DEVELOPMENT AND PRELIMINARY VALIDATION OF A COMPOST PROCESS SIMULATION MODEL

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INTRODUCTION

Physically based process models are key for design of industry and municipal scale bioconversion centers (Haug, 1993; Das and Keener, 1995, 1996,1997). Presently there are procedures for specifying carbon and nitrogen amounts in a crude manner. However, time required for a process to run its course because of the host of environmental variables and thermal/physical/chemical interactions bearing on the conversion process is an unknown without simulation modeling.

The complex and dynamic interactions within bioconversion systems are a fundamental component of the knowledge base necessary for developing a sustainable composting infrastructure. Physical and biological processes occurring in most bioconversion systems are not well understood primarily due to the myriad of possible substrates and highly dynamic temperature-moisture conditions. This lack of understanding has resulted in much empiricism being the norm in current bioconversion/composting literature. The current approach to designing commercial composting operations is the reliance on pilot project data. Golueke (1977) is recognized as a pioneer in the use of pilot project data for full scale design. Hansen et al. (1989), Keener et al. (1996, 1997) and Das et al. (1997a,b,c) used pilot scale approaches for developing full scale designs. They also began efforts to model the processes.

At present there is a reasonably good process model (Haug, 1993) for the bioconversion of biosolids (product from activated sludge treatment of municipal waste). These models have not been tested sufficiently for other substrates. Preliminary work to date suggests that serious shortcomings of the Haug (1993) approach must be overcome when generalizing to a broader range of substrates. Keener et al. (1996, 1997), Das and Keener (1997), and Das et al. (1997a,b,c) represent pioneering contributions to this end. They considered the compost reactor as a homogenous substrate mix. Stombaugh and Nokes (1996) developed an n layer model for evaluating effects of varying physical-microbiological parameters through the reactor.

Process models are evaluated by comparing predicted state variables with measured state variables in bench, pilot and full scale composting operations. Thoroughly documented process models enable one to design full scale operations without the costly steps of bench scale and pilot scale trials, except for the bench and pilot trials

required to develop and validate the model. Models may be deterministic, stochastic, steady-state or dynamic. All natural environmental bioprocesses are dynamic. Although conditions may often approach steady state, an understanding of the dynamics is essential if the influences of changes in conditions is to be predicted. A wide variety of platforms facilitate the development of dynamic models. Snape et al. (1995) reviews common modeling platforms. STELLA®, a PC-based simulation program with an excellent graphics interface will be used in this work.

In designing a bioconversion system for a previously untested waste stream, five steps are ideally performed. These are (1) Feedstock characterization, (2) Pilot scale process evaluation. (3) Product testing, 4) Design parameter evaluation, and (5) Scale up of system. The feedstock characterization includes a complete physical and chemical characterization as defined by the Compost Council. Respirometric data are also collected in the feedstock characterization. This data are modeled in the pilot phase, which produces product necessary for quality evaluation. Sound process models employing data gathered in the feedstock characterization and tested in the pilot phase are useful in the scale up phase. This procedure has been applied here to determine degradation coefficients of textile industry solids during composting. A systematic evaluation of the composting process at a pilot level including waste stream characterization, oxygen uptake, CO_2 evolution rates, amendments and degradation rates are described here.

The objective of this paper is to present a simple model evaluated using cotton gin trash and wool processing wastes.

MODEL DEVELOPMENT

The model, adapted from Haug (1993), is presented in simplified form. It is developed starting from the assumptions which follow below.

1. C/N ratio lies between 10 and 30 for good composting
2. Moisture content lies between 40% and 60% wet basis.
3. The carbon, nitrogen, oxygen and hydrogen in the biodegradable volatile solids fraction of the incoming substrate stream is known. Nonbiodegradable materials do not participate in the reaction.
4. First order kinetics are applicable and the biodegradable fraction can be characterized with one rate constant.
5. Temperature, oxygen, free airspace and moisture have multiplicative effects on the first order rate constant.
6. Aerobic metabolism stops at oxygen concentrations below 6% and the system does not become anaerobic.
7. Substrate mixture is homogeneous.
8. Particle size is sufficiently small such that particle geometry is compatible with pilot scale containers (e.g., largest particle dimension is 10 times smaller than the pilot scale reactor). Particle should be small enough such that oxygen diffusion into the particle is not limiting.
9. The compost reactor may be modeled as a continuous flow stirred tank reactor (CFSTR) at steady state.

