Multiphase Modeling of Flow, Transport, and Biodegradation in a Mesoscale Landfill Bioreactor

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Abstract

The need to control gas and leachate production and minimize refuse volume in municipal solid waste landfills has motivated the development of landfill simulation models to predict and design optimal treatment processes. We have developed a multiphase and multicomponent nonisothermal module called T2LBM for the three-dimensional TOUGH2 flow and transport simulator. T2LBM can be used to simulate aerobic or anaerobic biodegradation of municipal solid waste and the associated flow and transport of gas and liquid through the refuse mass. Acetic acid is used as a proxy for all biodegradable substrates in the refuse. T2LBM incorporates a Monod kinetic rate law for the biodegradation of acetic acid by either aerobic or anaerobic microbes as controlled by the local oxygen concentration. We have verified the model against published data, and applied it to our own mesoscale laboratory aerobic landfill bioreactor experiments. We observe spatial variability of flow and biodegradation consistent with permeability heterogeneity and the geometry of the radial grid. The model is capable of matching results of a shut-in test where the respiration of the system is measured over time.
Introduction

Concerns about air and water pollution emanating from landfills, coupled with limited suitable land available for the ever increasing needs of disposal of municipal solid waste (MSW), have led to landfill operations that involve active management of the refuse. For example, by law modern landfills in the U.S. must be lined with impermeable basal membranes to prevent leachate (i.e., water produced at the bottom of the refuse mass) from contaminating groundwater below. Leachate collection systems are then needed to control the depth of the leachate that ponds on the liner. Landfill top covers are also required by law in the U.S. to minimize infiltration and to isolate the refuse mass from the atmosphere. Top covers serve an additional purpose in capturing methane gas that is produced by anaerobic biodegradation of MSW. However, the top cover generally causes conditions that are too dry, leading to slow waste biodegradation, slow compaction, and low methane production rates (1, 2, 3). The slow rates of these stabilization processes extend the time period over which the refuse mass presents itself as a risk for contamination of air and water, and postpone potential land re-use.

Research suggests that stimulating aerobic processes in the refuse mass by injection of air along with leachate recirculation can speed up biodegradation, improve leachate composition, and increase compaction rate (4). In addition, aerobic stimulation prevents the formation of methane, leakage of which poses a threat to the environment as a greenhouse gas. The need for a new approach to landfill operations that controls gas and leachate production and minimizes refuse volume has motivated our studies of aerobic stimulation of MSW. These studies consist of (1) laboratory mesoscale experiments of
landfill biodegradation processes under various treatments, and (2) multiphase numerical simulation of landfill biodegradation processes. The former work is summarized in Borglin et al. (5). In this paper, we present the formulation and demonstration of the multiphase landfill bioreactor model called T2LBM and focus on the aerobic biodegradation reactions and associated gas production through comparison of model results to laboratory experiments of an aerobic landfill bioreactor.

With two exceptions (6, 7), prior landfill or composting models (e.g., 2, 8, 9, 10, and 11) are batch models that do not consider multiphase flow and transport within the refuse mass. Of the two studies that use nonbatch models, the Das and Keener (6) model is two-dimensional, and the Popov and Power (7) model considers each of the layers to be a different batch reactor, albeit with communication between the layers. Using the fully three-dimensional TOUGH2 framework, Nastev (12) considered the flow and transport of gas in detail, but used a prescribed time-varying generation rate for the evolution of gas rather than a process model of biological gas production. Another three-dimensional model is the TRAMP model (13) for aerobic and anaerobic biodegradation. However, TRAMP focuses on the biodegradation reactions insofar as they affect the substrate concentrations and microbial populations without consideration of the corresponding gas production and thermal effects.

T2LBM is a module for the TOUGH2 simulator (14) that implements a Landfill Bioreactor Model. The overall purpose of T2LBM is to provide simulation capability for aerobic and anaerobic biodegradation of MSW and multiphase flow and transport of gas and liquid through a heterogeneous refuse mass in one-, two-, or three-dimensions. The
ability to simulate the flow of liquid and gas is important because multiphase flow in MSW created by leachate recirculation, air injection, and gas production can lead to local conditions (e.g., anaerobic conditions, capillary barriers, gas pockets, low effective permeability barriers) that affect the overall treatment being applied (e.g., leachate recirculation, air injection). Understanding the potential effects and implications of heterogeneous conditions and processes will increase the likelihood of optimizing overall waste treatment.

