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T2LBM Version 1.0: Landfill bioreactor model for TOUGH2

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Publication Date

2001-11-01

T2LBM Version 1.0:
Landfill Bioreactor Model for TOUGH2

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November 2001

This work was supported by the Office of Science, U.S. Department of Energy under
Contract No. DE-AC03-76SF00098.

Abstract

The need to control gas and leachate production and minimize refuse volume in landfills has motivated the development of landfill simulation models that can be used by operators to predict and design optimal treatment processes. **T2LBM** is a module for the **TOUGH2** simulator that implements a **Landfill Bioreactor Model** to provide simulation capability for the processes of aerobic or anaerobic biodegradation of municipal solid waste and the associated flow and transport of gas and liquid through the refuse mass. T2LBM incorporates a Monod kinetic rate law for the biodegradation of acetic acid in the aqueous phase by either aerobic or anaerobic microbes as controlled by the local oxygen concentration. Acetic acid is considered a proxy for all biodegradable substrates in the refuse. Aerobic and anaerobic microbes are assumed to be immobile and not limited by nutrients in their growth. Methane and carbon dioxide generation due to biodegradation with corresponding thermal effects are modeled. The numerous parameters needed to specify biodegradation are input by the user in the SELEC block of the TOUGH2 input file. Test problems show that good matches to laboratory experiments of biodegradation can be obtained. A landfill test problem demonstrates the capabilities of T2LBM for a hypothetical two-dimensional landfill scenario with permeability heterogeneity and compaction.

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1. 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 significant active management of the refuse mass. For example, by law modern landfills in the U.S. must be lined with impermeable basal membranes to prevent leachate (i.e., water produced by the refuse mass) from contaminating groundwater below. However, to minimize the risk of leaks from the basal liner, conservative requirements have been established on the maximum depth of water allowed to pond on the liner at the base of the landfill. These requirements necessitate leachate collection systems to manage the amount of leachate that ponds on the liner.

Landfill top covers are also required by law in the U.S. to minimize rainfall infiltration that might ultimately migrate to the base of the refuse mass as leachate, as well as to isolate the refuse mass from the atmosphere. Top covers serve an additional purpose in some applications in capturing and collecting the methane gas that is produced by anaerobic biodegradation of MSW. Despite these apparent advantages of top covers for anaerobic landfills, the fact is that the top cover generally causes conditions that are too dry for optimal anaerobic biodegradation, leading to slow waste biodegradation, slow compaction, and low methane production rates (e.g., Farquhar and Rovers, 1973; EMCON, 1980; Reinhart, 1996). These slow 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.

The potential benefits of speeding up the anaerobic biodegradation process by active management of the refuse mass are higher methane production rates and increased compaction. It is also becoming recognized 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 (Stessel and Murphy, 1992). In addition, aerobic stimulation prevents the formation of methane, emissions of which are an increasing concern for global warming due to the role of methane in the atmosphere as a greenhouse gas. The need for

modern landfill operators to control gas and leachate production, along with minimizing the refuse volume motivate the development of landfill simulation models that can be used by operators to predict and design optimal treatment processes.

T2LBM is a module for the **TOUGH2** simulator that implements a **Landfill Bioreactor Model**. The overall purpose of T2LBM is to provide simulation capability for the processes of aerobic or anaerobic biodegradation of MSW that includes the flow and transport of gas and liquid through the refuse mass in zero-(batch), one-, two-, or three-dimensional space. Depending on the local oxygen concentration, T2LBM models either (i) nonisothermal anaerobic conversion of acetic acid to methane and carbon dioxide, or (ii) aerobic conversion of acetic acid to carbon dioxide and water. Schematics of the conceptualizations 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 (CH_3COOH , or *HAc*), to produce carbon dioxide (CO_2) and water (H_2O) and heat. In the absence of air injection, the bioreactor is anaerobic, under which condition anaerobic microbial biomass (*BN*) serves to biodegrade the refuse mass, modeled by proxy as acetic acid (*HAc*), to form methane (CH_4) and CO_2 and heat.

T2LBM uses a Monod kinetic rate law for the biodegradation reactions, and calculates an estimate of the pH of the aqueous phase and includes this value as primary output. Compaction of the refuse mass is modeled as an uncoupled process occurring at a constant rate over time. Because it is a module of TOUGH2, T2LBM includes all of the multiphase and multicomponent flow and transport capabilities of TOUGH2. For example, the flow of aqueous and gas phases may bypass local regions of the refuse mass leading to local aerobic or anaerobic biodegradation, both of which processes can occur simultaneously in different regions of the model refuse mass. T2LBM can be used to design and test different laboratory and pilot study configurations of anaerobic or aerobic treatments of MSW by leachate recirculation, air injection, temperature control, and waste placement.

