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Unsteady 2D coupled heat and mass transfer in porous media with biological and chemical heat generations

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1. Introduction

Sewage sludge is the inevitable end product of municipal wastewater treatment processes worldwide. For temporary disposal, the sewage sludge can be accumulated in compost piles. Municipal solid waste landfills often develop scenarios of self-heating causing negative environmental impacts by odors, gas generations and smoke production. Auto-ignition and resulting fires at landfill has been a non-desirable outcome in compost piles worldwide [\[1,2\].](#page-7-0) The conditions leading to spontaneous combustion in selfheating systems were revised for Buggeln and Rynk [\[3\].](#page-7-0) This sludge has particular biochemistry characteristics (organic carbon and micro-organisms) that combined with the compost process originate a very complicated system to analyze.

Chemical reactors have been proposed to study energy generation by carbonaceous materials [\[4\]](#page-7-0). Numerous efforts have been made for describing non-equilibrium systems using different strategies. One of the methods used in three studies is the statistical thermodynamics [\[5–7\].](#page-7-0) The thermodynamic coupling is not considered in this study. The use of a mathematical model coupling heat and mass transfer along the use of finite volume simulations is the way used in this work to investigate the diffusion in the compost pile and the auto-ignition processes. Finite differences, finite volumes and finite elements methods have been used along with

ABSTRACT

The coupled two-dimensional heat and oxygen diffusion in a compost pile of sewage sludge obtained from domestic wastewater treatment was studied. The unsteady, coupled, non-linear mathematical model, solved through the finite volume method, includes the volumetric heat generation caused by the action of aerobic bacteria and by the oxidation of cellulose in a porous media. The numerical simulation allows the prediction for the pile shape and size effects on the heat generated and on oxygen consumption. Temperature and oxygen concentration transient distributions within compost piles are presented for different geometries. Heat (temperature) and mass transfer (oxygen) results indicate that the pile height has an important effect on the heating process and that keeping the compost pile height lower than 1.7 m the self-combustion of sewage sludge can be avoided.

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different mathematical model in the prediction of the fluid dynamics and convective heat transfer in enclosures with porous media [\[8–21\].](#page-7-0)

Exothermic chemical reactions in porous media has been investigated by using numerical methods [\[22,23\].](#page-7-0) Effect of concentrations and temperature on the coupled heat and mass transport in liquid mixtures was studied for Demirel and Sandler [\[24\].](#page-7-0) The self-combustion phenomena originated by internal heat generation in piled solids such as charcoal, grains, garbage, sewage sludge, and others, can be described by the explosion theory developed by Semenov and Frank-Kamenetskii [\[25,26\]](#page-7-0). In the explosion model only the temperature rise is described by Arrhenius equation, which explains the starting point of self-combustion when the internal heat production–dissipation relationship reaches a point where the internal temperature is above a critical temperature. Analytical and numerical results were obtained for oxidation and combustion reactions in porous media described by Arrhenius equation forms [\[27–31\].](#page-7-0) Biomass combustion mathematical models have been proposed recently [\[32–34\].](#page-7-0) Thermal conversion optimization for biomass furnaces and products gas composition prediction have been two important targets in the models developed. A parametric equation to describe the biological processes activation and inactivation has been often used in aerobic biodegradation in order to calculate the organic fraction of municipal solid waste [\[35\]](#page-7-0) and for solid phase fermentation processes [\[36–39\].](#page-7-0) The theory developed by Semenov was used by Nelson et al. [\[40\]](#page-7-0) to describe the heat increase at low temperatures inside a pile as a

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Nomenclature

A pre-exponential factor for the oxidation $(m^3/kg s)$

result of exothermic biological activity, as well as the oxidation of cellulose and cellulose-like materials as fuels after the initial ignition. The Galerkin method has been used to obtain a semi-analytical solution to capture temperature increments in 1D and 2D compost piles due to micro-organisms undergoing exothermic reactions, which shows excellent agreements with a finite-difference solution [\[41\].](#page-7-0)

In this paper, auto-ignition and thermal explosion in compost piles are predicted by using the finite volume method developed by Patankar [\[42\]](#page-7-0) to solve the coupled two-dimensional heat and mass diffusion partial differential equations proposed by Sidhu et al. [\[43\]](#page-7-0). A general convection and radiation boundary condition is used in the lateral and top surfaces. The self-heating processes caused by biological effects and oxidation cellulosic materials are investigated in terms of the pile height. Unsteady temperature and oxygen distribution within the solids removed from water treatment are predicted; to assess the effect of geometrical changes for a trapezoidal, asymmetric and polynomial form of the compost pile.