Assumptions 1 and 2 assure that composting is generally possible. Assumptions 3 through 7 lie at the heart of the modeling effort to be described. Assumption 7 must be satisfied in the scaled up system. Assumptions 8 and 9 are important in the modeling effort and in scale up itself. It is commonly assumed that particle geometry effects may be safely ignored in the scale up process.

Invoking assumption 3, one may write the following relationship describing the fate of biodegradable solids in an aerobic composting system as

$$C_aH_bO_cN_d + \left(\frac{4a+b-2c-3d}{4}\right)O_2 \rightarrow aCO_2 + \frac{b-3d}{2}H_2O + dNH_3 \quad (1$$

where subscripts a,b,c,d describe the relative molar amounts of carbon, hydrogen, oxygen and nitrogen respectively in the dry portion of the biodegradable volatile solids fraction (BVS). The above equation indicates that biodegradable solids combine with additional oxygen to yield carbon dioxide, water and ammonia in stoichiometric quantities. Carbon dioxide and ammonia go off in gaseous form (further assuming that measures are not in place to trap the ammonia). The water evolved, along with the water comprising the moisture content of the incoming volatile solids, is available for evaporation which usually occurs during aeration. The equation says nothing about how fast or slow the reaction may occur. The equation in itself gives no hint of the temperatures one may expect during the course of the reaction.

Decomposition occurs as a first order reaction rate of the substrate available. The reaction rate is modeled using first order kinetics as described as

$$\frac{d(BVS*density*Vol)}{dt} = -k_d*(BVS*density*Vol) \qquad (2$$

where t represents time in days, k_d is the composite degredation rate constant, BVS represents the biodegradable volatile solids fraction in the reactor at time t (e.g., the term on the left of equation 1), density is the dry solids bulk density in the reactor, and Vol is the reactor volume. The product BVS*density*Vol represents the grams of BVS in the reactor. BVS is expressed in grams and time is expressed in seconds. BVS is computed by multiplying total solids (TS) by a factor representing the fraction of BVS in the substrate. Nonbiodegradable solids (NBS) is TS-BVS.

Following Haug (1993), the composite degradation constant is represented by multiplicative subfactors for temperature, oxygen, free air space and moisture content as

$$k_d = k_T \cdot k_{Moisture} \cdot k_{FAS} \cdot k_{O_2} \qquad (3$$

where k_T is the temperature correction, $k_{moisture}$ is the moisture content correction, k_{FAS} is the free airspace correction and k_{o_2} is the oxygen concentration correction.

Temperature is adjusted with the Arrhenius correction as

$$k_T = k_{dR1}[C_1^{(T-TR1)} - C_2^{(T-TR2)}] \qquad (4$$

where k_{dR1} is the degredation constant ideally obtained from respirometric studies, TR1 and TR2 are reference temperatures, C_1 and C_2 are Arrhenius temperature coefficients and T is the substrate temperature. Following Haug (1993) TR1=20C, TR2=60C, C_1=1.066 and C_2=1.21. These constants describe mixed mesophillic cultures commonly found in solid waste degredation and thus considered robust with respect to common substrates. The degredation coefficient k_{dR1} is particular to each substrate or substrate mixture and thus must be measured respirometrically (or estimated using curve fitting techniques. Haug (1993) discusses the derivation of degradation constants from respirometer data.

Moisture variation effects are modeled using an empirical logistic function. Haug (1993) found the following equation was adequate for biosolids composting.

$$k_{Moisture} = \frac{1}{e^{(-17.64[1-moisturefraction]+7.062} + 1} \qquad (5$$

where moisturefraction represents the moisture fraction (wet basis) of the substrate. Moisture fraction can vary with time in composting and can be calculated based on a moisture balance and solids balance to be discussed below. This relation in effect says that microbes function best in high moisture conditions and conversely do not function in dry conditions.