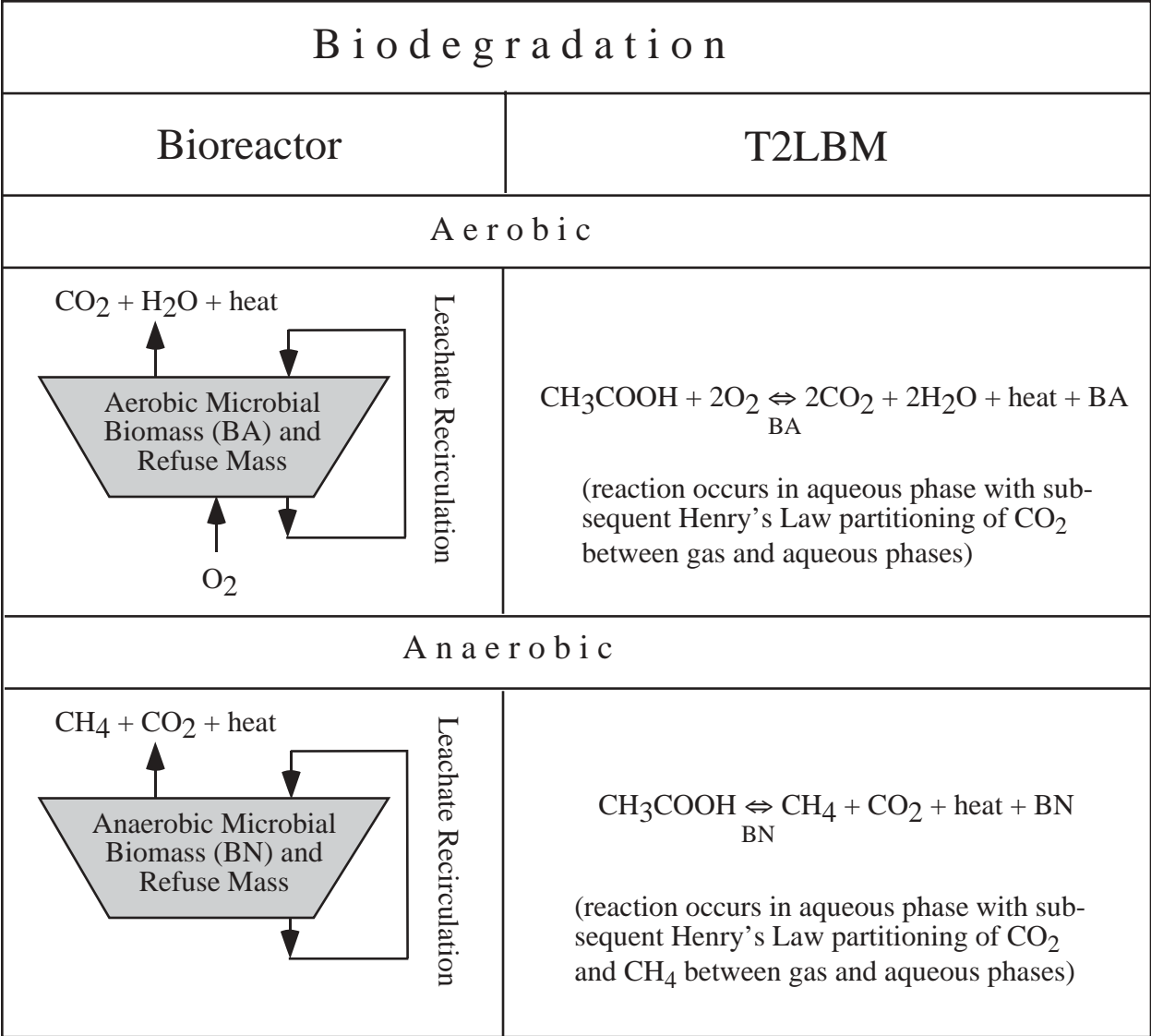


Figure 1. Schematic of bioreactor and T2LBM conceptualizations.

With a couple of exceptions (e.g., Das and Keener, 1997; Popov and Power, 1999), prior landfill or composting models (e.g., EMCON, 1980; Kaiser, 1996; Stombaugh and Nokes, 1996; Mohee *et al.*, 1998; and Lay *et al.*, 1998b) are batch models that do not consider local conditions due to flow and transport within the refuse mass. Of the two studies that use nonbatch models, the Das and Keener (1997) model is two-dimensional, and the Popov and Power (1999) model considers each of the layers to be a different batch reactor. Using the fully three-dimensional TOUGH2 framework, Nastev (1998) 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 rigorous model of the biological processes of gas production. Another fully three-dimensional model is the TRAMP model (Travis and Rosenberg, 1997) 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 builds upon the existing capabilities of the TOUGH2 framework for multidimensional flow and transport in porous media and adds biodegradation reactions and the corresponding gas and water production along with thermal effects.

In this report, the biodegradation reactions, the method of estimating pH, and the compaction model are presented along with their mathematical formulations as implemented in T2LBM. Input descriptions and formats, and instructions for using T2LBM are also provided, although users not familiar with TOUGH2 should refer to the TOUGH2 Users Guide (Pruess *et al.*, 1999) for additional information for successful application. Test problems are presented as code demonstrations and to give the reader examples of the use of the code.

2. Landfill Biodegradation Processes

2.1 Introduction

Biodegradation of MSW is an enormously complex and variable process. To make progress in the simulation of landfill processes, simplifications must be made. The approach chosen for T2LBM includes detailed process modeling of the flow and transport of gas and aqueous phases, with comparatively approximate process modeling of the biodegradation and gas generation processes. In particular, T2LBM models the biodegradation of a single substrate component (acetic acid, CH_3COOH) as a proxy for all of the biodegradable fractions 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 input that

specifies various local initial concentrations or variable generation rates of acetic acid. Below, the physical, chemical, and biological processes considered in T2LBM are presented in more detail.

2.2 Chemical components

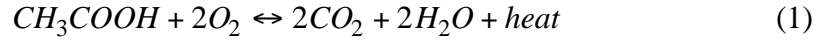
T2LBM includes six chemical components distributed between two phases as shown in Table 1. The water component, with or without dissolved acetic acid (HAc), is the main constituent of the aqueous phase, with minor amounts of the gaseous components carbon dioxide (CO₂), methane (CH₄), oxygen (O₂), and nitrogen (N₂) as controlled by the local solubility specified by Henry's Law. Note that all components except HAc can be present in the gas phase, again depending on the local solubility as modeled by Henry's Law. The N₂ and O₂ together approximate dry air in the model, where the two components are considered explicitly in order to track independently the concentration of O₂ insofar as its aqueous concentration determines whether aerobic or anaerobic conditions occur. In this formulation, O₂ can be consumed by aerobic reactions or injected along with N₂ as part of an air injection that a landfill operator might employ to stimulate aerobic biodegradation. The gas phase will normally be comprised of O₂, N₂, and water vapor, along with CO₂ and CH₄, if biodegradation reactions have occurred. In addition to the mass conservation equations that need to be solved for the six chemical components, there is a thermal energy equation solved to account for thermal effects including exothermic biodegradation reactions.