**Modeling Approach**

*Framework*

Simplifications must be made to make progress in the simulation of complex and variable landfill biodegradation processes. The approach chosen for T2LBM includes detailed process modeling of the flow and transport of gas and aqueous phases, with relatively simpler process modeling of the biodegradation and gas generation processes. In particular, T2LBM builds upon the existing capabilities of the TOUGH2 framework for multidimensional flow and transport in porous media and adds biodegradation reactions for acetic acid, which acts as a proxy for all the substrates in MSW, specifically, simple sugars, fatty acids, lipids, and proteins. This approach assumes implicitly that hydrolysis reactions occur to produce acetic acid, and places the model focus on the last biodegradation step, namely gas production. The earlier phases of biodegradation involving the formation of acetic acid can be phenomenologically modeled by the user through inputs that specify various local initial concentrations or variable generation rates of acetic acid.
Conceptualization

A schematic of the conceptualization of the bioreactor and the idealized biodegradation reactions modeled in T2LBM are shown in Figure 1. As shown, the addition of oxygen (O_2) in air injected at the base of the bioreactor promotes aerobic microbial biomass (BA) production that biodegrades the refuse mass, described by the proxy acetic acid (HAc, CH_3COOH), to produce carbon dioxide (CO_2), water (H_2O), and heat. In the absence of air injection, the bioreactor becomes anaerobic, under which condition anaerobic microbial biomass (BN) serves to biodegrade CH_3COOH to form methane (CH_4), CO_2, and heat.

As MSW biodegrades in landfills, it undergoes compaction due to loading of additional materials on top, loss of strength of individual pieces of refuse due to wetting and biodegradation, and mass loss by biodegradation and leaching. Compaction is important because of its potential to allow disposal of more refuse in a given volume of landfill. However, compaction can also decrease permeability and thus inhibit leachate recirculation and gas flow and production. A relatively detailed comparison of models and data on compaction has been presented by El-Fadel et al. (15). For simplicity, T2LBM uses a simple uncoupled model for compaction that assumes compaction is a linear function of time and occurs uniformly in the vertical (Z) direction. Compaction is neglected in the mesoscale laboratory experiments modeled in this paper.

Observable Properties

The biodegradation process gives rise to observable changes in landfill properties. For example, the primary gas production reactions involve mass transfer from the MSW...
to the gas phase, with corresponding production of CH$_4$ and CO$_2$ and reduction in mass of MSW. The volume of the MSW further changes due to compaction. Properties such as temperature, moisture content, pH, and gas and liquid compositions are additional observable properties that may be coupled with biodegradation. These observable changes can be used to constrain T2LBM.

*Chemical Components*

T2LBM includes six chemical components distributed between two phases as shown in Table 1. The water component, with or without dissolved acetic acid (HAc), is the main constituent of the aqueous phase, with minor amounts of CO$_2$, CH$_4$, O$_2$, and N$_2$ as controlled by the local solubility specified by Henry’s Law. Note that all components except HAc can be present in the gas phase depending on the local solubilities. The N$_2$ and O$_2$ together approximate dry air in the model, where the two components are considered explicitly in order to track independently the concentration of O$_2$ insofar as its aqueous concentration determines whether aerobic or anaerobic conditions occur. Pure water properties come from the steam tables (16), while the ideal gas law and simple mixing relations are used for properties of the gas mixtures, an excellent approximation for the low pressures encountered in landfills. The gas phase will normally be comprised of O$_2$, N$_2$, water vapor, CO$_2$ and CH$_4$. The solubility of air (composed of O$_2$ and N$_2$) is constant while the solubility of CO$_2$ and CH$_4$ are functions of temperature as given by Cramer (17). In T2LBM, O$_2$ can be consumed by aerobic reactions or injected along with N$_2$ as part of the air injection that a landfill operator might employ to stimulate aerobic biodegradation. In addition to the mass conservation equations that need to be solved for
the six chemical components, the thermal energy equation is solved to account for the
effects of phase change and exothermic biodegradation reactions.