Free air space (FAS) is important in composting environments because it is highly correlated with oxygen transfer within composting reactors. Data suggests that optimum moisture content for composting is between 55 - 65%. That optimum exists because of rate limiting moisture films which reduce oxygen diffusion in pilot scale and commercial scale systems. Reaction rates proceed most rapidly in an aqueous environment of 100% moisture (used in the respirometric evaluation), however above 65% pilot and commercial scale systems tend to become oxygen limited, thus the aerobic assumption becomes compromised. The moisture correction factor is 1 at 100% and decrease in a logistic curve as moisture content decreases. The FAS correction is given as

$$k_{FAS} = \frac{1}{1+e^{[-23.675*FAS+3.4945]}} \qquad (6$$

where nomenclature has been defined previously.

Free air space in reality decreases with time because particles constantly consolidate. However, free air space is left constant because the interactions of particles and moisture which affect FAS through the composting process on beyond the scope of this preliminary study.

Oxygen concentration (as measured from exhaust gas, Vol%O) can be limiting particularly when aeration is limited. Haug (1993) assumed a Monod type relationship written as follows to model oxygen limitation. The Monod relationship is given as follows.

$$k_{O_2} = \frac{Vol\%O}{Vol\%O+2} \qquad (7$$

The Vol%O is the percentage of oxygen in the incoming air. The constant 2 is the percentage of oxygen where the process is 50% limited. In reality, oxygen concentrations will be considerably above 6% to keep the reactor from becoming facultative or anaerobic. At oxygen percentages of 6% or above (see assumption 6) the k_{O_2} will not be less than 0.75. Consistent with the CFSTR reactor, it is assumed that the oxygen in the FAS in the reactor is the same as that measured in the exhaust gas.

Balances may also be written describing the state of solids, liquids and gases flowing through the compost reactor. Solids are typically partitioned into biodegradable and nonbiodegradable solids. Assuming a continuous flow stirred reactor may be used to model the process, the biodegradable solids may be written as

Rate of storage = input - output + sources - sinks (8a

or

$$\frac{d(BVS*Vol*density)}{dt} = ((BVSI-BVS)*through)+0-(k_d*BVS) \qquad (8b$$

where BVSIN is the biodegradable volatile solids entering the reactor (g/g dry solids), BVS is the biodegradable volatile solids fraction (g /g), the term density is the dry bulk density (g/m^3) at time t, through is the dry solids throughput rate (g/s), Vol is the reactor volume (m^3) and other nomenclature are as defined previously.

The nonbiodegradable solids balance reflects the addition of fixed nitrogen to the nonbiodegradable solids. Ammonia fixation represents approximately 1 % of the starting mass of compost. When microbes consume the substrate they fix some of the nitrogen into a stable organic form. This portion of N fixed is calculated from a 12% N composition of cells and a cell yield per gram of substrate. The mass of the fixed N is added to the non-degradable fraction of the compost.

Total solids may be represented as

$$DrySolidOut = (BVS + NBS) * through + D * \frac{17.01}{MoleWt} * \frac{d(BVS * Vol * density)}{dt} \qquad (8c$$

where the last term represents the fixed N contribution. The nonbiodegradeable materials (NBS) contains ash plus nonvolatile biodegradable. This assumes that the system is nitrogen limited.
Gas constituents of interest are carbon dioxide, oxygen and water vapor. The balance for CO_2 is given as

$$0.000501 * DryAirin = CO_2in = CO_2out - A(44 / MoleWt) * \frac{d(BVS * Vol * density)}{dt} \qquad (9a$$

where DryAirin is the ventilation rate (g/sec), A is the stoichoimetric factor in Equation 1 and MoleWt is the effective molecular weight of the biodegradable solids fraction. The derivative of BVS with respect to time is as given in Equation 2. The constant 0.000501 is the fraction of the incoming air which is CO_2. DryAirin can be calculated from the ventilation rate (m^3/s) from the gas law as shown in Haug (1993). The equation (in metric form) is given as

$$DryAirin = \frac{(Pair - PVI) * Qair * 28.96}{235.5 * (273 + Tairin)} \qquad (9b$$

where Pair is the atmospheric pressure (kPa) and PV is the vapor pressure (kPa), Qair is the volumetric ventilation rate (m^3/s), the constant 28.96 is the molecular weight of air, the constant 235.5 is the gas constant (kPa m^3/gm mole K) and Tair is air temperature in C. The saturated vapor pressure (kPa) corresponding to Tair can be computed using

$$PV_s = 3.38639[(0.00738Tair + 0.8072)^8 - 0.00019|1.8Tair + 48| + 0.001316] \qquad (9c$$

where PVs is the saturated vapor pressure (kPa). PV is found by multiplying PVs by the relative humidity (RH).