Table 1. Phases and components in T2LBM.

Phases (β)	Components (κ)					
1 – gas (g)	1 – H ₂ O	2 –	3 –CO ₂	4 –CH ₄	5 –O ₂	6 –N ₂
2 – aqueous (w)	1 – H ₂ O	2 – HAc	3 –CO ₂	4 –CH ₄	5 –O ₂	6 – N ₂

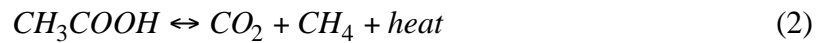
2.3 Biodegradation Reactions

Under aerobic conditions, the HAc (CH_3COOH) component acts as a substrate in the aqueous phase for a reaction where oxygen is consumed to produce carbon dioxide, water, and heat by



(Jakobsen, 1992). Implicit in this reaction is the formation of an aerobic biomass (BA) as the reaction proceeds. The reaction of Eq. 1 is the rate-controlling oxidation reaction in T2LBM assuming that nutrients such as nitrogen and phosphorous are plentiful and do not limit the degradation of the substrate. However, in addition to substrate and oxygen concentrations, many other factors such as temperature, biomass fraction, and removal of CO_2 also control the reaction rate and are included in the model as discussed below.

Under anaerobic conditions, HAc biodegrades to carbon dioxide, methane, and heat



(Popov and Power, 1999). Similar to the aerobic reaction, there is an implicit production of anaerobic biomass (BN) in Eq. 2. As for the aerobic reaction, it will be seen below that many factors control the rate of this anaerobic biodegradation reaction.

2.4 Kinetics of the Biodegradation Reactions

In general, the rate of substrate utilization by microbes can be approximated by the Monod kinetic rate equation, given by

$$\frac{dS}{dt} = -\frac{1}{Y} \left(\frac{dB}{dt} + \delta B \right) = -\frac{1}{Y} (\mu_B B + \delta B) \quad (3)$$

(see Nomenclature) where

$$\mu_B = \mu_{\max, B} f_B^T \frac{S}{K_{S, B} + S} - \delta \quad (4)$$

(e.g., Kaiser, 1996; Popov and Power, 1999). The Monod equation is analogous to the Michaelis-Menten relation and expresses the observation that the substrate utilization rate is controlled by the concentration of substrate, the concentration of microbes, and the temperature through the function f_B^T , along with the yield coefficient and the death rate of microbes. It is important to note that the total change in microbial mass is due to both substrate utilization and death rate. Despite their positive signs in Eq. 3, the death rate terms (δB) are present in order to remove the effects of mortality on the rate of change of microbial mass in order to relate directly the change in microbial mass to the change in substrate mass only. This kinetic rate equation is coded in T2LBM as the governing rate for the biodegradation reactions of Eqs. 1 and 2. Biomass (BA or BN) is monitored in T2LBM, but is not part of the mass balance equations that are solved for each formal component given in Table 1.

2.5 Heat Production and Transfer

The biodegradation reactions (Eqs. 1 and 2) are exothermic. The net heats generated by these reactions have been estimated and are on the order of $7.0 \times 10^6 \text{ J (kg HAc)}^{-1}$ for the aerobic reaction (e.g., Kaiser, 1996), and $2.7 \times 10^5 \text{ J (kg HAc)}^{-1}$ for the anaerobic reaction (Popov and Power, 1999). Note that the anaerobic reaction is only slightly exothermic relative to the aerobic reaction which can produce significant temperature increases. Upon including these source terms in the energy balance, no additional heat transfer processes need to be added as TOUGH2 models advection in gas and aqueous phases, conduction in the fluid phases and matrix, as well as enthalpy changes associated with water condensation and vaporization.

2.6 pH Estimation

The pH of the aqueous phase can be estimated by assuming the presence within MSW of a buffer such as calcium carbonate (Stumm and Morgan, 1996). In this case, the governing dissociation reaction is

$$2[Ca^{++}] + [H^+] \leftrightarrow C_T(\alpha_1 + 2\alpha_2) + [OH^-] + [HAc] \quad (5)$$

$$2[Ca^{++}] + [H^+] \leftrightarrow C_T(\alpha_1 + 2\alpha_2) + \frac{K_w}{[H^+]} + [HAc] \quad (6).$$

where the only unknown is $[H^+]$ in units of moles L^{-1} which can be solved by Newton-Raphson iteration. This is the same approach that was used by Popov and Power (1999), and is presented in more detail in Appendix A.

2.7 Compaction

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 of great interest to landfill operators 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.* (1999). 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. The total compaction ratio over the time of the simulation is specified by the user. Porosity reduction is modeled, while the corresponding permeability reduction is optional based on user input.

2.8 Observable Properties

The processes discussed above give 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 the temperature, moisture content, pH, and gas and liquid compositions are additional observable properties that

are affected by biodegradation in landfills. These changes can be used to constrain and test against T2LBM output of analogous property changes.

