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A NUMERICAL INTEGRATED MODEL OF COMPOSTING PROCESSES USING FINITE ELEMENTS METHODS

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ABSTRACT A dynamic finite element computer model of a composting system was created; it was temporally and spatially explicit. The modeled system was a cylindrical vessel, but it was conceptualized as a two-dimensional system on the assumption of radial symmetry. Air was blown in at the bottom through a distribution plenum and exited freely at the top. The evolution of the model was computed over time and space using multi-physics finite element modeling software (COMSOL™ version 3.5a). At each time step, the stationary solutions of the differential equations describing convection or diffusion were chosen, because those processes were assumed to occur much faster than any changes in the biomass. The compost was studied as a three-phase system. The water film around the solid particles hydrolyzed the nutrients that sustained the biomass and its chemical activities. Gases produced or consumed by the biomass – oxygen, carbon dioxide, ammonia – were exchanged with the gas phase through the water film. The gas concentrations and the temperature in the liquid or vapor phases were separately represented. Heat transfer was modeled as conductive through the liquid and solid phases, convective in the gas phase, and both convective and conductive therein. The population of micro-organisms was considered to be composed of mesophiles and thermophiles with different temperature-related growth coefficients. In order to model the heat and mass transfer between phases, a total of n growth characteristics were accounted for. Their development was computed through time and space. The modeling results and validation against physical experimental data are discussed.

Keywords: Numerical model, composting processes, finite element methods.

INTRODUCTION

Mathematical models of composting have been developed to improve the prediction of these processes and optimize their output by, for instance, by improving the quality of the resulting humus or reducing the emission of noxious gases. The equations in these models combine physics, chemistry and biology, but are often empirical approximations and thus there is a lack of uniformity among current models. Moreover, the complexity of these mathematical systems makes them difficult to solve with any high degree of

accuracy, precision, and speed. Finally, even if the mechanisms of the composting process are known, we often fail to effectively control the outputs.

Models have been developed of composting in windrows, piles, and vessels, and in which fresh air was provided through turning, passive aeration, or forced aeration. While windrows and piles, whether turned or passively aerated, are closer to the conditions in most composting factories, aerated vessel are widely used as the basis for modeling exercises because they lend themselves well to research, and because the dynamics of the airflow are easier to model.

Biomass plays a central role in composting processes. Early models represented compost as a homogeneous unit with external interactions like entering and exiting gases or heat loss. Temperature, substrate and oxygen availability were generally assumed to have a multiplicative impact on biomass growth. Though the rate functions used were initially piecewise linear, later studies employed smoother and more realistic functions - some of them based on Arrhenius' equation (Nielsen and Berthelsen 2002). Humidity (Ekinci 2004) and the carbon-to-nitrogen ratio of the compost also influence the biomass growth rate and were accounted for in more recent models (Sole-Mauri, Illa et al. 2007).

Research has gradually increased the spatial resolution of models of in-vessel composting. As mentioned, early computational models represented compost as a single unit. More recent models represent the composting vessel as being divided into discrete, internally uniform, layers, with transition conditions between them (Stombaugh and Nokes 1996). Furthermore, some of the latest models have considered space as a continuous variable and implemented spatial partial differential equations (Bongochgetsakul and Ishida 2008).

More recent models take into account increasingly complex physical processes. Early models considered only a single variable, like temperature, humidity, or oxygen content within the compost (Stombaugh and Nokes 1996). Later on, the temperature of the solid and gas phases were modeled separately (Petric and Selimbasic 2008). Eventually, models included a different variable for each phase – gas, liquid, and even solid – for temperature, moisture, or gas concentrations. Recent studies have implemented diffusion and convection in the liquid and gas phases (Bongochgetsakul and Ishida 2008).

No model, however, has yet combined complex physical processes and high spatial resolution. Furthermore, researchers usually configure models to represent specific composting conditions as determined by the composition of the compost substrate or the geometry of the vessel, and thus the models are single-use. The increase of precision and adaptability of composting models will help further work on the optimization of the composting process. Some major improvement would be the increase of the quality of resulting humus, less emissions of noxious gases, and a faster composting process.

We hypothesize that an integrative model can be developed which will include every important process that has been shown to occur in composting, with high spatial resolution that will increase its predictive accuracy. We also want to demonstrate that it is possible to have a user-friendly model that is easily adaptable to any kind of compost or composting apparatus.