<table>
<thead>
<tr>
<th>Phases (β)</th>
<th>Components (κ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – gas (g) 1 – H₂O 2 – 3 –CO₂ 4 –CH₄ 5 –O₂ 6 –N₂</td>
<td></td>
</tr>
<tr>
<td>2 – aqueous (w) 1 – H₂O 2 – HAc 3 –CO₂ 4 –CH₄ 5 –O₂ 6 – N₂</td>
<td></td>
</tr>
</tbody>
</table>

Anaerobic and aerobic microbes (BN and BA, respectively) are modeled in T2LBM insofar as local biomass is updated after each time step as the biomass population may grow or decline. However, biomass is not transported with the flowing phases, nor does it partition into the gas phase. Conceptually, the biomass is effectively held immobile onto the wetted surfaces of the solid matrix.

Process Model Equations

The main model equations are presented in Table 2, with symbols defined in the nomenclature. As shown in Table 2, the model equations consist essentially of the mass conservation (flow and transport) equations for NK components and heat (κ = NK+1) (Eqns. 1–5) coupled to equations governing the biodegradation of acetic acid (Eqns. 9–15). T2LBM uses a multiphase version of Darcy’s law for liquid and gas phase fluxes with capillary pressure and relative permeability for handling two-phase gas-liquid flow.
interaction (Eqns. 6, 7). Various options for relative permeability and capillary pressure functions are available in TOUGH2 (14). Henry’s law with temperature-dependent coefficients is used for two-phase component partitioning (Eqn. 8). T2LBM models the exothermic biodegradation of acetic acid as a proxy for all biodegradable substrates (Eqns. 9, 10). A Monod kinetic rate law is used for the aerobic and anaerobic reaction kinetics (Eqns. 11, 12). The kinetic rate law models substrate utilization as controlled by the concentration of substrate, microbial biomass, and temperature. For low oxygen concentrations where the system is prone to oscillate between aerobic and anaerobic conditions, a dual Monod rate law is used to avoid small time steps (Eqn. 13).

Temperature dependence of the reaction rate is controlled by the equation suggested by Kaiser (8) (Eqn. 14). The microbial biomass as controlled by the yield coefficient and microbial death rate is updated at the end of the time step (Eqn. 15). Similarly, the local aqueous phase oxygen mass fraction is also updated after convergence at each time step.

Two landfill process models included in T2LBM but not tested in this study are compaction and pH calculation. For compaction, T2LBM uses a simple uncoupled model wherein the refuse is assumed to compact uniformly in space and time as given by the final refuse height \( h_{r\text{final}} \) specified by the user. Porosity reduction is modeled, while the corresponding permeability reduction is optional based on user input. The pH of the aqueous phase can be estimated by assuming the presence within MSW of a buffer such as calcium carbonate (18). Although the compaction and pH are calculated in T2LBM, neither process is directly coupled to biodegradation in the current version and both are
therefore omitted from Table 2 and from further consideration in this study. Future research will be aimed at evaluating the effects of compaction and pH on biodegradation.

Table 2. Main model equations solved in T2LBM.

