are the development of mathematical tools to allow the integration of the knowledge concerning the considered phenomena, to orientate the experimental design, to evaluate experimental results, to test the hypothesis, to reveal relationships between variables, to predict the evolution of a system and, definitively, to design optimised process and management strategies.

Composting process models present a higher complexity than those for aerobic and anaerobic wastewater treatment, because of the solid medium heterogeneity. Models described in the literature are focused on the biological or the physical aspects of composting.

Models describing the aerobic composting process has focused mainly on design and the biological aspect has been often ignored. Nevertheless, Hamelers (1993) introduced the biological component in a model at the particle level, Stombaugh and Nokes (1996) described the evolution of substrate, oxygen, water and microbial growth using Monod kinetics, whereas Kaiser (1996) proposed a model where different populations of microorganisms populations and substrates were considered. However, there is a need for models that include the thermal, physical and biological characteristics of the process.

A new approach, integrating biological and physical phenomena in a dynamic structured model for aerobic composting, was the objective of the present work.

MODEL DEVELOPMENT

The model considered a three-phase system, with mass and heat transfer, and biological processes including hydrolysis, growth, lysis and decomposition by microorganisms. In the solid-liquid phase the organic matter was decomposed by microorganisms, with release of gases and heat, and oxygen uptake. Between the liquid and gas phases, mass transfer of gases and water, through evaporation or condensation, was considered.

Twelve hydrolysis processes were used in the model to simulate the transformation of a particulate substrate into its soluble monomers and this was represented by Contois kinetics.

The soluble substrates were oxidized by bacteria, actinomycetes and fungi to carbon dioxide, ammonia and water. The different capability of each group of microorganisms to degrade different substrates was applied to the model in 29 growth processes. Monod growth kinetics for multiple substrate was used, in conjunction with temperature and oxygen

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dependence functions, for better describing the influence of temperature on the growth of microorganisms and to reduce growth rates when oxygen was limited.

Microorganism lysis was represented by 6 processes modelled by first order kinetics, and its products were maintained in the system as death biomass. Death biomass decomposition on soluble and inert substrates was also modelled by first order kinetics.

Modelled physical processes were mass transfer of oxygen, carbon dioxide, ammonia and water and heat transfer, both sensible and latent, between the liquid and gas phases, considered at different temperatures. All biological reactions were assumed to occur in the solid-liquid interphase.

The system was described by 31 state variables (Table 1) and 53 processes, following 31 ordinary non-linear differential equations, with proper initial and boundary conditions.

Table 1. State variables

<i>i</i>	State variable	<i>i</i>	State variable	<i>i</i>	State variable	
1	X _C	Carbohydrates	12	X _{MF}	Mesophilic fungi	
2	X _P	Proteins	13	X _{TF}	Thermophilic fungi	
3	X _L	Lipids	14	X _{DB}	Death biomass	
4	X _H	Hemicelluloses	15	S _{S1}	Soluble substrate 1	
5	X _{CE}	Celluloses	16	S _{S2}	Soluble substrate 2	
6	X _{LG}	Lignins	17	S _{S3}	Soluble substrate 3	
7	X _I	Inerts	18	S _{S4}	Soluble substrate 4	
8	X _{MB}	Mesophilic bacteria	19	S _{S5}	Soluble substrate 5	
9	X _{TB}	Thermophilic bacteria	20	S _{S6}	Soluble substrate 6	
10	X _{MA}	Meso. actinomycetes	21	S _{O2}	Soluble oxygen	
11	X _{TA}	Thermo. actinomycetes	22	S _{CO2}	Soluble carbon dioxide	
				23	S _{NH4+}	Soluble ammonium
				24	IW	Water
				25	n _{O2}	Oxygen gas
				26	n _{CO2}	Carbon dioxide gas
				27	n _{NH3}	Ammonia gas
				28	n _{H2Ov}	Water vapour
				29	n _{N2}	Dinitrogen
				30	θ	Gas temperature
				31	T	Sol.-liquid temperature