In this study, we implemented complex physical chemical and biological processes and took into account gas, liquid, and solid phases. We built this model with the software COMSOL™, which simulates multi-physics processes. The solver algorithms of this software are based on finite element methods with a spatial resolution that can be set to be as fine as wished. The interface of this software simplifies the modification of parameters so that the model can fit any experimental situation. The model is validated by comparing predicted and measured results of composting experiments using a cylindrical vessel. The model has also been compared to published results. Our user-friendly model shows great adaptability and successfully predicts the evolution of more parameters of composting processes with higher resolution than existing models.

METHODOLOGY:

Description of the model:

The overall objective of this study is to understand and optimize the composting process in order to obtain good quality compost as quickly as possible. As many studies have already shown, adequate provision of oxygen is necessary to meet these goals. This study will focus on forced aeration systems, for passive aeration can be considered an extreme case of forced aeration: with a ventilation quasi null.

The model describes the evolution of compost in a cylindrical vessel. This shape was chosen because of its simplicity and symmetry, and because it is a common style of vessel in the literature. A cylinder is, apart from the sphere, the shape that maximizes the ratio of volume over surface area, lowering the heat loss through the sides. The configuration of the vessel is shown in Figure 1.

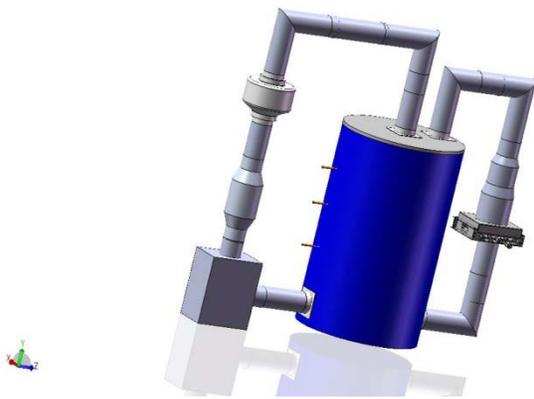


Figure1

the compost is in the blue cylinder. The two tubes are here for the recirculation of air and the air sampling.

The circulation of air will be implemented by one inlet valve at the bottom of the barrel and one exit valve at the top where the air exit unimpeded. A fan will provide a constant pressure drop across the compost bed. Ambient air will be blown from the bottom. A grid will support the compost to create an aeration plenum extending several centimetres above the inlet valve in order to uniformly distribute the supply air. In the model it is

assumed that a constant and homogeneous air flow is blown from the bottom of the cylinder.

The compost within the barrel is assumed to remain static, and is not turned or changed during the simulation. The vessel prevents any entry or exit of gases other than through the aforementioned vents.

As the vertical air flow and the horizontal loss of heat through the sides of the vessel suggest that, even with initially homogeneous compost, some spatial variability will arise. This model has high spatial resolution in order to follow the development of such variability. The finite element methods already implemented in COMSOL Multiphysics™ (COMSOL AB, Stockholm) were used to solve the partial differential equations of the model.

The biomass:

The compost quality is heavily dependent on its carbon to nitrogen ratio, and its potassium and phosphorus content. Changes in these nutrient concentrations are monitored during the simulation to track the overall quality of the compost. It is not possible, however, to model the evolution of only a few parameters without modeling the whole system.

This model is centered on the growth of microbial biomass. The growth of the biomass is modeled using the classic Equation 1:

$$\frac{dX}{dt} = (\mu - k_d)X \quad (1)$$

Where μ is the growth factor and k_d is holds for the proportion of death within the population. The growth factor depends on several parameters like temperature, oxygen content, humidity, substrat. Hence we have $\mu = \mu_{max} * f_{O_2}(O_2) * f_T(T) * f_{H_2O}(H_2O) * f_S(S)$, where f_{O_2} , f_T , f_{H_2O} , and f_S are functions with values ranging from 0 to 1 and which represent the impact of oxygen, temperature, moisture content and substrate on the growth of microbial biomass (Stombaugh and Nokes 1996).

The biomass is often assumed to be composed of two kinds of microbes: mesophilic and thermophilic. The mesophiles dominate at temperatures from 25 to 40°C. However those microorganisms are more sensible to heat than the thermophilic and stop growing after 40°C. At higher temperatures, thermophilic organisms are responsible for the degradation.

