

PREDICTION OF TEMPERATURE AND OXYGEN DISTRIBUTIONS DURING AEROBIC MICROBIAL GROWTH

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AEROBIC DECOMPOSITION IS the basis of many processes which are of current commercial or environmental interest. For example, it is being studied commercially as a means of energy production and has long been used for horticultural purposes such as composting. Environmental examples of aerobic decomposition include various types of waste disposal, strip mine reclamation, and the decomposition of oil spills in the ocean.

Although aerobic microbial growth has been used for centuries, e.g., in composting, it is often practiced more as an art than a science. This is not surprising when one considers the complexity of the biochemical processes by which materials are decomposed. The microorganisms which carry out the decomposition require a suitable environment in terms of nutrients in the substrate, temperature range, oxygen content, and moisture content. In addition, a biochemical source of energy is needed for the decomposition to occur. Thus, in order to develop an accurate mathematical model of the aerobic microbial process it is necessary to consider oxygen transfer into as well as carbon dioxide and thermal diffusion out of the decomposing mass.

DEVELOPMENT OF EQUATIONS

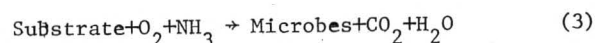
THE THERMAL AND mass diffusion aspects of decomposition are described by Fourier's and Fick's Laws, respectively. When chemical reaction source and sink terms are included, the following equations for the temperature and oxygen distributions result:

$$R = -\frac{k}{H} \frac{d^2 T}{dy^2} \quad (1)$$

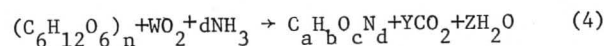
$$-R = -c\bar{D} \frac{d^2 X}{dy^2} + \frac{d}{dy} \left(X \sum_i N_i \right) \quad (2)$$

It is more difficult to determine the mathematical form of the reaction term, R , in Equations 1 and 2, i.e., the rate expression for the complex biochemical reactions taking place during decomposition.

The energy for the numerous biochemical reactions occurring during decomposition comes from the biological oxidation of some of the available carbon.^{1, 2} The biological oxidation of organic compounds to carbon dioxide and water is a complicated process being made up of several successive enzyme catalyzed reactions.³ However, the overall reaction (unbalanced) can be written as



If one considers the substrate to decompose via carbohydrate oxidation a balanced form of Equation 3 can be written



The values of a , b , c , d , W , Y and Z can be calculated from mass balances on the carbon, oxygen and hydrogen. Assuming the composition of cell material to be similar to yeast which is 47% C, 6.5% H, 31% O and 8.5% N⁴ and that about 0.4 g of cell material are produced per gram of substrate, the values of a , b , c and d are: $a = 2.82n$; $b = 4.69n$; $c = 1.40n$; $d = 0.436n$. Using these

values, a mass balance for the oxygen gives

$W = 3.03 n$, moles CO_2 /mole substrate consumed
Similarly, mass balances for the carbon and hydrogen give

$Y = 3.18 n$, moles CO_2 /mole substrate consumed
 $Z = 4.31 n$, moles CO_2 /mole substrate consumed

The respiratory quotient (RQ) of a reaction is a measure of the amount of CO_2 produced per unit of O_2 consumed, i.e.,

$$\text{RQ} = \frac{\text{moles } \text{CO}_2 \text{ produced}}{\text{moles } \text{O}_2 \text{ consumed}} = Y \quad (5)$$

The reaction shown in Equation 4 has a respiratory quotient of 1.05. Experimental studies^{5, 6} have measured the respiratory quotient of laboratory compost piles undergoing aerobic decomposition and found that it is approximately 0.9. From this experimental evidence and Equation 5 it can be deduced that the biological oxidation of the substrate is the predominant oxidative reaction taking place during aerobic decomposition. This is not surprising since the other reactions taking place during aerobic decomposition rely upon the biological oxidation to supply the energy necessary for these reactions to proceed. Therefore, in the mathematical model the biological oxidation will be the limiting reaction considered.