2. Mathematical model

The mathematical model considers transient coupled twodimensional heat and oxygen diffusion in a porous media [\[43\].](#page-7-0) The pile bottom is assumed to be adiabatic, as shown in Fig. 1. Cellulosic oxidation and micro-organism activity inside the pile are incorporated in the model by volumetric heat generation. For simplicity, local thermal equilibrium is assumed which is a common assumption for porous medium and packed particle beds [\[44\]](#page-7-0).

$$
(\rho C)_{\text{eff}} \frac{\partial T}{\partial t} = k_{\text{eff}} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q_c (1 - \varepsilon) A_c \rho_c C_{\text{ox}} \exp \left(\frac{-E_C}{RT} \right) + Q_b (1 - \varepsilon) \rho_b \rho_c \left(\frac{A_1 \exp \left(\frac{-E_1}{RT} \right)}{1 + A_2 \exp \left(\frac{-E_2}{RT} \right)} \right)
$$
(1)

Greek symbols

- β inclination angle of the lateral right wall
- Γ diffusion coefficient
- Δt time step (s)
- ε porosity
- ρ density (kg/m³)
- θ inclination angle of the lateral left wall
- ϕ dependent variable

Subscripts

Superscript

 $k, k+1$ iteration number

 $\varepsilon \frac{\partial C_{ox}}{\partial t} = D_{\text{eff}} \left(\frac{\partial^2 C_{ox}}{\partial x^2} + \frac{\partial^2 C_{ox}}{\partial y^2} \right)$ In Eqs. (1) and (2), A_c is the pre-exponential factor for the oxidation of the cellulose; and E_c , E_1 and E_2 are the activation energy for the cellulose, biomass growth and inhibition of biomass growth, respec-

defined in terms of the pile porosity
$$
\varepsilon
$$
,

 ∂y^2

 $(2c - 2c)$

$$
k_{\text{eff}} = \varepsilon k_{\text{air}} + (1 - \varepsilon)k_{\text{c}} \tag{3}
$$

tively. Heat and mass transfer properties in the porous media are

 $- (1 - \varepsilon) A_c \rho_c C_{ox} \exp \left[\frac{-E_c}{RT} \right]$ (2)

$$
(\rho C)_{\text{eff}} = \varepsilon \rho_{\text{air}} C_{\text{air}} + (1 - \varepsilon) \rho_{\text{c}} C_{\text{c}} \tag{4}
$$

$$
D_{\rm eff} = \varepsilon D_{\rm air,c} \tag{5}
$$

where k_{eff} and D_{eff} are the effective properties which are considered independent of temperature and concentration, and C_c is the specific heat capacity of the cellulose. The heat produced due to the cellulosic material oxidation is represented by the second term on the right-hand side of Eq. (1). This term is expressed as a function of the oxygen concentration and it is responsible of the self-heating. The last term in Eq. (1) represents heat generated due to biological

Fig. 1. Physical situation.

activity within the pile, caused by micro-organism growth. Oxygen content variation is included in Eq. [\(2\).](#page-1-0) Initially oxygen content in the pile has the same concentration than in the external air. The micro-organisms growth followed by organic matter oxidation produce the oxygen depletion. These assumptions are incorporated by the second term on the right-hand side of Eq. [\(2\).](#page-1-0)

Details in the formulation of the term representing the heat generated by the biomass have been given by Chen and Mitchell [\[45\].](#page-7-0) The parameter values used in the mathematical model were obtained from Ref. [\[43\]](#page-7-0).