For oxygen the mass balance appears as

$$0.2314 * DryAirin = O_2in = O_2out + \left[\frac{4A + B - 2C - 3D}{4}\right] * (32 / Molewt) * \frac{d(BVS * Vol * density)}{dt} \qquad (9d$$

where A,B,C,D are the stoichiometric coefficients of Equation 1 and the constant 0.2314 is the fraction of dry air represented by oxygen. Other nomenclature are defined as above. The water vapor pressure at the exit may be estimated as (Haug, 1993)

$$PVO = PVI + \{[PVSO - PVI] * k_{moisture}\} \qquad (9e$$

where PVO is the exit vapor pressure, PVI is the incoming vapor pressure, PVSO is the saturated vapor pressure at the exit. The PVSO is estimated using an equation similar to 9c based on the temperature of the reactor which is as yet unknown.

The total dry gas out (DryAirout, g/s) is given as

$$DryAirout = DryAirin + GasFactor * \frac{d(BVS * Vol * density)}{dt} \qquad (9f$$

where GasFactor is the summation of stoichiometric O_2 (negative) and CO_2 (positive) contributions. GasFactor is written as

$$GasFactor = A * \frac{44}{MoleWt} - (4A + B - 2C - 3D) * \frac{32}{MoleWt} \quad (9g$$

The steady state water balance is written as

output = input + sources - sinks (10a

or,

Mcoutdb*Vol*density*through +VaporOut=MCindb*Vol*density*through+VaporIn +Wadd+Wprod (10b

where MCoutdb is moisture content at exit expressed as fraction dry basis, MCindb is incoming moisture rate expressed as fraction dry basis. VaporIn is the moisture rate coming in as a vapor, Wadd is the water addition rate(g/s), Wprod is the stoichiometric water production rate and VaporOut is the rate of water vapor movement out of the system. The left hand side of Equation 10b represents moisture leaving the system. The term (BVS + NBS) represents dry material leaving the system. One may modify Equation 9b to predict VaporIn by substituting the vapor pressure of water (PV) in the incoming airstream by substituting PV in place of Pair-PV. Similarly, one may also substitute PVO in place of Pair-PV in Equation 9b to compute VaporOut. ProdWat is computed as

$$\Pr odWat = \left[\frac{B - 3D}{2}\right] * \frac{18.01}{MoleWt} * \frac{d(BVS)}{dt} \qquad (10c$$

where nomenclature has been defined previously. The moisture fraction needed in the computation of $k_{Moisture}$ can now be computed using

$$MoistureFraction = \frac{MCoutdb * Vol * density}{(1 + MCoutdb) * Vol * density} \qquad (10d$$

The temperature of the reactor at time t is required to compute the water vapor exiting the system. Temperature of the reactor is determined based on an energy balance. The energy balance can be constructed as follows.

Rate of change of energy = energy in - energy out + sources -sinks =0 (11a

The energy in is the sensible heat content of the dry substrate and the incoming water. This can be written as

energy in =MCdbin*through*CPSOL*(Tin-Tref) +Wadd*CPWAT(Tin-Tref) +Qair*CPAIR*(Tin - Tref) (11b

energy out = MCdbout*through*CPSOL*(Treact-Tref)+Qair*CPAIR*(Treact-Tref)+Latent (11c

where Latent is the latent heat contained in the saturated air leaving the system, Tin (assumed same as Tair) is the incoming temperature(C) of the substrate, added water (Wadd) and of the incoming air. Tref is an arbitrary reference temperature(C). The specific heat of air, CPAIR, is taken to be Latent heat (λ, kJ/g) may be computed as follows.

$$Latent = Qair * (Vaporin - Vaporout) * \lambda \qquad (11d$$

Vaporin and Vaporout are the water vapor in the incoming air and outgoing air respectively (gms water/gms dryair). The symbol λ is the latent heat of evaporation given as

$$\lambda = 2.501 - 0.002361 * Treact \qquad (11e$$

Vaporin and Vaporout are computed using (ASAE, 1997)

$$Vaporin = \frac{0.6219 * PVI}{Pair - PVI} \qquad Vaporout = \frac{0.6219 * PVO}{Pair - PVO} \qquad (11f,g$$