Using this model the rate of substrate decomposition according to Michaelis-Menten kinetics (assuming oxygen limitation) is given by the Monod equation:

$$R = \frac{\mu_{\max} (M)X}{K_s + X} \quad (6)$$

Since the reaction rate is assumed to be limited by the rate of oxygen diffusion, $K_s \gg X$, and therefore

$$R = \frac{\mu_{\max}}{K_s} (M)X \quad (7)$$

The temperature sensitivity of μ_{\max} is given by

$$\mu_{\max} = A' e^{-E/R_g T} \quad (8)$$

Substituting this into Equation 7 one gets

$$R = \frac{A'}{K_s} e^{-E/R_g T} (M)X \quad (9)$$

If we further assume that the microorganisms are in a linear growth phase, their concentration

would remain relatively constant and under these conditions Equation 9 reduces to

$$R = A e^{-E/R_g T} X \quad (10)$$

where $A = \frac{A'}{K_s} (M)$. This equation can now be substituted into the transport Equations (1 and 2) to give

$$\frac{d^2 T}{dy^2} = - \frac{AH}{k} e^{-E/R_g T} X \quad (11)$$

$$\frac{d^2 X}{dy^2} - \frac{1}{cD} \frac{d}{dy} (X \sum_i N_i) = + \frac{A}{cD} e^{-E/R_g T} X \quad (12)$$

According to the model the bulk diffusion term is given by

$$\sum_i N_i \sim N_{\text{O}_2} + N_{\text{CO}_2} \quad (13)$$

But Equation 4 indicates that the oxygen and carbon dioxide are approximately in a state of equimolar counterdiffusion and therefore $\sum_i N_i \sim 0$. This reduces Equation 12 to

$$\frac{d^2 X}{dy^2} = + \frac{A}{cD} e^{-E/RT} X \quad (14)$$

Converting Equations 11 and 14 to dimensionless variables gives

$$\frac{d^2 T^*}{dy^{*2}} = - D e^{-B/T^*} X^* \quad (15)$$

where

$$\frac{d^2 X^*}{dy^{*2}} = + C e^{-B/T^*} X^* \quad (16)$$

$$B = E/R_g; \quad C = \frac{AL^2}{cD}; \quad D = \frac{AH X_o L^2}{k(T_m - T_o)}$$

The temperature in the exponential term is not made dimensionless since doing so would not simplify the solution of the equations. Equations 15 and 16 can now be solved simultaneously with the proper boundary conditions to get the temperature and oxygen distributions desired.

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ANALOG COMPUTER PROGRAM

THE ANALOG COMPUTER was chosen to solve this problem since it provided the flexibility to study the effects of changes in the parameters B, C and D as well as give a rapid solution to Equations 15 and 16. The program used to determine the temperature and oxygen distributions is shown in Figure 1. Table 1 summarizes the potentiometer values and amplifier outputs.

The portion of the program in the upper half of Figure 1 is devoted to calculating the forcing function, $e^{(D'-B/T)X}$, where $D' = \ln D$. The value of B, which is related to the activation energy, is controlled by P3. The value of P3 must actually be set at $B/20,000$ in order to get proper scaling. P7 controls the value of the pre-exponential constant, D, and it accomplishes this by being set at the value of $10 e^{(D'-B/T)|_0}$. The output of A6 is $e^{D'-B/T}$ and as can be seen in Figure 1, this is generated by an internal integration loop. This method for generating the exponential function is discussed by Cadman and Smith⁸ and eliminates the problems caused by the use of a non-linear exponential circuit.