The initial temperature and oxygen distribution within the pile are assumed to be the same as those corresponding to the surrounding ambient conditions

$$
T(x, y, 0) = T_0; \quad C_{ox}(x, y, 0) = C_{ox, 0}
$$
 (6)

Adiabatic and impermeable boundary conditions, are considered at the pile base

$$
y = 0 : \frac{\partial T}{\partial y}\Big|_{y=0} = 0; \quad \frac{\partial C_{ox}}{\partial y}\Big|_{y=0} = 0 \tag{7}
$$

Exchange with the surroundings at the outer pile surface considers heat transfer caused by a combined action due to convection and radiation through impermeable walls:

$$
y = H: -k_{\text{eff}} \frac{\partial T}{\partial x}\Big|_{y=H} = q''_{\text{conv}} + q''_{\text{rad}}; \quad D_{\text{eff}} \frac{\partial C_{\text{ox}}}{\partial y}\Big|_{y=H} = 0 \tag{8}
$$

$$
-k_{\text{eff}}\frac{\partial T}{\partial n}\bigg|_{y=H} = q''_{\text{conv}} + q''_{\text{rad}}; \quad D_{\text{eff}}\frac{\partial C_{\text{ox}}}{\partial n}\bigg|_{y=H} = 0 \tag{9}
$$

$$
q''_{\text{conv}} = h[T - T_{\text{a}}(t)] \tag{10}
$$

The heat transfer convective coefficient is assumed to change with ambient air velocity v [\[46\]:](#page-7-0)

$$
h = 5.7 + 3.8 \times \nu \tag{11}
$$

External thermal radiation incorporates incoming daily solar radiation and nocturnal heat losses in terms of a function that periodically changes with time according to

$$
q''_{\text{rad}} = a \cdot \sin(w \cdot t) \tag{12}
$$

An idealized two-dimensional domain was considered to assess the effects of the pile geometry. Three cases were considered for the compost piles investigated: (1) symmetric trapezoidal; (2) asymmetric trapezoidal; and (3) fifth polynomial contour.

3. Numerical procedure

The system of equations that governs this problems (1) – (12) was solved numerically using the finite volume method, Patankar [\[47\].](#page-7-0) Each one of the governing equations was written in the general form of the transport equation, with unsteady, diffusion and linearized source terms:

$$
\frac{\partial \phi}{\partial t} = \text{div}(F \cdot \text{grad}\phi) + Sc + Sp \cdot \phi \tag{13}
$$

The first-order accuracy in time was used in the numerical scheme to account for the unsteady heat and mass terms

$$
\frac{\partial \phi}{\partial t} = \frac{\phi^{t + \Delta t} - \phi^t}{\Delta t} \tag{14}
$$

The diffusion coefficient (Γ) and source terms (Sc, Sp) for each dependent variable ϕ are given in Table 1.

An original computational program, written in FORTRAN language, with a combination of the TDMA and Gauss–Seidel method

Table 1

Diffusion coefficient and source terms for the mathematical model.

an iterative solver [\[47\]](#page-7-0), was used to predict temperature and oxygen concentration inside the compost pile.

The pile geometry was discretized using three uniform grids: 100×100 , 200×200 and 300×300 nodes in the x- and y-directions, respectively, to verify that the results obtained were not influenced by the mesh size. Numerical simulations were carried out for four piles: 1.7, 1.8, 2.5 and 3.0 m height.

Temperature was noticed to increase initially smoothly with time while oxygen decreased slowly with time until sudden changes, caused by the cellulosic heat generation, were noticed for both temperature and oxygen concentration.

Therefore, a strategy based on the use of dynamic time steps was implemented, with lower time steps when the unsteady terms were higher. The different values of the time steps used in the unsteady calculations were in the interval

$$
300s \leqslant \Delta t \leqslant 3600s \tag{15}
$$

The iterative procedure ended at each time step when the maximum difference between iteration for $\phi = T$, C _{ox}, satisfied in each control volume the convergence criteria

$$
\phi_{ij}^{k+1} - \phi_{ij}^k \leq 10^{-4} \tag{16}
$$

4. Results and discussion

4.1. Validation of results

In order to validate the mathematical model and the numerical simulations a 2.5 m high, 8.5 m long and 7.0 m wide compost pile was built, with a 3D trapezoidal shape, with a 2.5 m wide top surface. Temperature was recorded using type K thermocouples (Ni–Cr) 0.1 m long and 0.0015 m in diameter, built with a type G junction and a silver end, provided with a 5-m long cable with flexible stainless steel coating. The thermocouples were connected to an LA/AI-A8 Cole Parmer data acquisition system coupled to a PC computer provided with the InstaTrend software programmed to collect temperature data every 10 min. Every week the values of the computer collected data were averaged and plotted. The temperature measurement points were located in the pile center (z-axis) at 2.1, 1.25 and 0.35 m depth. The pile was built with sewage sludge produced by a municipal waste water treatment plant located in the city of Santiago, Chile (El Trebal) in a landfill belonging to the same plant. The sewage sludge was produced in July 2004 and was used to build the pile in the third week of February 2005.