Stoichiometric coefficients were presented in matrix form $[v_{i,j}]$, where $1 \leq i \leq 31$ and $1 \leq j \leq 53$. Reaction rates for each process constituted the vector $[\rho_j]$, and $[m_{i0}]$ and $[m_{i1}]$ were the mass flows entering and exiting the system. The whole mass balance was

$$\frac{d[m_i]}{dt} = [m_{i0}] - [m_{i1}] + [v_{j,i}] \cdot [\rho_j],$$

and the two energy balance equations for the solid and gaseous phase were

$$\frac{d\theta}{dt} = \frac{Q_c + (\theta_0 - \theta) \left(\sum_k \beta_k \cdot n_{k0} \right) + (T - \theta) \sum_k \beta_k \max\{0, R_k^T\}}{\sum_k n_k \beta_k},$$

$$\frac{dT}{dt} = \frac{Q_{cw} + Q_G - Q_c^T - \sum_k (\max\{0, R_k^T\} h_j(T) + \min\{0, R_k^T\} h_j(\theta)) - (T - 273) \left(c_{pw} \frac{dm_w}{dt} + \sum_i c_{pi} \frac{dm_i}{dt} \right)}{C_{con} + c_{pw} m_w + \sum_i c_{pi} m_i},$$

with the initial values $(m_i)_{t=0}$, $(\theta)_{t=0}$ and $(T)_{t=0}$ completing the ordinary differential equation sets.

NUMERICAL APPROXIMATION AND RESULTS

A 4-5 Runge-Kutta-Fehlberg adaptive method was used for approaching the solution of the set of differential equations.

The model presented 179 parameters: 24 in hydrolysis, 144 in microorganisms growth, 7 in microorganisms lysis, and 4 liquid-gas mass transfer coefficients. For the preliminary test of the model, a set of parameters defined, estimated from different parameter values obtained

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from the literature (Nakasaki et al., 1985; Stombaugh and Nokes, 1996; Kaiser, 1996; Das and Keener, 1996).

For illustrating the capability of the model, simulations were run by considering a mixture of poultry manure and straw (Soliva, 2001; Haug, 1993) with the data shown in Table 2.

Table 2. Initial conditions (units in kg, if it is not specified, related to 100 kg fresh matter)

X _C	3.183	X _{M_B}	0.040	S _{S1}	2.0	S _{O2}	0.0006	n _{O2}	6.7E-3	kmol
X _P	2.975	X _{T_B}	0.008	S _{S2}	3.0	S _{CO2}	0.0000	n _{CO2}	0.000	kmol
X _L	0.895	X _{M_A}	0.010	S _{S3}	2.0	S _{NH4⁺}	0.0050	n _{NH3}	0.000	kmol
X _H	4.577	X _{T_A}	0.020	S _{S4}	1.0	IW	60.0	n _{H2O_v}	3.86E-4	kmol
X _{CE}	4.036	X _{M_F}	0.010	S _{S5}	0.5			n _{N2}	2.52E-2	kmol
X _{LG}	3.142	X _{T_F}	0.100	S _{S6}	0.5			g	293.15	K
X _I	1.997	X _{D_B}	0.000					T	293.15	K

The simulation results were qualitatively compared with experimental values described in the literature and a good approximation was obtained.

Changes in the populations were well predicted by the model (Fig.1). Bacteria and actinomycetes appeared during the mesophilic stage as reported by Epstein (1997). Their activity produced an increase in the temperature and thermophilic bacteria, actinomycetes and fungi replaced the previous populations, as described by Poincelot (1975) and Haug (1993). Substrate degradation followed the pattern of microorganism succession, with carbohydrates, proteins and lipids being degraded rapidly, whereas hemicellulose, cellulose and lignin did not suffer any important transformation during the first hours (Fig. 2). This succession was reported by Poincelot (1975). Mesophilic microorganisms consumed the most readily decomposable carbohydrates and proteins. Thermophilic bacteria decomposed protein, non-cellulose carbohydrate and lipid. Actinomycetes attacked hemicellulose but not cellulose and lignin, which were degraded by fungi. All these results were consistent with the results obtained by Gray et al. (1973) and Poincelot (1975).