Nomenclature has been previously defined. The heat lost by conduction (e.g., the major sink term) is assumed zero. The major heat source is given by the combustion of the BVS, written as follows.

$$Source = \frac{d(BVS * Vol * density)}{dt} * HeatCnt \qquad (11h$$

where heat content (HeatCnt) is in units of kcal/gm BVS. Values for heat content may be found in Haug (1993). Equations 11b through 11h may be substituted into Equation 11a for the energy balance. All terms in Equation 11i are constant except for Treact. The energy balance presumes no condensation. Equations 3 through 11 must be solved over time, where all parameters are known or hypothesized except for the reactor temperature Treact. Software packages such as STELLA® allow one to impose conditional aeration rates (e.g., rate dependant on reactor temperature). One may also impose moisture conditions on which one may add water at a specified rate.

MODEL VALIDATION

Substrate: Data from Das et al. (1997b) composting of duster and gin trash was compared to model results. The compost process used in Das et al. (1997b) was conducive to modeling. The material was mixed and placed in a barrel with temperature control aeration. The compost was only mixed weekly as opposed to continually as the model suggests, which explains the discrepancies in the temperature during mixing. Moisture content (wet basis) was maintained at above 55% but was adjusted only weekly. The model was set to add water whenever the moisture content dropped below 55%. One kg of substrate was used. Data points for the composting are actually a four hour moving averages. The O_2 concentrations are samples taken over a minute. This varies from the data displayed by the model which are 6 hour averages of 7.2 averages. Selected model inputs are given in Table 1.

Table 1. Selected model inputs

	Unit Formula (refer to Equation 1)				ASH	BVS	MC	K_d	Energy content
	A	B	C	D	%	%	%	Day^{-1}	MJ/Kg
Duster, Wool & Gin Trash	9	11	3	1	40	19	69.1	.015	20*

* The K_d value was evaluated by qualitative best fit to experimental data

The model can incorporate changes in humidity and ambient temperature that affect energy into the system. The climate data is not available for this model and therefore not included. The temperature was set at a constant 26°C and 50% relative humidity.

Aeration: The aeration for Das et al. (1997b) was set at 40.8 m^3/day when vessel temperature exceeded 55°C. Below 55°C the flow rate was set to 0.45 m^3/day. The initial mass of the composting vessel was then used to determine specific flow rates of 7.7 m^3 /day above 55°C and 0.085 m^3/day below 55°C.

Results: Comparisons between predicted mass, temperature and oxygen were made to validate the model. The fraction of remaining solids matches within two percentage points. The actual data was collected and weighed weekly. Selected simulation results are shown in Figure 1. The dry mass decays exponentially as one would expect. The temperature and airflow dynamics behave as one would expect with aeration being controlled by temperature.