The experimental and numerical data are compared in [Fig. 2.](#page-3-0) Data obtained from numerical calculations were plotted considering daily output at 12:00 AM. The experimental and predicted data follow the same general trends. Near the surface (0.35 m depth) during the third week the main differences found are not larger than 3° C. The best description of the experimental data was obtained at a depth of 2.1 m.

Fig. 2. Comparison between experimental and numerical temperature values during 6 weeks.

4.2. General analysis for the temperature time evolution

A fundamental process in compost pile is to achieve a temperature level higher enough to cause the pathogen micro-organisms death along to the carbonaceous material degradation. The field practice indicates that an adequate compost process may be achieved when the temperature range inside the pile is between 313 K and 353 K. Initially, temperature inside the pile increases slowly from 293 K up to 353 K due to micro-organism growth, as described by the last term in the right-hand side of Eq. [\(1\).](#page-1-0) As the temperature increases beyond 353 K the death of different micro-organisms colonies is followed by a sudden increment in the cellulose oxidation, included as a volumetric heat generations in the second term in the right-hand side of Eq. [\(1\).](#page-1-0) The cellulose oxidation is accounted for in terms of the oxygen concentrations in the heat generation term of Eq. [\(1\)](#page-1-0) and in its counter-part term of oxygen depletion in the last term of the mass diffusion equation [\(2\)](#page-1-0). The sudden temperature increment is known as a thermal explosion. Compost physical properties change dramatically when the soil has experienced a thermal explosion and hence the compost material cannot be used as a soil fertilizer. Field control of such a sudden temperature increment is a very difficult task and often thermal explosion occur in practice, with the lost of the compost material.

A first case of self-heating in a rectangular porous pile, with 2.5 m height (H) and 5 m length (L) , was investigated using three grids, with 100 \times 100, 200 \times 200 and 300 \times 300 nodes, and three time steps: 300 s, 600 s and 3600 s. The temperature time evolution was calculated in the three positions: (f) $H/4$, $L/4$; (g) $H/2$, L/2 and (h) 3H/4, 3L/4. Results of the time needed to cause autoignition, in days, are shown in Table 2, for the three positions. The use of a time step of 600 s and a grid with 300×300 nodes allows to calculate a time for auto-ignition: 247, 246 and 250 days, at the three vertical positions, respectively, independently of the time a space discretizations.

Table 2

[Fig. 3](#page-4-0) shows the time evolution results of temperature in the (f) position: $H/4$, $L/4$, calculated with a grid of 300 \times 300 nodes using two time steps: 300 s and 3600 s. A typical heating curve depicting four stages is observed in the [Fig. 3a](#page-4-0). A first phase, lasting 35 days, where temperature increases from 293 K up to 340 K is observed. The growth and activities caused by aerobic micro-organisms, included in the mathematical model by a volumetric heat generation, originated the initial pile heating. A second phase, from day 35 up to day 246, with a very slow heating process in which temperature increases from 340 K up to 370 K is originated initially by thermophilic micro-organisms, that progressively are decreasing in number as temperature increases, followed by the cellulosic oxidation of the wood chips (used to increase the pile mechanical strength), incorporated as the first heat generation term in the right-hand side of Eq. [\(1\)](#page-1-0). Auto-ignition at H/4, L/4 occurs after 247 days, during the third stage, in which temperature increased suddenly in one day from 370 K to 515 K. A complex system of solid, liquid and gaseous fuels as a final result of the cellulosic oxidation originated a volumetric heat generation causing the self-ignition process. Temperature decreasing in time, characterized the fourth and last stage, in which the fuel reserves in the location are exhausting.