An easy way to model this behaviour is to implement two strains of microorganisms with different curves of response to temperature and to split the biomass into two accordingly.

The function f_T used was $f_T = \frac{A_T e^{-\frac{E_1}{RT}}}{1 + K_T e^{-\frac{E_2}{RT}}}$ and is a modified version of the Arrhenius

equation, to take into account the activity of the enzymes that moderate the microorganisms' growth (Nielsen and Berthelsen 2002). In this expression, E_1 and E_2 are the energies of activation and inhibition of one strain of bacteria, and differ between mesophiles and thermophiles.

The microorganisms were assumed to be aerobic. It has been shown that biomass activity is highly dependent on oxygen concentrations when the latter is low. However, when the oxygen content is higher than a specific threshold, its influence on the growth of the microorganisms plateaus. The impact of the oxygen content on the growth of the biomass was represented with a Monod function.

$$f_{O_2} = \frac{O_2}{K_{O_2} + O_2}$$

The impact of the substrate availability is assumed to have the same form as that of oxygen, hence the function:

$$f_S = \frac{S}{K_S + S}$$

As the biomass grows within the water film, the water availability determines the volume in which the microbial activity will take place. Thus, increasing the water content improves the growth capacity of the biomass by decreasing the effect of overpopulation. However, the thickness of the water film increases with the water content. The thickness of the water film disturbs the diffusivity of the dissolved oxygen and prevents the growth of the biomass. The impact function of the water content on the growth of the biomass must reflect both of these effects. We chose a piecewise linear function (in this definition, H_2O is the moisture content from 0 to 1):

$$f_{H_2O}(H_2O) = \begin{cases} 0, & 0 < H_2O < 0.2 \\ \frac{H_2O - 0.2}{0.4 - 0.2}, & 0.2 < H_2O < 0.4 \\ 1, & 0.4 < H_2O < 0.6 \\ \frac{0.6 - H_2O}{0.6 - 0.8}, & 0.6 < H_2O < 0.8 \\ 0, & 0.8 < H_2O < 1 \end{cases}$$

The amount of substrate is reduced by the quantity is reduced by the microbial biomass in two ways, as described with equation 2:

$$\frac{dS}{dt} = \min\left(\frac{dX}{dt}, 0\right) - \eta_{max} \cdot f_{O_2}(O_2) \cdot f_T(T) \cdot f_{H_2O}(H_2O) \cdot f_S(S) \cdot X \quad (2)$$

Where the first term represents the consumption of substrate required for the increase of the biomass due to its growth: $Y_{X \rightarrow S}$ is the yield coefficient of the creation of biomass and is negative. This term only exists when the microorganisms are dividing faster than they are dying, hence the maximum. The second term stands for the uptake of the existing biomass to sustain itself, η_{max} being the maximum microbial maintenance coefficient. (Stombaugh and Nokes 1996)

Physical processes:

Compost is a three phase system. The solid part, the organic waste, is slowly dissolved in the water film that surrounds it. All the biomass activity happens in this liquid phase. Microorganism consumes dissolved substrat and oxygen to grow. The growth of biomass releases water and heat as a side effect. Heat and water will be exchanged at the interface with the gas. The gas is continuously replaced by fresh air through the ventilation system. Here we assumed that all the substrat is already dissolved and available to the biomass so that we can focus on the liquid and gas phases.

In order to model the physical properties of compost, one needs to model them on both liquid and gas phases. The evolution of the biomass happens over weeks, whereas the physical processes like heat and mass transfer, convection and conduction of air happen within hours. Because of the huge difference in time scales, we assume that the physical processes reach instantaneously the equilibrium. Looking at stationary solutions for the physical aspects greatly simplifies the problem under study. The following equations will be displayed according to this assumption.

The equation of diffusion of heat in the air is:

$$-k_{air}\Delta\theta = Q_{ex} - \rho_{air}\langle\vec{u}|\overline{grad\theta}\rangle \quad (3)$$

Where θ is the temperature of air, k_{air} the thermal conductivity, Q_{ex} the heat exchanged with the liquid phase, ρ_{air} the density of air and \vec{u} the airflow. This equation takes into account diffusion (the term on the left), convection (the right term), and the heat exchanges. In the air phase, there is no heat source.(Petric and Selimbasic 2008)

In the liquid phase, the biomass releases heat as part of its activity. Also, there is assumed to be no convection. The heat equation in the liquid is then

$$-k_{liq}\Delta T = -Q_{ex} + Q_{bio} \quad (4)$$

Where k_{liq} is the thermal conductivity of the liquid phase, and Q_{bio} is the heat released by the biomass.