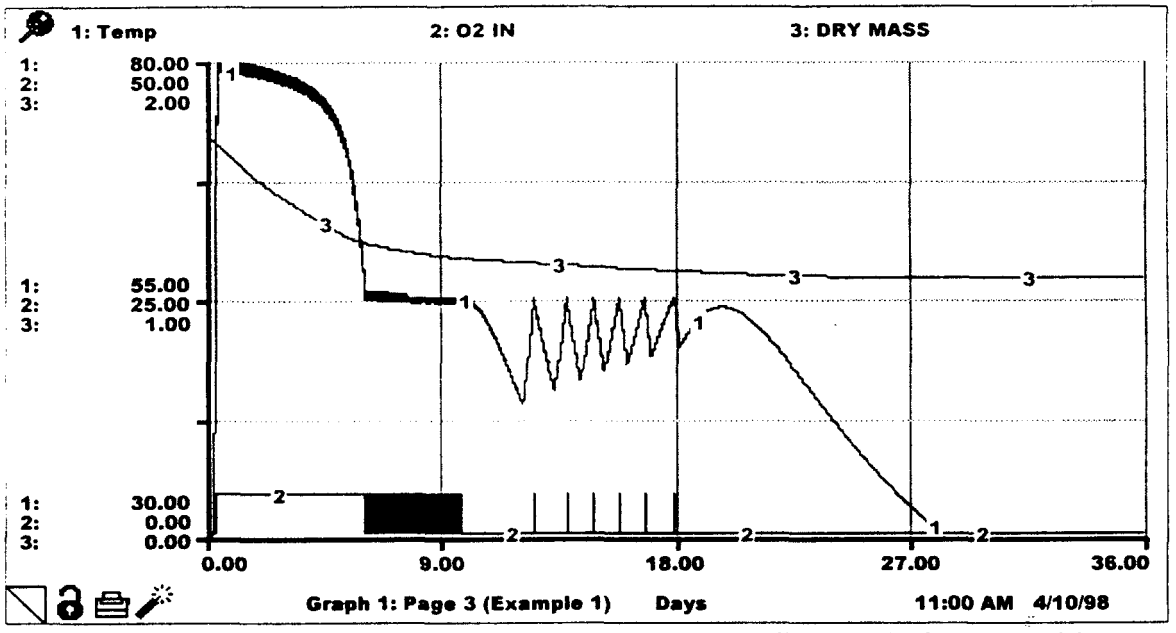

Figure 1. Selected dry mass, temperature and oxygen concentration predicted results from the model.

The temperature results appear to not match closely, particularly the time at which the reactor cools. Two reasons explain the discrepancies : incomplete mixing and excessive aeration rates. When mixing is incomplete, non-degradable material encapsulates BVS which becomes inaccessible to microbial activity. Excessive aeration rates can actually be explained as a function of incomplete mixing. The model distributes the aeration evenly. In reality, channeling through the substrates exists. The channeled air has higher velocities and a higher effective cooling of the vessel temperature. The channeling allows for hot pockets to exist in the vessel creating temperature readings which are lower than the average vessel temperature.

Note the reheating occurs in the actual data on days 7, 14, and 21 (Figure 2.). The increased reheating suggests more BVS are freed for degradation. Also, if the below 55°C aeration rate is increased the temperature will drop off sooner. Doubling the low aeration rates generates a temperature curve more closely related to the actual data. The improved fit suggests doubling the aeration rate for non-continuous mixed systems. The reason channeling does not affect the high aeration rate is because the same average aeration rate can be generated by longer run times at a lower aeration rates, particularly if the actual high aeration is over designed.

Dramatic temperature drop while aerating does not necessarily mean a finished product, but means degradation, and therefore, heat production, has slowed below the cooling affect of the aeration. During the slow degradation the pile can removed for curing or the aeration can be reduced to match the decomposition.

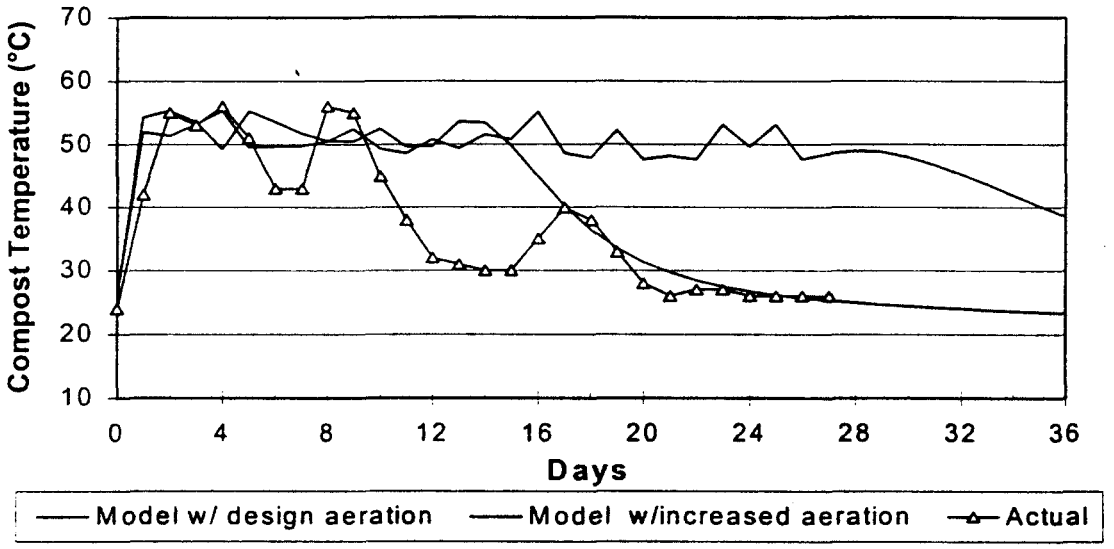

Figure 2. Temperature in composts as a function of aeration rate.