[Fig.](#page-4-0) 3b, a zoom view of [Fig. 3a](#page-4-0) for the time interval between days 240 and 255, shows that a time step reduction from 3600 s to 300 s allows to determine a more accurate prediction (within 1 day) for the time needed to insatiate the self-ignition in a 2.5 m height compost pile.

Due to the previous analysis, a mesh with 300×300 nodes and a dynamic time step with 300 s during the auto-ignition and 3600 s in other stages were used in all calculations.

4.3. Height pile effect on temperature and oxygen concentration

In this section, a critical pile height of 1.8 m for the thermal explosion to occur has been found. Heating curves at three different positions (H/4, H/2 and 3H/4) located at the mid horizontal section of four rectangular piles (5 m wide) with 1.7, 1.8, 2.5 and 3.0 m heights are shown in [Fig. 4](#page-4-0). Temperature is observed to increase up to 369 K in the 1.7 m height pile, at $H/4$ and $H/2$ vertical locations, and to 353 K at the position 3H/4, after 728 days. A sudden temperature increment, taking place at around 240 days for the 2.5 and 3.0 m height piles, and at 397 days (in $H/4$), at 374 days (in $H/2$) and 409 days (in 3H/4) can be observed to characterize the initial time for the self-ignition process. Compost piles with heights larger than 1.7 m are observed to initiate self-ignition in a time that is inversely proportional to the pile height.

Changes in the oxygen content with time, calculated inside compost piles with 1.7, 1.8, 2.5 and 3.0 m height, are described in [Fig. 5,](#page-4-0) at three vertical positions $(H/4, H/2)$ and $3H/4$). As a result of the coupling between heat and mass transfer caused by the cellulose oxidation in both diffusion equations, sudden oxygen depletions are observed at the three positions for 1.8, 2.5 and 3.0 m pile heights, that occurs at the time when fast increments in temperature were noticed. When pile height is 1.7 m, oxygen concentration inside the pile remains almost constant during the 728 days interval used in the analysis. The oxygen reduction to low levels in the domain coupled to the high temperatures achieved in the same regions destroys the aerobic thermophilic micro-organisms.

[Table 3](#page-5-0) summarized the results obtained after the analysis for self-ignition calculated from the time evolution of temperature and oxygen concentration distributions inside the four rectangular piles with different heights. Temperature and oxygen distributions results show that when the ratio between pile volume and heat transfer external area, V/A, is larger or equal to 1.05 the self-ignition inside the pile occurs.

Fig. 3. Temperature evolution in time calculated with two time steps 300×300 mesh, in position $H/4$, $L/4$, for a 2.5 m height pile: (a) full time scale and (b) during thermal explosion.

Fig. 4. Time evolution of temperature for four piles with different heights.

Fig. 5. Time evolution of the oxygen concentrations for four piles with different heights.

Micro-organism and cellulosic heat generations inside piles, calculated at a position located at mid section and 3H/4, for four different heights are presented for the rectangular pile in Fig. 6. A rapid initial growth followed by a fast fall in the micro-organism volumetric heat generated can be noticed for the four height pile investigated. While cellulosic heat generation inside a 1.7 m pile height is seen to increase to a value that remains almost constant after 450 days, piles higher or equal to 1.8 m show a monotonous increment that is followed by a sudden increment, causing selfignition The heat generated by the biological activity of microorganisms becomes equal to the heat generated by the cellulose oxidation after 102 days for the 1.7 m, 105 days for 1.8 m, 84 days for 2.5 m height pile and 77 days for the 3.0 m height piles. In the 1.7 m height pile, after 100 days, the cellulosic oxidation keeps the temperatures for all time simulation, the oxygen consumption increases until 500 day, after decreases. Maximum values of heat generation for the cellulose oxidations are 2.4 \times 10 5 W/m 3 , 5.7×10^5 W/m³ and 6.4×10^5 W/m³ for 1.8 m, 2.5 m and 3.0 m heights pile, respectively.

In the water treatment industries, the piles are about 1.5 m in height and 120 m in length. Numerical results verified by experimental observations show that temperature increment in the pile is a function of the volume. Therefore, the pile height must be considered a very important factor in the thermal explosions.When the initial oxygen content within the pile is in adequate concentrations micro-organisms and temperature increments are observed. This occurs until temperature reaches a value of 353 K when two phenomena occur: the death of the micro-organisms and the cellulosic

Table 3 Rate V/A in four piles with different heights.