3. T2LBM Process Modeling

3.1 General

The general conservation equations solved by the integral finite difference method (IFDM) in TOUGH2 consist of balances between mass accumulation and flux and source terms over all grid blocks V_n into which the flow domain V has been partitioned:

$$\frac{d}{dt} \int_{V_n} M^\kappa dV = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma + \int_{V_n} q^\kappa dV \quad (7)$$

(see Nomenclature for definition of symbols). In Eq. 7, the index $n = 1, \dots, N$ corresponds to the grid blocks with volume V_n and surface area Γ_n . The index $\kappa = 1, \dots, NK+1$ corresponds to the NK fluid components and heat. The mass accumulation term (M) in Eq. 7 is given by

$$M^\kappa = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta X_\beta^\kappa \quad (8)$$

where β indexes the phases, in this case the gas and aqueous phases. The flux term has contributions from both the phase flux and from molecular diffusion and can be written

$$\mathbf{F}^\kappa = \sum_{\beta=1}^{NPH} \left(X_\beta^\kappa F_\beta - \phi \tau_o \tau_\beta \rho_\beta d_\beta^k \nabla X_\beta^\kappa \right) \quad (9).$$

The first term on the right-hand side of Eq. 9 is the phase flux term which accounts for the flux of component κ arising from Darcy flux of the phases containing κ . The second term on the right-hand side of Eq. 9 is the dispersion term, which includes only molecular diffusion in

T2LBM. In Eq. 9, one observes that the molecular diffusivity coefficient (d_β^k) is modified by porosity (ϕ), a tortuosity factor arising from the porous medium (τ_o), and a tortuosity factor (τ_β) arising from the phase saturation (see Pruess *et al.*, 1999). The heat flux term has analogous contributions from heat conduction and phase flux and is given by

$$\mathbf{F}^{NK+1} = -\lambda \nabla T + \sum_{\beta}^{NPH} h_{\beta} \mathbf{F}_{\beta} \quad (10).$$

(Heat transport from diffusive fluxes is neglected in T2LBM as it is in TOUGH2).

The phase flux term for either gas or aqueous phases is given by the multiphase version of Darcy's Law,

$$\mathbf{F}_{\beta} = -k \frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \quad (11)$$

where $k_{r\beta}$ is the relative permeability and

$$P_{\beta} = P + P_{c\beta} \quad (12)$$

and where $P_{c\beta}$ is the capillary pressure of phase β . Various options for relative permeability and capillary pressure functions are available in TOUGH2 as described in Pruess *et al.* (1999).

3.2 Liquid and Gas Phase Properties

As in TOUGH2, pure water properties (density, specific enthalpy, viscosity, saturated vapor pressure) for aqueous and gas phases are calculated from the steam table equations as given by the International Formulation Committee (1967). Because the aqueous phase is expected to be comprised almost entirely of water due to low concentrations of HAc and low solubility of the gas components, the properties of the aqueous phase are assumed to be independent of composition. Water vapor is assumed to be in equilibrium with the aqueous

phase at the saturation vapor pressure (100% relative humidity) corresponding to the local pressure and temperature. Mixtures of water vapor with the main gas components N_2 , O_2 , CO_2 , and CH_4 are modeled using ideal gas approximations for all species. This approximation is expected to be accurate for the low (ambient) pressures encountered in landfill systems. Simple mixing relations are used to calculate the density and viscosity of the gas phase as a function of gas composition. The solubility of N_2 and O_2 in the aqueous phase is assumed to be constant ($K_H = 1 \times 10^{10}$ Pa) as for air in TOUGH2/EOS3 (see Pruess *et al.*, 1999), while CO_2 and CH_4 solubilities vary with temperature as in TOUGH2/EWASG (see Battistelli *et al.*, 1997; Pruess *et al.*, 1999).

3.3 Chemical Components and Heat

Six chemical components are modeled in T2LBM. These are H_2O , CH_3COOH , CO_2 , CH_4 , O_2 , and N_2 . The chemical components are transported by advection and molecular diffusion in both the gas and liquid phases with the exception of HAC which is assumed to be nonvolatile and therefore is only transported in the liquid phase. For the aerobic reaction (Eq. 1), HAC and O_2 are consumed while CO_2 , H_2O , and aerobic biomass (*BA*) are created. Similarly, for the anaerobic reaction (Eq. 2), HAC is consumed while CO_2 and CH_4 are created along with anaerobic biomass (*BN*). The N_2 is passive in T2LBM in that it is not involved in any transformation reactions. For the purposes of calculating density, viscosity, and internal energy, the sum of the mass fractions of O_2 and N_2 is considered to give the mass fraction of air, and properties of air are used as properties of O_2 and N_2 . Furthermore, the solubility and molecular weights of O_2 and N_2 are assumed to be the same as those of air for solubility and gas density calculations. T2LBM assumes further that O_2 is only consumed and that the gas phase can never become enriched in O_2 beyond its concentration in ambient air. Upon initialization, the proportions of O_2 and N_2 are checked and set to those of ambient dry air (23% O_2 and 77% N_2 by mass) if the O_2 concentration is larger than that of ambient air. Essentially, the method used here

treats air as a two-component mixture (O_2 and N_2) of two identical components that can be tracked individually as O_2 is consumed in the aerobic biodegradation reaction.

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, one should think of the biomass as being held immobile onto the wetted surfaces of the solid matrix. Local biomass mass fractions can be input into the model in the INCON file as initial conditions and for restarts. Similarly, the local biomass mass fractions are written to file SAVE at the end of each simulation run. However, it is important to remember that the biomass mass fraction is a mass fraction in name only, in that no mass balance is carried out for biomass as it is for the chemical components.

Heat advection and conduction as well as enthalpy effects associated with phase change are modeled in T2LBM as they are in TOUGH2. In addition, T2LBM models enthalpy changes due to the exothermic biodegradation reactions (Eqs. 1 and 2).