The output of A7 is the forcing function, $e^{D'-B/T}X$, which is then integrated twice to get T^* as a function of y^* . Actually the output of the second integrator is $10T^*$ for scaling purposes. In many systems, the temperature and oxygen fluxes at $y^* = 0$ are approximately zero. When this condition is met Equations 15 and 16 indicate that X^* is linearly related to T^* . The linear relationship between X^* and T^* is derived as follows:

$$dX^*/dy^* = - (C/D) dT^*/dy^* \quad (17)$$

$$X^* = - (C/D) \int \frac{dT^*}{dy^*} dy^* + X^*|_0 \quad (18)$$

$$T^* = \int \frac{dT^*}{dy^*} dy^* + T^*|_0 \quad (19)$$

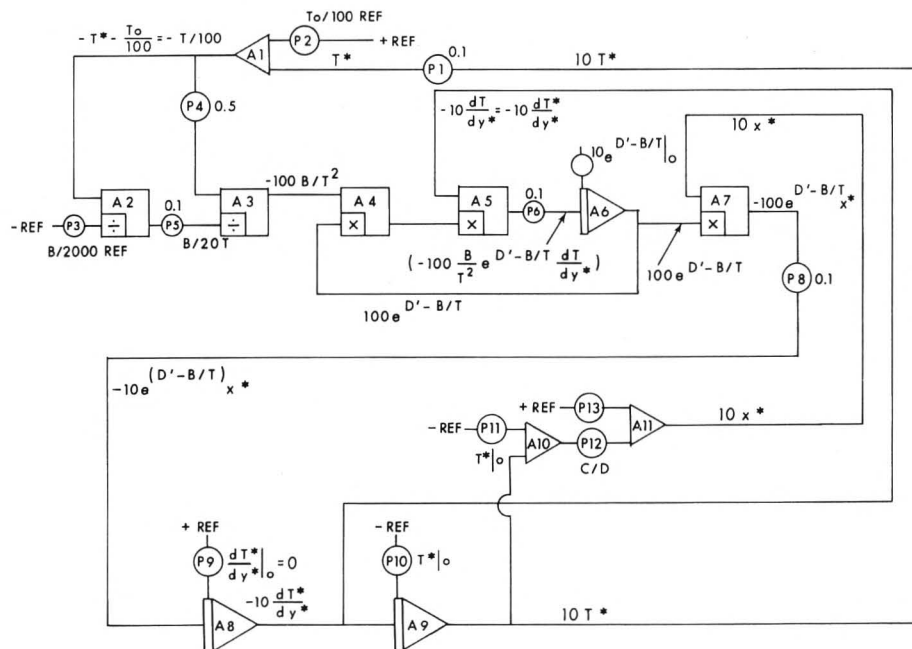


Figure 1: ANALOG COMPUTER SOLUTION

$$X^* = - (C/D) (T^* - T^*|_0) + X^*|_0 \quad (20)$$

$$\text{at } y^* = 0: \quad dT^*/dy^*=0, dX^*/dy^*=0, T^*=T^*|_0$$

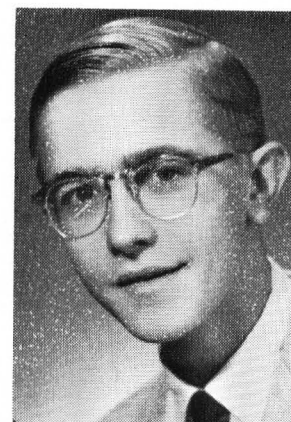
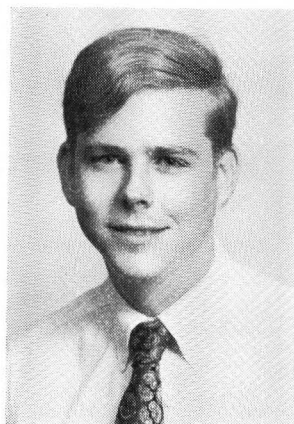
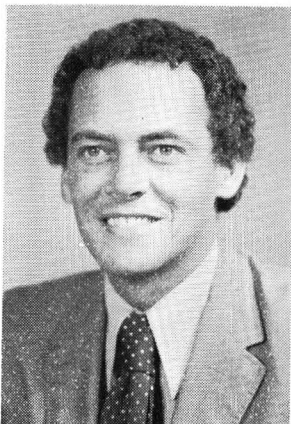
$$\text{at } y^* = 1: \quad X^* = 1$$

This linearity is used to simplify the program by replacing the integrators for X^* with a much simpler circuit and indeed, this is the way in which X^* , or to be more exact, $10X^*$, is generated. P12 controls the value of C/D , P13 controls $X^*|_0$ and P10 and P11 are both set at the value of $T^*|_0$.