<table>
<thead>
<tr>
<th>Description</th>
<th>Equation (number)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conservation of mass or energy</td>
<td>( \frac{d}{dt} \int_M M^\kappa dV = \int F^\kappa \cdot n , d\Gamma + \int q^\kappa dV )</td>
<td>14</td>
</tr>
<tr>
<td>Mass accumulation</td>
<td>( M^\kappa = \phi \sum_{\beta=1}^{NP} (S_\beta \rho_\beta X^\kappa_\beta) )</td>
<td>14</td>
</tr>
<tr>
<td>Component flux</td>
<td>( F^\kappa = \sum_{\beta=1}^{NP} \left( X^\kappa_\beta F_\beta - \phi \tau_\alpha \tau_\beta \rho_\beta \frac{d}{dt} X^\kappa_\beta \right) )</td>
<td>14</td>
</tr>
<tr>
<td>Heat accumulation</td>
<td>( M^{N\kappa+1} = (1 - \phi) \rho_K C_R T + \phi \sum_{\beta} S_\beta \rho_\beta u_\beta )</td>
<td>14</td>
</tr>
<tr>
<td>Heat flux</td>
<td>( F^{N\kappa+1} = -\lambda \nabla T + \sum_{\beta} h_\beta F_\beta )</td>
<td>14</td>
</tr>
<tr>
<td>Phase flux</td>
<td>( F_\beta = -k_{r,\beta} \rho_\beta \left( \nabla P_\beta - \rho_\beta g \right) )</td>
<td>14</td>
</tr>
<tr>
<td>Pressure and capillary pressure</td>
<td>( P_\beta = P + P_{c,\beta} )</td>
<td>14</td>
</tr>
<tr>
<td>Henry’s law</td>
<td>( P_g^\kappa = F_{H,kappa} )</td>
<td>14</td>
</tr>
<tr>
<td>Aerobic biodegradation</td>
<td>( CH_3COOH + 2O_2 \Leftrightarrow 2CO_2 + 2H_2O + heat )</td>
<td>19</td>
</tr>
<tr>
<td>Anaerobic biodegradation</td>
<td>( CH_3COOH \Leftrightarrow CO_2 + CH_4 + heat )</td>
<td>7</td>
</tr>
<tr>
<td>Biodegradation kinetics</td>
<td>( \frac{dS}{dt} = -\frac{1}{Y} \left( \frac{dB}{dt} + \delta B \right) = -\frac{1}{Y} \left( \mu_B B + \delta B \right) )</td>
<td>8, 20, 7</td>
</tr>
<tr>
<td>Monod rate law</td>
<td>( \mu_B = \mu_{max,B} \frac{T}{K_{S,B} + S} - \delta )</td>
<td>8, 7</td>
</tr>
<tr>
<td>Multiple Monod for low ( X_{O_2}^{\kappa \alpha} )</td>
<td>( \frac{dS}{dt} = \left( \frac{X_{O_2}^{\kappa \alpha}}{X_{O_2,crv}^\kappa + X_{O_2,liq}^\kappa} \right) \left( -\frac{1}{Y} \left( \mu_B B + \delta B \right) \right) )</td>
<td>21, 22</td>
</tr>
<tr>
<td>Temperature dependence</td>
<td>( f_B^T = \frac{1}{2} \frac{T}{T_{max,B}} \left( T_{max,B} - T \right) )</td>
<td>8</td>
</tr>
<tr>
<td>Microbial biomass update</td>
<td>( B = B_o (1 - \delta \Delta t) - Y \Delta S )</td>
<td>22</td>
</tr>
</tbody>
</table>
Mathematical Methods

T2LBM uses the integral finite difference method, where the domain (one-, two-, or three-dimensional) is discretized into gridblocks between which heat and mass can flow and in which conservation of heat and mass are rigorously imposed. T2LBM uses a residual-based formulation in which the discretized mass balance equations and energy equation are solved simultaneously at each time step. Newton-Raphson iteration is used to reduce all of the residuals to small fractions of the accumulation terms. Solution of the sparse Jacobian matrix system of linear equations is accomplished with direct or iterative matrix solvers as specified by the user. An inner Newton-Raphson iteration is carried out to solve for the change in moles of HAc due to biodegradation, whereupon other reactants and products are correspondingly updated at each time step, including the enthalpy to account for thermal effects of biodegradation. In this way, the primary variables pressure, mass fractions of HAc, CO₂, CH₄, O₂, gas saturation, and temperature are determined and all secondary parameters (e.g., liquid saturation, relative permeability, etc.) can be calculated. Details of the methods used in TOUGH2 can be found in Pruess et al. (14), while details of the methods used in T2LBM can be found in Oldenburg (22). T2LBM was tested and agreed well against published solutions of aerobic and anaerobic biodegradation (8, 23, 22).

Mesoscale Bioreactor Simulation

The mesoscale laboratory experiments carried out by Borglin et al. (5) provide a controlled system for testing T2LBM. Conditions, experimental design and results are
presented in Borglin et al. (5). In this section, we present our approach and results for
the T2LBM simulations of the mesoscale aerobic landfill bioreactor.

The 55-gallon clear acrylic tanks used for the experiments can be conveniently
approximated for modeling by a radially symmetric r-Z grid as shown in Figure 2. With a
radius of 0.33 m and height of 0.60 m, the MSW volume is 0.208 m$^3$ (55 gal). A 0.06 m
thick layer of gravel is added at the bottom, along with a 0.03 m thick layer of acrylic for
the sidewall. The domain is discretized into 132 gridblocks with a row of gridblocks just
below the top headspace for leachate injection and just above the gravel layer for air
injection. The boundary conditions are constant pressure in the headspace and gravel
layers, and constant temperature of 20$^\circ$C along the impermeable outer perimeter to model
the laboratory ambient temperature. The moisture content of the wetted MSW was 0.17
as measured in the lab. With a porosity assumed to be 0.5, we assumed in the model that
one half of the moisture resides within the MSW and the other half is in the pore space.
Therefore, the initial average liquid saturation in the pore space is approximately 0.17.