3.4 Biodegradation Reactions

The biodegradation reactions are coded in a subroutine called BIOREACT that is called from subroutine MULTI in analogy to subroutine QU for sinks and sources. Depending on the local concentration of O_2 in the aqueous phase, effects of either the aerobic or anaerobic reactions are modeled. The approach taken to solve Eq. 3 for the new substrate concentration is Newton-Raphson iteration as follows. We start by writing the ordinary differential equation describing the rate of reaction,

$$\frac{dS}{dt} = -\frac{1}{Y}(\mu_B B + \delta B) = -\frac{B}{Y} \left(\mu_{\max} f_B^T \frac{S}{K_{S,B} + S} \right) \quad (13)$$

where

$$B = B_o - Y \frac{dS}{dt} \Delta t - \delta B_o \Delta t \quad (14).$$

Substitution of Eq. 14 into Eq. 13 yields

$$\frac{dS}{dt} = -\frac{1}{Y} \left(\mu_{\max} f_B^T \frac{S}{K_{S,B} + S} \right) \left(B_o - Y \frac{dS}{dt} \Delta t - \delta B_o \Delta t \right) \quad (15)$$

which simplifies to

$$\frac{dS}{dt} = \frac{-\frac{B_o}{Y} \mu_{\max} f_B^T \frac{S}{K_{S,B} + S} (1 - \delta \Delta t)}{\left(1 - \mu_{\max} f_B^T \frac{S}{K_{S,B} + S} \Delta t \right)} \quad (16).$$

We then discretize this as a first-order reaction in time as

$$\Delta S = S_2 - S_1 = \frac{dS}{dt} \Delta t \quad (17)$$

which can then be solved for the new substrate concentration, S_2 , by Newton-Raphson iteration

$$f(S_2) = \left. \frac{dS}{dt} \right|_{S_2} \Delta t + S_1 - S_2 = 0 \quad (18)$$

$$f(S_2^{k+1}) = f(S_2^k) + (S_2^{k+1} - S_2^k) \frac{df(S_2)}{dS_2} \quad (19)$$

where k is the iteration index and a numerical derivative is calculated using the same increment for S_2 as used in calculating elements of the Jacobian matrix in TOUGH2. Note that the derivative of Eq. 18 is approximately equal to -1 due to the $-S_2$ term. Thus this inner iteration converges rapidly. Based on the iteratively calculated S_2 (the new HAc mass fraction), the corresponding change in moles of HAc is calculated by dividing by the molecular weight of

HAc. From the change in moles of HAc, all of the corresponding changes in moles for the reactants in Eqs. 1 and 2 are computed and then converted back to mass fraction changes. These changes in mass fractions are converted to mass changes in each gridblock, with appropriate updating of the right-hand side vector and Jacobian elements since these changes in component masses are computed at the state point and once for each incremented primary variable. The enthalpies are likewise considered to update the heat accumulation terms. The initial biomass mass fractions are input by the user and then tracked in terms of growth and decline throughout the simulation. Upon convergence, the microbial mass fraction is updated according to

$$B = B_o(1 - \delta \Delta t) - Y\Delta S \quad (20).$$

In essence, the biomass is assumed to remain immobile on the solid grains and in the aqueous phase within each gridblock and no mass balances are carried out for biomass. Therefore, the biomass is not a formal mass fraction, but rather a convenient way to quantify biomass for the biodegradation reactions. In short, changes in biomass mass fraction are due only to growth and death.

For aerobic reactions, an additional rate dependence arises from the dependence of Eq. 1 on oxygen concentration. This dependence is included according to the assignment

$$\frac{dS}{dt} = \left(\frac{X_{liq}^{O_2}}{X_{O_2,crit} + X_{liq}^{O_2}} \right) \frac{dS}{dt} \quad (21).$$

This rate dependence on oxygen concentration was added to combat the very poor convergence that results at low oxygen concentrations when conditions oscillate between aerobic and anaerobic. With this additional rate dependence, T2LBM effectively models a multiple Monod process (e.g., Borden and Bedient, 1986).

The production of HAC in landfills is by hydrolysis reactions with the MSW. For example, cellulose breaks down to form acetic acid as water interacts with it. This process of hydrolysis is not formally modeled in T2LBM, but the rate of production of HAC can be arbitrarily controlled by the user through the GENER option to create a heuristic model of the hydrolysis process.

Temperature dependence of the biodegradation is included through the function f_B^T in Eq.

4. The approach of Kaiser (1996) is used in T2LBM wherein

$$f_B^T = \frac{T(T_{\max,B} - T)}{\left(\frac{1}{2}T_{\max,B}\right)^2} \quad (22)$$

where $T_{\max,B}$ is temperature (°C). As can be seen by inspection of Eq. 22, f_B^T is a parabola with a maximum value of 1 at $T = 1/2T_{\max,B}$, and is equal to 0 at $T = 0$ and $T = T_{\max,B}$.

T2LBM is coded so that both the aerobic and anaerobic reactions are calculated at each iteration, with the results weighted by an arctan switching function

$$a = \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left(\text{switchf}(X_{\text{liq}}^{O_2} - X_{\text{crit}}^{O_2}) \right) \quad (23).$$

In Eq. 23, a varies from ~ 1 for $X_{\text{liq}}^{O_2} > X_{\text{crit}}^{O_2}$, to ~ 0 for $X_{\text{liq}}^{O_2} < X_{\text{crit}}^{O_2}$. The steepness of the transition around $X_{\text{crit}}^{O_2}$ is controlled by the user through the variable *switchf* entered as FE(44) in the input file. This approach makes possible a smooth transition from aerobic to anaerobic conditions, and has been used in other applications where process changes occur at critical points and thresholds (e.g., Oldenburg and Spera, 1994). The term aerobicity is given to the function a and is given as primary output from T2LBM to delineate aerobic and anaerobic regions of the domain.