In working with the program, the most sensitive parameter has been found to be the exponential part of the forcing function, $e^{D'-B/T}$. The value of B, which is related to the activation energy, can usually be estimated from data in the literature. Thus in fitting experimental data the value of P3 is known independently and the values of P7, P10, P12 and P13 are adjusted to get the best data fit. P11 is set to exactly equal P10 ($T^*|_0$) and therefore is not an independent parameter. P10 and P13 control the values of the boundary conditions, $T^*|_0$ and $X^*|_0$ respectively. Therefore, the computer predictions are essentially controlled by two parameters, C and D, which are controlled by P12 and P7 respectively.

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Theodore W. Cadman is engaged in teaching and research directed to process control and simulation. He serves as Director of the Laboratory for Process and Simulation at University of Maryland.

Dr. Cadman received his BS, MS, and PhD from Carnegie Mellon University. He is a member of the AIChE, ACS, NSPE and ISA. (Above right)

TABLE 1
Amplifier Outputs And Potentiometer Settings

Component	Output or Value	Estimated Max. Value	Scaled Value
Amp. 1	-T	-400 °K	-T/100
2	B/T	20	B/2T
3	-B/T ²	-0.1 °K ⁻¹	-100 B/T ²
4	$\frac{B}{T^2} e^{D'-B/T}$	0.01 °K ⁻¹	1000 $\frac{B}{T^2} e^{D'-B/T}$
5	$-\frac{B}{T^2} e^{D'-B/T} \frac{dT}{dy^*}$	-0.01	-1000 $\frac{B}{T^2} e^{D'-B/T} \frac{dT}{dy^*}$
6	$e^{D'-B/T}$	0.1	100 $e^{D'-B/T}$
7	$-e^{D'-B/T} X^*$	-0.1	-100 $e^{D'-B/T} X^*$
8	$-\frac{dT^*}{dy^*}$	-1.0	-10 $\frac{dT^*}{dy^*}$
9	T*	1.0	10T*
10	$-T^* + T^* _0$	1.0	$-10T^* + 10T^* _0$
11	X*	1.0	10X*
Pot 1	0.1		0.1
2	T ₀	300	T ₀ /100 Ref.
3	B	6000	B/2000 Ref.
4	0.5		0.5
5	0.1		0.1
6	0.1		0.1
7	$e^{D'-B/T} _0$	0.1	10 $e^{D'-B/T} _0$
8	0.1		0.1
9	$\frac{dT^*}{dy^*} _0$	0	0
10	T* ₀	1.0	T* ₀
11	T* ₀	1.0	T* ₀
12	C/D	10	C/D
13	X* ₀	1.0	X* ₀

RESULTS

THE VALIDITY OF Equations 15 and 16 were tested against available data from compost piles. The boundary conditions used were

$$\text{at } y^* = 0 \quad dT^*/dy^* = 0, dX^*/dy^* = 0, \\ T^* = T^*|_0 \quad \text{at } y^* = 1 \quad X^* = 1$$

where $y^* = 0$ represents the center of the pile and $y^* = 1$ represents the outside surface. The experimental data of temperature distributions in actual compost heaps was supplied by the Butler County Mushroom Farms.† The value for the activation energy was determined from rate versus temperature data on laboratory compost heaps⁵ and was found to be 1.11×10^4 cal/mole. The experimental compost data were then fitted by varying the values of the other model parameters. The shape of the computer was very sensitive to changes in the pre-exponential constants and were affected to a much smaller degree by the boundary conditions.