Simulation of the mesoscale experiments begins with the creation of a permeability
field broadly representative of the MSW-filled tank. Although for radial symmetry the
statistical representation of heterogeneity should be altered to reflect increasing domain
volume as a function of radius, we used standard simulated annealing techniques to
generate a permeability field with correlation length of 0.09 m in the horizontal and 0.03
m in the vertical directions and mean permeability of 10$^{-10}$ m$^2$. The permeability field is
shown in Figure 3a along with gas flow vectors (see below). We believe this permeability
field is broadly representative of the laboratory tanks and serves to demonstrate
preferential flow. Future studies may be undertaken to investigate sensitivity of model results to permeability through simulations of multiple realizations of permeability structure.

The model hydrologic properties are presented in Table 3. With the conceptualization for substrate used in T2LBM, the porous medium matrix is inert while the biodegradable MSW modeled by HAc is mobile as a dissolved constituent of the aqueous phase. As such, the user must carefully control the mobility of the aqueous phase to model a system that consists of immobile MSW. This control can be easily accomplished through the relative permeability term as discussed below. Note that for simplicity in this problem, the capillary pressure has been set to zero. The injection and biodegradation properties for the problem are shown in Tables 4 and 5. The biodegradation parameters were chosen after Kaiser (8) with some minor changes to match our experimental data. The critical oxygen mass fraction ($X_{O2, crit}$) is an input parameter and was chosen to be one-half the initial $X_{O2}$, i.e., anaerobic conditions were assumed to begin when the oxygen concentration reached one-half of the initial value.
### Table 3. Hydrologic properties of model system.

<table>
<thead>
<tr>
<th>Model system property</th>
<th>Symbol</th>
<th>MSW</th>
<th>Gravel</th>
<th>Acrylic sidewall</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>$\phi$</td>
<td>0.5</td>
<td>0.54</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>466.</td>
<td>2700.</td>
<td>1200.</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>Heat capacity</td>
<td>$C_R$</td>
<td>1300.</td>
<td>zero</td>
<td>1297.</td>
<td>J kg$^{-1}$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\lambda$</td>
<td>0.50</td>
<td>1.8</td>
<td>0.15</td>
<td>J s$^{-1}$ m$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>Thickness</td>
<td>$D$</td>
<td>0.60</td>
<td>0.06</td>
<td>0.03</td>
<td>m</td>
</tr>
<tr>
<td>Permeability (heterogeneous)</td>
<td>$k$</td>
<td>Mean 1.0 x 10$^{-10}$</td>
<td>0.0</td>
<td></td>
<td>m$^2$</td>
</tr>
<tr>
<td>Relative permeability, $k_r$</td>
<td>$\gamma'$</td>
<td>0.72</td>
<td>All phases</td>
<td>none</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$S_{br}$</td>
<td>0.04</td>
<td>perfectly</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$S_{ls}$</td>
<td>1.0</td>
<td>mobile.</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$S_{gr}$</td>
<td>0.005</td>
<td></td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Capillary pressure</td>
<td>$P_c$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>Pa</td>
</tr>
</tbody>
</table>

### Table 4. Model system injection rates and temperatures.

<table>
<thead>
<tr>
<th>Model system property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total air injection rate</td>
<td>$q_{air}$</td>
<td>2.0 L min$^{-1}$ (4.0 x 10$^5$ kg s$^{-1}$)</td>
</tr>
<tr>
<td>O$_2$ injection rate</td>
<td>$q_{O2}$</td>
<td>9.2 x 10$^{-6}$ kg s$^{-1}$</td>
</tr>
<tr>
<td>N$_2$ injection rate</td>
<td>$q_{N2}$</td>
<td>3.1 x 10$^{-5}$ kg s$^{-1}$</td>
</tr>
<tr>
<td>Air injection temperature</td>
<td>$T_{air}$</td>
<td>20 °C</td>
</tr>
<tr>
<td>Total leachate injection rate</td>
<td>$q_{leachate}$</td>
<td>20 mL min$^{-1}$ (3.3 x 10$^{-4}$ kg s$^{-1}$)</td>
</tr>
<tr>
<td>H$_2$O injection rate</td>
<td>$q_{H2O}$</td>
<td>3.3 x 10$^{-4}$ kg s$^{-1}$</td>
</tr>
<tr>
<td>HAc injection rate</td>
<td>$q_{HAc}$</td>
<td>1.65 x 10$^{-5}$ kg s$^{-1}$</td>
</tr>
<tr>
<td>Leachate injection temperature</td>
<td>$T_{liq}$</td>
<td>20 °C</td>
</tr>
</tbody>
</table>
Table 5. T2LBM biodegradation properties for the mesoscale landfill bioreactor problem.