3.5 Estimating pH

An estimate of the aqueous phase pH is made in a subroutine called ESTPH that is called from BIOREACT prior to carrying out the biodegradation reactions. The pH is estimated by the methods described above using Newton-Raphson iteration of Eq. 6 where the equation to be solved is

$$f([H^+]) = 2[Ca^{++}] + [H^+] - C_T(\alpha_1 + 2\alpha_2) - \frac{K_w}{[H^+]} - [HAc] = 0 \quad (24)$$

With the substitutions given in Appendix A, we obtain

$$f([H^+]) = 2 \left(\frac{\frac{K_{SO}}{K_H P_{CO_2}} \alpha_1}{\alpha_2} \right) + [H^+] - \frac{K_H P_{CO_2}}{\alpha_o} (\alpha_1 + 2\alpha_2) - \frac{K_w}{[H^+]} - [HAc] = 0 \quad (25)$$

where the only unknown $[H^+]$ can be solved for by Newton-Raphson iteration. Details and definitions of the variables in Eq. 25 are presented in Appendix A. The pH is calculated in this version of T2LBM for the current time step and printed in the output file, but it is not coupled to the rate equations.

3.6 Compaction

A simple compaction model has been included in T2LBM to model compaction as a function of time. The user inputs the total compaction ratio (cr) over the period of simulation. For example, if the final height of the refuse mass (hr_{final}) is 80% of the initial height ($hr_{initial}$), the user would input 0.20 for the input variable $acomact$ (FE(46)) as calculated by the relation

$$cr = 1 - \frac{hr_{final}}{hr_{initial}} \quad (26).$$

The code uses the compaction factor, calculated by

$$z_c = 1 - \frac{t}{t_{final}} cr \quad (27)$$

to compute a variety of properties at each time step such as the connection distances for vertical connections, gridblock volumes, and porosity by

$$D_1 = D_1 z_c \quad (28)$$

$$V_n = V_n z_c \quad (29)$$

$$\phi_n = \phi_n z_c \quad (30).$$

The permeability can be modified according to the Kozeny-Carman equation upon engaging the permeability modifier capability (see Pruess *et al.*, 1999, p. 71)

$$k_{new} = \frac{\frac{\phi^3}{(1-\phi)^2}_{new}}{\frac{\phi^3}{(1-\phi)^2}_{old}} k_{old} \quad (31).$$

3.7 Overview of T2LBM Processes

The model implementation discussed above includes inherently all of the existing processes modeled in TOUGH2, for example, flow by Darcy's law of liquid and gas phases, transport of chemical components by advection and molecular diffusion, gas-liquid phase partitioning assuming Henry's law and local equilibrium, nonisothermal effects of vaporization, and heat transfer by conduction and convection. T2LBM extends TOUGH2 to model gas production by aerobic and anaerobic biodegradation of acetic acid. The resulting flow and transport of gas and aqueous phases along with the chemical components and heat are fully coupled. Furthermore, the kinetics of the reactions are fully coupled. That is, the properties

controlling the biodegradation rates are based on most recently updated values. One exception to this is oxygen, the concentration of which is based on the oxygen concentration from the prior time step. The pH of the aqueous phase is estimated, but it is not used to control any process. Compaction is calculated at the beginning of the time step based on the time, but it is not directly coupled to the reaction progress. However, the effects of compaction in terms of gridblock volume, porosity, and permeability are fully engaged. The properties modeled by T2LBM and which can be compared against laboratory or field studies include the concentrations of gas and liquid phase components (O₂, N₂, CO₂, CH₄, H₂O, and HAc) temperature, biomass, pH, moisture content, and mass fluxes of the components and phases. A summary of T2LBM program units and their functions is presented in Appendix B.

Table 2. Biodegradation variable names in T2LBM.

Variable	Symbol in Eqns	Units	Name in code (aerobic)	Name in code (anaerobic)
HAc concentration	S	Mole or mass fraction	XAC (mass fraction)	XAC (mass fraction)
Yield coefficient	Y	kg (kg substrate) ⁻¹	YIELDCA	YIELDCA
Maximum microbial growth rate	μ_{max}	s ⁻¹	AMUMAXA	AMUMAXN
Maximum temperature for microbial growth	$T_{max,B}$	°C	TMAXA	TMAXN
Saturation constant	$K_{S,B}$	kg (kg waste) ⁻¹	AKSBA	AKSBN
Microbial death rate	δ	s ⁻¹	DEATHA	DEATHN
Initial biomass mass fraction	B_0	mass fraction	BAI	BNI
Biomass mass fractions	B	mass fraction	BA	BN
Enthalpy of reaction	ΔH_B	J (kg HAc) ⁻¹	ENBA	ENBN
Critical oxygen mass fraction	$X_{crit}^{O_2}$	-	XO2CRIT	XO2CRIT
Compaction ratio	cr	-	ACOMPACT	ACOMPACT

4. Using T2LBM

4.1 Compilation

The compilation instruction for T2LBM on an IBM RS/6000 workstation is as follows:

```
xlf -qautodbl=dblpad t2cg2b2.f meshm.f t2lbm2.f t2fb2.f t2solv.f ma28.f
```

The italics indicate the new program units of T2LBM. Note that duplicate subroutine name warnings may arise from some compilers. Depending on the compiler, it is possible that duplicate main programs and subroutines may have to be eliminated from the source code. Alternatively, one can change the names of later occurrences of the same subroutine (e.g., an unwanted version of CYCIT could be renamed CYCITx).

4.2 Input Formats

All of the new input data required for T2LBM are input in the SELEC block of the input file. In addition, some existing input data blocks require input changes to engage T2LBM as follows:

MULTI keyword to input number of components and phases.

MULTI.1 format(5I5)

NK, NEQ set equal to 6, 7 to model 6 mass components, 7 equations (6 for mass, 1 for energy)

NPH, NB set equal to 2, 8 for 2 phases and 8 secondary parameters.