Correlations between the model and two sets of data are shown in Figures 2 and 3. $y^* = 0$ represents the center of the compost pile with the outside surface being at $y^* = 1$. The temperature range in the two graphs is from 27°C ($T^* = 0$) to 127°C ($T^* = 1$) and the oxygen combination range is from 0% O_2 ($X^* = 0$ to 21% O_2 ($X^* = 1$).

The two sets of data were taken from separate compost piles at a height of 3 feet from the bottom of the pile. The piles were 7 feet wide and approximately 6½ feet high. The computer predictions were within 1°C of the measured temperatures for 9 of the 14 data points, i.e., 64% of the points, and were within 2°C for 13 of the 14 data points. The maximum deviation between the model predictions and the measured temperatures was 3°C. The oxygen distributions predicted are reasonable in that they predict low oxygen concentrations in the interior of the pile, as have been found experimentally^{9, 10} The model further predicts that the oxygen concentration rises rapidly as the outer edge of the pile is approached until at the surface the oxygen concentration is equal to atmospheric conditions ($X^* = 1$ or 21% by volume).

The values of the model parameters used to obtain the computer predictions in Figures 2 and 3 are given in Table 2. The dimensionless parameter C, which is related to the oxygen distribution varies by 7% of the average value for the two data sets, while D, which is related to the temperature distribution, varies by 8% of the average. The relative constancy of the model parameters would be expected since the data were obtained on similar compost piles and therefore only small variations were anticipated.

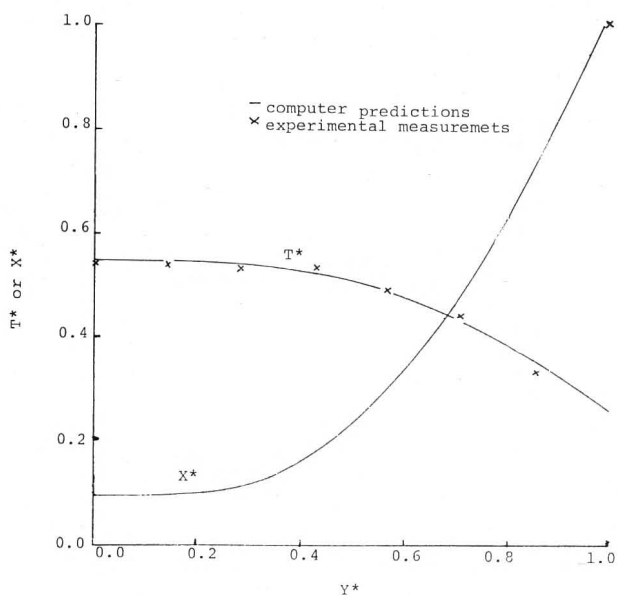


FIGURE 2. Correlations For Compost Heap 1.

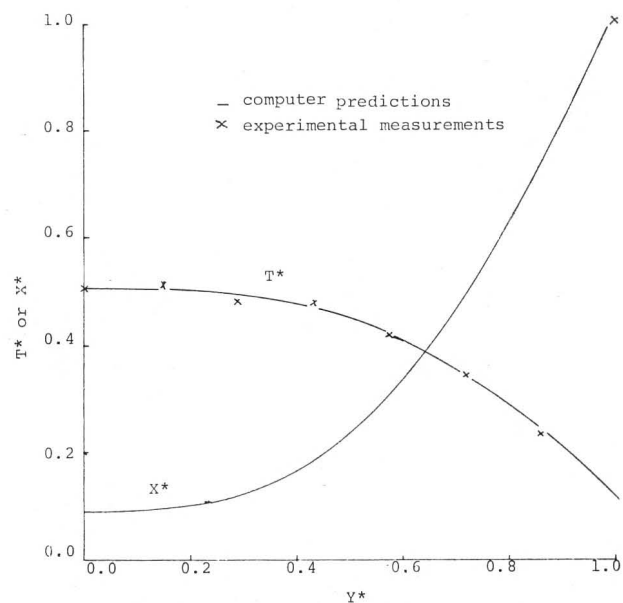


FIGURE 3. Correlations For Compost Heap 2.