We have: $Q_{bio} = \Delta_{HCT} \frac{dS}{dt}$ and

$$Q_{ex} = h_{trans}(T - \theta) + c_{H_2O} \max\left(0, -\left(H_2O_{liq} - \frac{psat(\theta)}{R\theta}\right)\right)T - c_{H_2O} \min\left(0, -\left(H_2O_{liq} - \frac{psat(\theta)}{R\theta}\right)\right)\theta \quad (5)$$

Where h_{trans} is the convective heat transfer coefficient and represents the convective heat transfer at the liquid-gas interface. c_{H_2O} is the capacity coefficient of the water, $psat(\theta)$ is the saturated pressure of water in the air at the temperature θ . R is the gas

constant. The two last terms stand for the heat exchange through the evaporation or liquefaction of water.(Petric and Selimbasic 2008)

The evolution of water is modeled by the equations (6) for the gas phase and (7) for the liquid phase.

$$-D_{air}\Delta H_2O_{gas} = W_{ex} - \langle \vec{u} | \overrightarrow{grad}(H_2O_{gas}) \rangle \quad (6)$$

$$-D_{liq}\Delta H_2O_{liq} = -W_{ex} - Y_{S \rightarrow w} \frac{dS}{dt} \quad (7)$$

Where D_{air} and D_{liq} are the respective coefficient of diffusion of water in the air and the porous media. $Y_{S \rightarrow w}$ is the yield coefficient of the creation of water due to the consumption of substrat by the biomass.

$$W_{ex} = \left(H_2O_{liq} - \frac{psat(\theta)}{R\theta} \right) H(H_2O_{liq}) \quad (8)$$

Where $H(H_2O_{liq})$ is a Heaviside function that has the value 1, when the volumetric water content is higher than the residual water content and 0 otherwise. It the model the fact that in a porous media, a part of the water is imprisoned, due to surface tension and cannot go away through evaporation.

The oxygen is consumed by the biomass in the water film. New oxygen is provided by the inlet of fresh air and the convective exchange at the liquid/gas interface. The equations of evolution of oxygen in the gas (9) and liquid (10) phases are:

$$-D_{O_2gas}\Delta O_2_{gas} = O_{2ex} - \langle \vec{u} | \overrightarrow{grad}(O_2_{gas}) \rangle \quad (9)$$

$$-D_{O_2liq}\Delta O_2_{liq} = -O_{2ex} + -O_{2consumption} \quad (10)$$

Where D_{O_2gas} and D_{O_2liq} are the respective diffusion coefficients of the oxygen in the gas and liquid phase. $O_{2consumption} = Y_{O_2 \rightarrow S} \frac{dS}{dt}$, where $Y_{O_2 \rightarrow S}$ is the yield consumption of oxygen, represents the consumption of oxygen by the biomass. The oxygen exchange at the liquid-gas interface follows Henry's Law: $O_{2ex} = k_{LaO_2} \left(H_{eO_2}(T) \cdot O_{2liq} - O_{2gas} \cdot R \cdot \theta \right)$. $H_{eO_2}(T)$ is the Henry's constant and depends on the temperature. k_{LaO_2} is the mass transfer coefficient of oxygen.(Petric and Selimbasic 2008)

The emission of gas (carbone dioxide, ammonia) by the biomass is linearly linked to its activity (e.g. growth) and has not been modeled yet.

RESULTS

COMSOL Multiphysics™ solves the problem with regards to time and space. It is possible to follow the evolution of each parameter over time at any point of the composting vessel, and even to have a color map of the slice of the vessel for any parameters.