<table>
<thead>
<tr>
<th>Model system property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aerobic yield coefficient</td>
<td>$Y$</td>
<td>0.2 kg microbe (kg waste)$^{-1}$</td>
</tr>
<tr>
<td>Aerobic microbial growth rate</td>
<td>$\mu_{\text{max}}$</td>
<td>$1.2 \times 10^{-5}$ s$^{-1}$</td>
</tr>
<tr>
<td>Anaerobic microbial growth rate</td>
<td>$\mu_{\text{max}}$</td>
<td>0.0 s$^{-1}$</td>
</tr>
<tr>
<td>Critical oxygen mass fraction</td>
<td>$X_{\text{crit}O_2}$</td>
<td>$1.8 \times 10^{-6}$</td>
</tr>
<tr>
<td>Maximum T for microbial growth</td>
<td>$T_{\text{max},B}$</td>
<td>80 °C</td>
</tr>
<tr>
<td>Saturation constant</td>
<td>$K_s$</td>
<td>0.02</td>
</tr>
<tr>
<td>Death rate of aerobic microbes</td>
<td>$\delta$</td>
<td>$2.8 \times 10^{-7}$ s$^{-1}$</td>
</tr>
<tr>
<td>Initial mass fraction acetic acid</td>
<td>$X_{\text{aq}HAc}$</td>
<td>~0.05</td>
</tr>
<tr>
<td>Initial mass fraction microbes</td>
<td>$BA$</td>
<td>0.01</td>
</tr>
<tr>
<td>Heat of reaction</td>
<td>$\Delta H_a$</td>
<td>$1.5 \times 10^7$ J (kg HAc)$^{-1}$</td>
</tr>
</tbody>
</table>

The second step was the simulation of a steady-state leachate recirculation and air injection flow field with no biodegradation occurring (microbial growth rate set to zero).

This was accomplished by injecting $O_2$ and $N_2$ in the proportions appropriate for air (23% $O_2$, 77% $N_2$ by mass) into the gravel at the bottom while allowing leachate to drain through the gravel. Simultaneously, water and HAc in proportions such that the initial $X_{\text{aq}HAc} = 0.05$ are injected into the top of the domain to simulate leachate recirculation.

**Results and Discussion**

Using the steady-state flow field as the initial condition, the biodegradation terms are turned on by setting the biodegradation rate to a non-zero value (see Table 5). The gas and liquid and gas flow fields at 28.5 days are shown in Figures 3a and b along with permeability and liquid saturation, respectively. Note the variability of the gas phase velocity vectors in the MSW that results from the heterogeneous permeability field. Note further the large flow of air downward into the leachate collection system. This phenomenon was observed also in the laboratory experiment (5), and results from the fact

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that in many cases the effective permeability of the gravel and leachate collection system is larger than the effective permeability of the MSW, the result of which is return flow of injected air back into the leachate collection system.

The temperature and CO₂ mass fraction in the gas are shown at \( t = 28.5 \) days in Figure 4. The highest temperatures are in the middle of the domain while the lowest temperature is at the bottom where the 20 °C air is injected. The lack of large temperature increase for the aerobic tank in the model result agrees well with the laboratory experiments, and results from the small size of the tanks and associated conductive cooling through the acrylic sidewalls, along with the injection of 20 °C air.