CONCLUSION

THE SUCCESS WITH which the model predicted temperature and oxygen distributions gives strong support to the assumptions made in its development. Specifically, proof of the oxygen limitation assumption is very important in commercial activities such as composting since the rate at which the process is carried out could be significantly increased by improved aeration. The mathematical model presented here will be used to study the effects of process modifications to improve such activities. Similarly, the use of the biological oxidation reaction as the predominant oxidative reaction is important in helping to understand and control aerobic microbial growth.

It should also be noted that the basic mathematical form of the model is applicable to any problem in which simultaneous heat transfer, mass transfer and reaction are taking place. The analog computer program that was developed can be adapted to solve the resulting coupled differential equations by simply varying the model parameters and boundary conditions. Although the equations and computer program were developed for a cartesian coordinate system, they could be extended to solve problems in other coordinate systems, e.g., radial distributions in cylindrical or spherical systems. □

(Continued on page 100.)

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A	= $A'(M)/K_s$
A'	= pre-exponential kinetic constant
B	= E/R_g
c	= oxygen concentration, moles/liter $\frac{AL^2}{cD}$
D	= $\frac{AH X_o L^2}{k(T_m - T_o)}$
D'	= $\ln D$
D	= diffusivity of oxygen
E	= activation energy
H	= heat of reaction (per unit of O_2 consumed)
k	= thermal diffusivity
K_s	= Michaelis constant
L	= thickness of decomposing mass
(M)	= concentration of microorganisms
N_i	= molar flux of species i
R	= rate of substrate decomposition
R_g	= universal gas constant
T	= temperature, °K
T_m	= maximum anticipated temperature
T_o	= minimum anticipated temperature $T/(T_m - T_o)$
$T^* _o$	= value of T^* at $y^* = 0$
μ	= specific growth rate of microorganisms
μ_{max}	= maximum specific growth rate of microorganisms
X	= oxygen concentration, mole fraction
X_o	= oxygen concentration in the atmosphere
X^*	= X/X_o
$X^* _o$	= value of X^* at $y^* = 0$
y	= distance from center of the decomposing mass
y^*	= y/L

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ChE Book Review Continued from page 99.

some areas of comparatively recent development and there is no other reference where a useful introduction can be found in one place. This demands an introduction to probability theory which is provided in chapter 4 where the concept of the random variable and its characterisation is carefully explained. Next comes a discussion of stochastic processes, their description and governing equations. Of particular value here is the explanation of the differences between the calculus of Ito and that of Stratonovich. The sixth chapter on the theory of residence time distributions discovers a habitat where the behavior of both deterministic and stochastic models can be observed.

The remainder of the book is devoted to parameter estimation and process identification, the former being the appropriate task when the structure of the model is fully known, the latter when it is unknown. In both cases there is a natural distinction between linearity and nonlinearity with a simpler set of methods for the linear. In the estimation problem, algebraic, differential equation and stochastic models are discussed, as are frequency domain, moment, gradient and search methods. There follows a valuable chapter on the design of experiments in the light of the estimation problem.

In introducing the subject of the realization of systems for which the structure of the model is unknown the dual concepts of controllability and observability are first explained and some specific algorithms are then developed. The final chapter is on process identification of nonlinear systems, a problem of peculiar difficulty which brings the student near to the frontier of the subject.

For anyone giving a course in methods of process analysis at a graduate level this book will provide a splendid text, while, for the student wanting to study the subject on his own, its organization and clarity make it equally useful. Altogether it is one of the best books in the Prentice-Hall Series in the Physical and Chemical Engineering Sciences.