NKIN set equal to number of mass components in INCON file or leave blank if reading from T2LBM INCON file.

PARAM keyword to input computational parameters.

PARAM.1 format(2I2, 3I4, 24I1, 2E10.4)

NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), DIFF0, TEXP

See TOUGH2 User's Guide (Pruess *et al.*, 1999) for description of all of the above parameters except the following:

MOP(5) selects amount of printout from SUBROUTINE EOS and SUBROUTINE BIOREACT.

Set equal to 3 or larger for printout indicating aerobicity and mass changes due to biodegradation at each iteration for each gridblock.

SELEC keyword to introduce a data block with landfill biodegradation properties.

SELEC.1 format(8I5)

IE(1),

IE(1) set equal to 6 to read six additional data records.

SELEC.2 format(E10.4)

P_o reference pressure, Pa. Set equal to negative number to make acetic acid have the same thermophysical properties as pure water.

SELEC.3 format(3E10.4)

$v(i)$, $i=1,3$

$v(i)$ coefficients for correction to aqueous phase viscosity due to acetic acid. Not engaged if P_o is set to a negative number in SELEC.2.

SELEC.4 format(2E10.4)

ALPHAT, ALPHAL

The dispersion coefficients are not used in T2LBM.

ALPHAT transverse dispersivity, m.

ALPHAL longitudinal dispersivity, m.

SELEC.5 format(7E10.4)

Aerobic kinetic parameters:

YIELDCA aerobic yield coefficient, kg (kg substrate)⁻¹.

AMUMAXA maximum aerobic microbial growth rates, s⁻¹.

TMAXA maximum temperatures for aerobic microbes, °C.

AKSBA saturation constants of aerobic microbes, kg (kg waste)⁻¹.

DEATHA aerobic microbial death rates, s⁻¹.

BAI initial aerobic biomass mass fractions, -.

ENBA enthalpies of the aerobic reaction, J (kg substrate)⁻¹.

SELEC.6 format(7E10.4)

Anerobic kinetic parameters:

YIELDCN anaerobic yield coefficient, kg (kg substrate)⁻¹.

AMUMAXN maximum anaerobic microbial growth rates, s⁻¹.

TMAXN maximum temperatures for anaerobic microbes, °C.

AKSBN saturation constants of anaerobic microbes, kg (kg waste)⁻¹.

DEATHN anaerobic microbial death rates, s⁻¹.

BNI initial anaerobic biomass mass fractions, -.

ENBN enthalpies of the anaerobic reaction, J (kg substrate)⁻¹.

SELEC.7 format(6E10.4)

O2CRIT critical oxygen mass fraction in the liquid.

BFAC reduction factor criterion for local Newton Raphson iteration to reduce substrate residual.

PHFAC reduction factor criterion for local Newton Raphson iteration to reduces pH estimate residual

SWITCHF coefficient in arctan switching function.

EFFCP enthalpy modification factor for changing effective heat capacity of aqueous phase.

ACOMPACT compaction ratio.

INCON keyword to introduce gridblock-specific initial conditions. See Pruess et al. (1999) for complete description of INCON block.

INCON.1 format(A3, I2, 2I5, 3E15.8)

EL,NE code name of gridblock.

NSEQ number of additional gridblocks with same initial conditions.

NADD increment between code numbers of two successive gridblocks with same initial conditions.

PORX porosity; if zero or blank, porosity will be taken as specified in ROCKS block if START is used (see Pruess *et al.*, 1999).

BA, BN mass fraction of aerobic and anaerobic biomass; if zero or blank, biomass will be taken from SELEC block of input file (BAI, BNI).

INCON.2 format(4E20.13)

X1 pressure in Pa.

X2 liquid mass acetic acid.

X3 liquid mass fraction CO₂.

X4 liquid mass fraction CH₄.

INCON.3 format(3E20.13)

 X5 liquid mass fraction O₂.

 X6 gas saturation plus 10.

 X7 temperature, °C.

5. Sample Problems

5.1 Aerobic Biodegradation (Composting)

In this sample problem, the simulated dynamics of the aerobic biodegradation of a small batch composter under interval aeration are compared against results from the laboratory experiment of Kaiser and Soyez (1990) as documented in Kaiser (1996). A schematic of the simple system under investigation is shown in Figure 1. In this experiment, moist air was injected periodically into a pile of plant matter contained within an insulated reactor and allowed to vent out the top. Although the system appears very simple, it involves complex coupled biological processes. The problem was simulated with T2LBM using one active gridblock and one boundary gridblock to model the vent to the atmosphere. The geometry of the composter itself is zero-dimensional, i.e., a batch process.

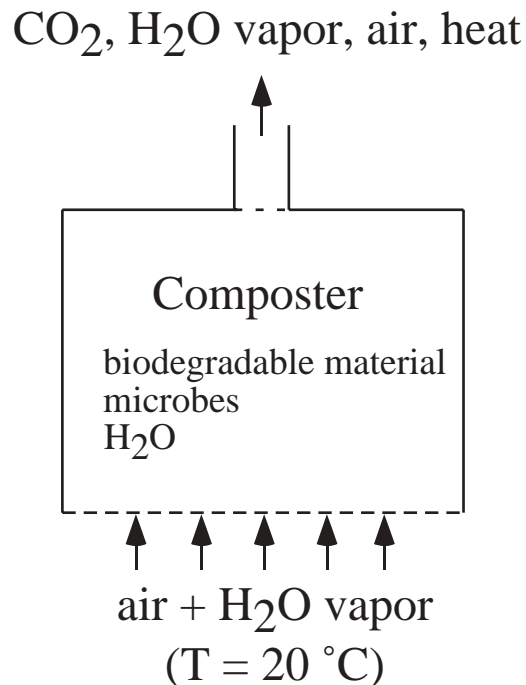


Figure 2. Schematic of the Kaiser and Soyez (1990) experiment.