As all the parameters are linked, the trends of evolution of each parameter can be seen in that of another. For instance the color graph of the temperature and the biomass are close, even if they do not deal with the same quantities. Where the biomass is important, so is the temperature but along with it the oxygen and water content are low. However, the pattern of evolutions repeats themselves. At first, the activity lies in the top part of the vessel. The reason is that at first, there is no shortage of oxygen or water. The limiting factor is temperature. At $t=0$, the conditions are the same everywhere, so is the beginning growth of the biomass and the production of heat. The heat produced is elevated through the airflow and one point in the compost takes profit to the heat produced by the other points below it. The top part is the one that accumulates the maximum heat. As the temperature is higher at the top, so is the growth of the biomass. Because the growth of the biomass is improved at the top, it releases more heat, thus self-perpetuating the process.

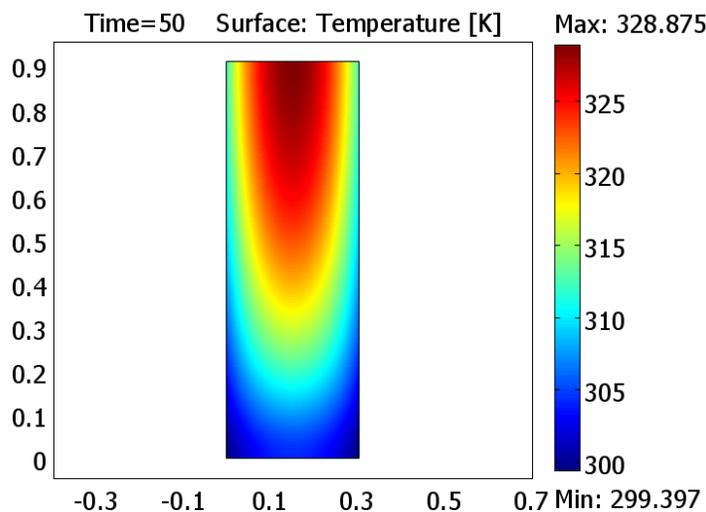


Figure 2. Temperature distribution in a vertical slice of a cylinder vessel of compost after 50 hours. The temperature scale is on the right in Kelvin. The scales of the bottom and left are in meters.

However, the nutrients, oxygen and water are being consumed faster as the biomass population increases. After some time, the uptake of the biomass in the lower part of the vessel will be such that the upper parts of the vessel will not have enough oxygen. Then the activity of the biomass will decrease as well as the heat released by this activity. Because heat is blown away by the airflow, the temperature on the upper part will decrease, and only the bottom of the vessel will reach high temperature.

The evolutions of several parameters were assessed in a specific point in the upper part of the composting vessel. The graphs obtained have the same format to what can be found in the literature and show the same kind of behaviour.

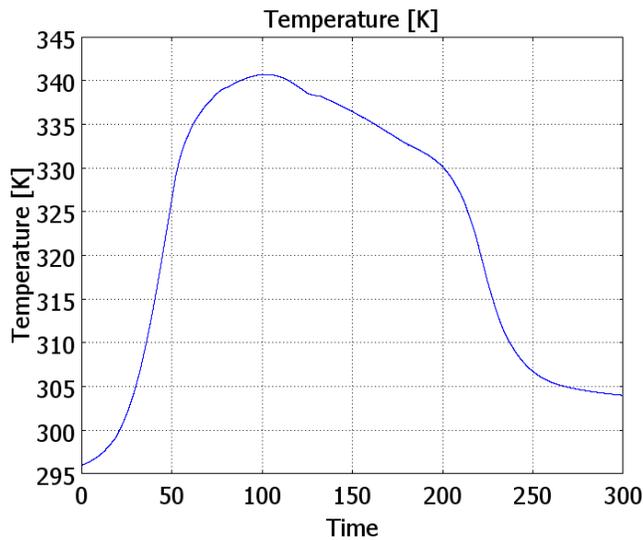


Figure 3. Temperature evolution with time (in hours) in the upper part of the composting vessel

CONCLUSION

We model composting processes in a cylinder-shaped vessel using complex physics. The equations are solved with COMSOL Multiphysics™, which uses finite element methods. The preliminary results show correlations to what can be found in literature.

Some aspects are still to be implemented. Right now the carbon to nitrogen ratio is not taken into account. However, it will just need to split the substrat into separate variables. The emission of noxious gases is not taken into account, but, as they do not interfere with the other processes, they can be added at the very end.

Now we are trying to find heat and mass transfer equations that model the specificities of the porous media. We are also implementing passive convection due to the buoyancy forces.

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