High pile (m)	Area $(m2)$	Volume (m^3)	Rate V/A (m)	Self-ignition
1.7 1.8 2.5 3.0	8.4 8.6 10	8.5 12.5 15	1.01 1.05 1.25 1.36	No occur Occur Occur Occur

oxidation. The numerical results shown in [Figs. 4–6](#page-4-0) reproduce the biochemical processes described before, resulting in sudden changes in both oxygen and temperature in piles higher or equal to 1.8 m.

4.4. Geometry effects

Heat and mass transfer characteristics are described in terms of temperature and oxygen concentration distributions, at four times, in the nearby of the self-ignition time in [Figs. 7–9.](#page-6-0) These results were obtained by numerical simulations using the proposed model, Eqs. [\(1\)–\(12\)](#page-1-0). In [Fig. 7](#page-6-0) the evolution in time of temperature and oxygen concentration distributions for a symmetrical trapezoidal 3 m height pile with 8 m at the base and lateral walls inclined in 45° , are shown. A maximum temperature of 440 K is reached after 208 days in the pile lower-central section, which increases in the day 216 up to 519 K and is located at H/3, in the central region. Temperatures higher than 500 K can be observed in the central pile region for 60 days. Oxygen content inside the pile is observed to tend towards zero in an increased growing lower-central section of the pile from 216 to 252 days. Almost all the pile can be noticed to be in self-ignition in day 225 but the regions close to the lateral and top areas.

Heat and mass transfer inside a non-symmetric trapezoidal sludge pile, 8 m at the base and lateral inclined walls with angles θ = 56.3° and β = 33.7°, caused by chemical and biological reactions, are described in terms of temperature and oxygen distributions in [Fig. 8.](#page-6-0) Self-ignition is initiated in day 215 where a maximum temperature of 513 K is achieved. A narrow region with high temperature gradients can be observed in the lower-central region of the pile at day 217. At this time, the self-ignition front is closer to the larger lateral wall (with $\beta = 33.7^{\circ}$) and hence that smoke production can be expected to initiate there. During self-ignition the zone with maximum temperatures, in the range 516–519 K, reached between days 217 and 253 is closer to the shorter inclined wall.

Time evolution for temperature and oxygen concentration distributions at 209, 247, 275 and 300 days, for a non-symmetrical

Fig. 6. Time evolution of energy and oxygen consumption generation for four piles with different heights.

Fig. 7. Distribution of temperature and oxygen concentration within a compost pile, trapezoidal geometry.

Fig. 8. Distribution of temperature and oxygen concentration within a compost pile, asymmetric geometry.

compost pile with two different height bumps, with a maximum height of 3 m and 8 m in the base, are depicted in Fig. 9. Self-ignition occurs near the base of the taller region, at day 258 with a

Fig. 9. Distribution of temperature and oxygen concentration within a compost pile, polynomial geometry.

maximum temperature equal to 493 K, propagated towards the central zone of the taller region and then migrates towards the pile section with lower height (1.5 m), where a maximum temperature equal to 502 K can be noticed at day 300. The self-combustion zone can be easily detected as the region in which the oxygen content is zero that in day 300 can be observed to extend from the pile base to a region close to the external walls.

5. Conclusions

Self-combustion of sewage sludge generated as the end product of municipal wastewater treatment processes was studied. The relation between compost pile height and the self-combustion phenomenon was studied under convection and radiation boundary conditions. A two-dimensional mathematical heat and mass diffusion model, solved through the finite volume method, that includes heat and oxygen diffusion as well as heat generation from cellulose oxidation and micro-organisms was used to predict the pile heating process. Numerical simulations indicate that self-combustion does not take place when the piles are smaller than 1.8 m in the height. The results show that the heating process is initiated by the volumetric heat generation by micro-organisms, and the thermal explosion is caused by cellulose oxidation when the volume to area ratio exceeding 1. The time required to initiate selfcombustion is inversely proportional to the pile height. Internal distribution of the temperature and oxygen concentration depends on the geometry of the compost pile.

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