We simulated the respiration test conducted in the laboratory experiments starting at \( t = 28.5 \) days. The respiration test is carried out by turning off the leachate recirculation and air injection and monitoring the changes in gas concentrations in the headspace. We simulated the respiration test by turning off the injection of water and HAc at the top of tank and turning off the air injection at the bottom. Because gravity is acting on the water, leachate will tend to continue to drain from the model system after leachate recirculation is stopped. In the model system where the HAc substrate is dissolved in the aqueous phase, this results in unrealistic drainage of model MSW. To prevent this, we arbitrarily set the relative permeability of the aqueous phase to zero for the duration of the respiration test (\( t = 28.5 \) to 31.5 days). This effectively holds the HAc stationary consistent with the immobile MSW in the laboratory experiment. To compare results between the model and laboratory experiment, we averaged the gas compositions in the headspace in the simulation to model the mixing that occurs in the lab.
experiment. Following the end of the shut-in period at \( t = 31.5 \) days, the aqueous phase relative permeability is restored and the leachate and air injection are turned back on.

We present in Figure 5 a comparison of the results of the actual and simulated respiration test. As shown, the volume fraction of \( \text{O}_2 \) in the gas begins at ambient levels (21% by volume) and falls slowly as aerobic biodegradation of HAc occurs. The system at this time is marginally aerobic, as biodegradation consumes \( \text{O}_2 \) while enriching the system in \( \text{CO}_2 \). Starting at \( t = 28.5 \) days, the air injection and leachate recirculation are stopped and the tank is shut in. As shown, the \( \text{O}_2 \) concentration falls quickly as excess \( \text{O}_2 \) is consumed by the aerobic reactions until anaerobic conditions are reached after approximately 0.5 days. At \( t = 31.5 \) days, the leachate recirculation and air injection are turned on again and the \( \text{O}_2 \) concentration increases. The reason that the \( \text{O}_2 \) does not reach the concentration levels that existed prior to the shut in is that the rate of biodegradation is increasing due to the growth of aerobic microbial biomass, and the rate of \( \text{O}_2 \) consumption is greater than the rate of resupply by air injection. Also shown in Figure 5 is the simulated volume fraction of \( \text{CO}_2 \) in the gas, showing the complementary relation of \( \text{CO}_2 \), a product of the aerobic reactions, and \( \text{O}_2 \), a reactant in the reaction.

The model requires many properties as input parameters, most of which are not well constrained. We have used many property values from Kaiser (8) appropriate for green waste composting. These properties were adjusted slightly in some cases to match the experimental results, but no formal inverse modeling was undertaken. It appears from our studies that rather generic properties can be used to obtain plausible results. The good agreement between the laboratory experiment and T2LBM for a relatively complex
process involving flow, transport, biodegradation, and gas production suggests that
T2LBM is modeling fundamental processes active in the mesoscale bioreactor. With the
T2LBM framework in place, improvements in process modeling detail such as coupling
with compaction and pH can be made as the need arises from additional MSW
biodegradation and gas production applications. This modeling capability can be used for
sensitivity and optimization studies to improve the processing of MSW in landfills.

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Energy, contract No. DE–AC03–76SF00098.

Nomenclature

\[ B \] microbial concentration \( \text{kg microbes (kg aqueous phase)}^{-1} \)

\[ BA \] aerobic biomass concentration \( \text{kg microbes (kg aqueous phase)}^{-1} \)

\[ BN \] anaerobic biomass concentration \( \text{kg microbes (kg aqueous phase)}^{-1} \)

\[ CR \] matrix heat capacity \( \text{J kg}^{-1} \text{ °C}^{-1} \)

\[ d \] molecular diffusivity \( \text{m}^2 \text{ s}^{-1} \)

\[ f_B T \] coefficient of T-dependent growth \( - \)

\[ F \] Darcy flux vector \( \text{kg m}^2 \text{ s}^{-1} \)