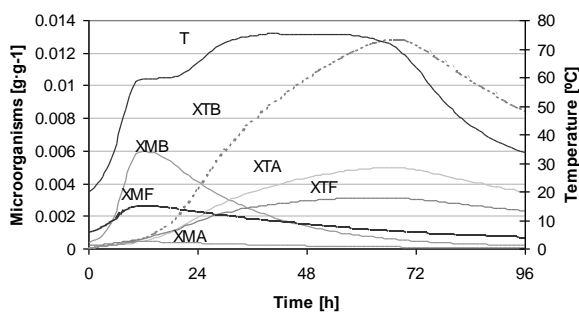


Fig. 1. Microorganisms and temperature evolution

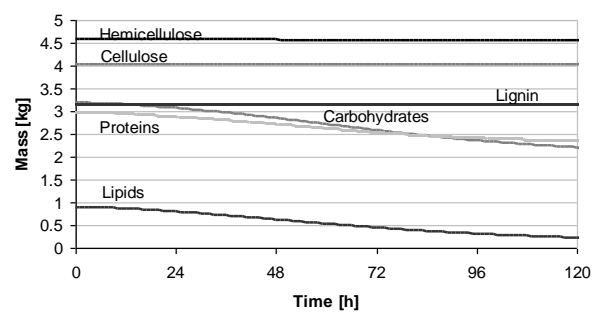


Fig. 2. Substrate evolution

The sensitivity analysis performed orientates the experiments for further calibration, focusing the experiments on parameters and state variables requiring special attention and evaluating the relative importance of each parameter of the model. Parameters were varied individually by -25, -50, -75, +25, +50 and +75% from their default value. When a parameter was varied, all other parameters were maintained at their default value. A total of 20 objective functions were examined during a simulation time of 360 h and with the initial conditions described in Table 2.

In general terms, parameters with a greater sensitivity of the objective functions were those related with proteins or protein hydrolysis products. Also important were carbohydrates

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and lipids (no significant difference was noticed between glycerol and LCFA), whereas hemicelluloses had minor sensitivity and celluloses and lignins had a similar behaviour. In reference to microorganisms, thermophiles were more sensible than mesophiles.

From the 194 parameters of the model, 20 resulted in great sensitivity for a minimum of 7 of the 20 objective functions. In the hydrolysis process, the saturation constant of the Contois kinetics showed no response with a variation of +/-75%. This indicated that hydrolysis may be modelled better by first order kinetics than by Contois kinetics. The maximum specific growth rate and decay rate of thermophilic bacteria and thermophilic actinomycetes showed high sensitivity. Variations in the maximum specific growth rate for thermophilic fungi and the decay rate for mesophilic microorganisms also induced a response in the objective functions. Variations in the initial conditions were also considered, and the most important were the initial concentration of the thermophilic microorganisms and the hydrolysis products of carbohydrates, proteins and lipids (glycerol).

CONCLUSIONS

A useful mathematical tool has been developed and simulations provided good approximations to the evolution of the composting process.

The consideration of different populations and substrates in the biochemical part of the model was shown to be a key point for predicting the transformations that occur during the composting process.

The sensitivity analysis performed showed that 1) hydrolysis may be considered by a first order kinetics, 2) differentiation between lipids-glycerol and lipids-long chain fatty acids can be ignored, 3) mesophilic actinomycete populations were not significant for the model, 4) hydrolysis constants, maximum specific growth rate and decay rate were key parameters; experiments need to be designed in order to determine these values.

Further work will be directed towards modifying the model in order to introduce the conclusions of the sensitivity analysis, to design experiments for calibrating the model and finally to validate it.

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