The maximum oxygen consumption rate measured, 2.7 g/mg-DM/hr, is within 15% of the modeled rate of 2.3 g/mg-DM/hr. The maximum rate measured occurred within the first day while the modeled peak does not occur until day 6. This discrepancy can point directly to an error in the model. The logistic function which accounts for oxygen limitation uses a ratio of the oxygen supplied and maximum consumption in an unlimited oxygen atmosphere. This ratio causes maximum O_2 consumption to occur after the potential maximum oxygen consumption has decreased and therefore increasing the ratio.

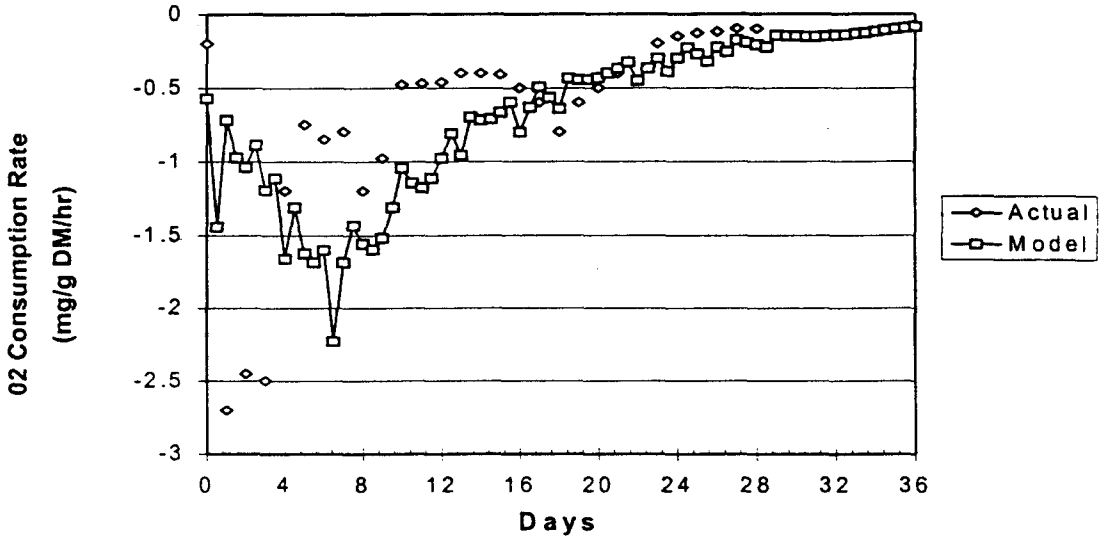

Figure 3. O_2 consumption rates.

The measurement of the O_2 consumption is questioned, because a sample of air from the head space is taken for a minute every hour. Depending on the cycling of the fan, the measurement can be skewed. If the fan is cycling during sampling it will give a false low reading and vice versa. Changing the time period that the O_2 consumption is averaged makes a large difference. The data here is a 6 hour average. The hourly averages are higher and the six minute average goes as high as 40 mg/g-DM/hr.

MODEL USES

The model can be used to evaluate "what if" questions associated with virtually all operational parameters. For example, one may develop different aeration regimes to optimize the composting process. One possibility is to develop variable speed aeration motors to maximize ramp up temperatures and prevent excessive cooling. While temperature ramp up is not a concern in steady state system, in reality substrate variability does occur. One may evaluate reactor vessel sizing in relation to the product throughput rate. A model can predict required changes to keep a composting system running optimally or to prevent system failure.

Another component an operator must control is water addition. Adding ambient temperature water has a large impact on the energy balance of the system. Modeling the affects of water addition can also help optimize that process. A difficult parameter in compost modeling to determine is the degradation coefficient. Evaluating a computed calculated degradation coefficient based on data collected at the pilot scale as was done in this study is another use of a process model.

Much remains to be done with respect to modeling the compost process. Many assumptions are necessary in terms of input parameters as well as model structure. Modeling the process enables researchers to structure their work in light of a large integrative picture.

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