\[ g \] acceleration of gravity vector \( \text{m s}^{-2} \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tbody>
<tr>
<td>$\Delta H_B$</td>
<td>enthalpy of biodegradation reaction</td>
<td>J kg$^{-1}$</td>
</tr>
<tr>
<td>$hr$</td>
<td>refuse height ratio</td>
<td>-</td>
</tr>
<tr>
<td>$k$</td>
<td>permeability</td>
<td>m$^2$</td>
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<tr>
<td>$K_H$</td>
<td>Henry’s Law coefficient</td>
<td>Pa$^{-1}$</td>
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<tr>
<td>$K_{S,B}$</td>
<td>saturation constant</td>
<td>kg substrate (kg aqueous phase)$^{-1}$</td>
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<tr>
<td>$M$</td>
<td>mass accumulation term</td>
<td>kg m$^3$</td>
</tr>
<tr>
<td>$n$</td>
<td>inward unit normal vector</td>
<td></td>
</tr>
<tr>
<td>NK</td>
<td>number of mass components (species)</td>
<td></td>
</tr>
<tr>
<td>NPH</td>
<td>maximum number of phases present</td>
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<tr>
<td>$P$</td>
<td>pressure</td>
<td>Pa</td>
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<tr>
<td>$P_c$</td>
<td>capillary pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$q$</td>
<td>component source term</td>
<td>kg m$^3$ s$^{-1}$</td>
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<tr>
<td>$r$</td>
<td>radial coordinate</td>
<td>m</td>
</tr>
<tr>
<td>$S_\beta$</td>
<td>phase saturation</td>
<td>-</td>
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<tr>
<td>$S$</td>
<td>substrate (acetic acid) concentration</td>
<td>kg substrate (kg aqueous phase)$^{-1}$</td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
<td>s, days</td>
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<tr>
<td>$T$</td>
<td>temperature</td>
<td>°C</td>
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<td>$V$</td>
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<tr>
<td>$X$</td>
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<tr>
<td>$Y$</td>
<td>yield coefficient</td>
<td>kg microbes (kg substrate)$^{-1}$</td>
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<tr>
<td>$zc$</td>
<td>compaction factor</td>
<td>-</td>
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Z  Z-coordinate  m

Greek symbols

\( \gamma \)  van Genuchten (1980) parameter  -
\( \delta \)  microbial death rate  s\(^{-1}\)
\( \Gamma \)  surface area  m\(^2\)
\( \lambda \)  thermal conductivity  J m\(^{-1}\) K\(^{-1}\) s\(^{-1}\)
\( \mu \)  dynamic viscosity  kg m\(^{-1}\) s\(^{-1}\)
\( \mu_B \)  microbial growth rate  s\(^{-1}\)
\( \mu_{\text{max},B} \)  maximum microbial growth rate  s\(^{-1}\)
\( \phi \)  porosity  -
\( \rho \)  density  kg m\(^{-3}\)
\( \theta \)  moisture content  -
\( \tau \)  tortuosity  -

Subscripts and superscripts

\( aq \)  aqueous
\( B \)  biomass, microbes
\( \text{crit} \)  critical
\( g \)  gas
\( l \)  liquid
\( ls \)  liquid satiated
\( \text{max} \)  maximum
$R$  rock

$\omega$  reference value, initial value

$\beta$  phase index

$\kappa$  mass components

**Literature Cited**


Biodegradation

<table>
<thead>
<tr>
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<th>Bioreactor</th>
<th>T2LBM</th>
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<td></td>
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<td>Aerobic</td>
<td>CO₂ + H₂O + heat</td>
<td>CH₃COOH + 2O₂ ⇌ 2CO₂ + 2H₂O + heat + BA&lt;sub&gt;BA&lt;/sub&gt;</td>
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<td>Aerobic Microbial Biomass (BA) and Refuse Mass</td>
<td>(reaction occurs in aqueous phase with subsequent Henry’s Law partitioning of CO₂ between gas and aqueous phases)</td>
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<td>Leachate Recirculation</td>
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<tr>
<td>Anaerobic</td>
<td>CH₄ + CO₂ + heat</td>
<td>CH₃COOH ⇌ CH₄ + CO₂ + heat + BN&lt;sub&gt;BN&lt;/sub&gt;</td>
</tr>
<tr>
<td></td>
<td>Anaerobic Microbial Biomass (BN) and Refuse Mass</td>
<td>(reaction occurs in aqueous phase with subsequent Henry’s Law partitioning of CO₂ and CH₄ between gas and aqueous phases)</td>
</tr>
<tr>
<td></td>
<td>Leachate Recirculation</td>
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</table>

Figure 1. Schematic of bioreactor and T2LBM conceptualizations.
Figure 2. Domain and boundary conditions for the mesoscale landfill bioreactor.

Figure 3. (a) Model permeability field with gas flow velocity vectors, and (b) Liquid saturation and leachate flow velocity vectors at $t = 28.5$ days.
Figure 4. (a) Temperature field, and (b) Mass fraction CO$_2$ in the gas at $t = 28.5$ days.
Figure 5. Volume fractions of O$_2$ from the laboratory experiment and T2LBM and volume fraction CO$_2$ from T2LBM.