Many properties of the system can be used directly from the specifications given in Kaiser (1996). However, some other properties must be derived due to the specific process model conceptualization of T2LBM. For example, T2LBM assumes that biodegradation occurs within the aqueous phase, and that HAc is the biodegradable substrate. With this assumption, there is no solid biodegradable material, e.g., plant matter, in the model. The biodegradable material is the HAc and it is dissolved in the liquid phase. Therefore, the model system contains much more water by mass than the actual experimental system. Specifically, the model system contains 420 kg of water as opposed to an estimated 65.2 kg in the experimental system. This additional water creates additional mass that must be heated to effect temperature changes. To accommodate this difference, the heat capacity of water was scaled by a factor of 0.024 (see SELEC.7, EFFCP) and the heat capacity of the matrix was set to $132 \text{ J kg}^{-1} \text{ K}^{-1}$. With these changes, the coupled system consisting of water and the solid matrix has a heat capacity of $9 \times 10^4 \text{ J K}^{-1}$ as specified in the experiment. Another difference is that T2LBM assumes that there is only one biodegradable substrate as opposed to five considered by Kaiser (1996). This difference was treated by adjusting the microbial growth rate until a reasonable match was obtained. The final value turned out to be about 80% of the geometric mean of the five growth rates presented by Kaiser (1996).

Presented in Tables 3 and 4 are relevant properties of the experimental system and the model system, respectively. Note that the air injected into the model system is actually injected on a component basis with 23% O_2 , 76% N_2 , and approximately 1% H_2O by mass making up the $2 \text{ m}^3 \text{ hr}^{-1}$ injection. The purpose of the 1% H_2O injection is to inject humid air, and thereby avoid the large evaporative cooling effects that will occur if dry air is injected. Note further that a nominal constant background N_2 injection rate of $1 \times 10^{-6} \text{ kg s}^{-1}$ was included to make a positive pressure in the composter so that backflow would not occur from the vent gridblock. The initial microbial mass fraction in the liquid for the model system is derived from the total amount of water present (420 kg) by the relation $0.53 \text{ kg}/420 \text{ kg} = 1.3 \times 10^{-3}$. For this problem, the

anaerobic reaction in T2LBM was turned off by setting the anaerobic microbial growth rate to zero resulting in no methane generation regardless of the oxygen concentration in the liquid.

Table 3. Properties for the Kaiser and Soyez (1990) composting problem.

Experimental system property	Symbol	Value
Volume	V	0.7 m ³
Mass of waste (biodegradable matter)	M_{ref}	106 kg
Initial moisture content	θ_0	0.60
Yield coefficient	Y	0.2 kg microbe (kg waste) ⁻¹
Growth rates		
Bacteria	μ_{max}	5.5 x 10 ⁻⁵ s ⁻¹
Actinomycetes	μ_{max}	2.8 x 10 ⁻⁵ s ⁻¹
Brown-rot fungi	μ_{max}	1.4 x 10 ⁻⁵ s ⁻¹
White-rot fungi	μ_{max}	8.3 x 10 ⁻⁶ s ⁻¹
Geometric mean of μ_{max}	μ_{max}	2.1 x 10 ⁻⁵ s ⁻¹
Saturation constants for all substrates	K_s	0.02
Death rate of microbes	δ	2.8 x 10 ⁻⁷ s ⁻¹
Initial mass of microbes	M_{mic}	0.53 kg
Heat of reaction	ΔH_{bio}	1.4 x 10 ⁷ J (kg O ₂) ⁻¹
Heat capacity of composter	$C_{p,comp}$	849 J kg ⁻¹ K ⁻¹
Air injection temperature	T_{intake}	20 °C
Air injection rate	q_{air}	6.7 x 10 ⁻⁴ kg s ⁻¹ (2 m ³ hr ⁻¹)

Table 4. T2LBM properties for the Kaiser and Soyez (1990) composting problem.

Model system property	Symbol	Value
Volume	V	1.0 m ³
Porosity	ϕ	0.70
Initial liquid saturation	S_{l0}	0.60
Aerobic yield coefficient	Y	0.2 kg microbe (kg waste) ⁻¹
Aerobic microbial growth rate	μ_{max}	1.5 x 10 ⁻⁵ s ⁻¹
Anaerobic microbial growth rate	μ_{max}	0.0 s ⁻¹
Maximum T for microbial growth	$T_{max,B}$	80 °C
Saturation constant	K_s	0.02
Death rate of aerobic microbes	δ	2.8 x 10 ⁻⁷ s ⁻¹
Initial mass fraction acetic acid	X_{liq}^{HAc}	0.015
Initial mass fraction microbes	BAI	1.3 x 10 ⁻³
Heat of reaction	ΔH_a	1.5 x 10 ⁷ J (kg HAc) ⁻¹
Heat capacity of matrix	Cp	132 J kg ⁻¹ K ⁻¹
O ₂ injection rate	q_{O2}	1.4 x 10 ⁻⁴ kg s ⁻¹
N ₂ injection rate	q_{N2}	5.2 x 10 ⁻⁴ kg s ⁻¹
H ₂ O vapor injection rate	q_{H2O}	5.2 x 10 ⁻⁶ kg s ⁻¹
Total interval air injection rate	q_{air}	6.65 x 10 ⁻⁴ kg s ⁻¹
Air injection temperature	T_{intake}	20 °C
Constant background N ₂ injection rate	$q_{N2,const}$	1.0 x 10 ⁻⁶ kg s ⁻¹
Critical oxygen mass fraction	X_{crit}^{O2}	1.0 x 10 ⁻⁶

With constraints on many properties of the system prescribed by the experimental specifications, there are at least two important parameters to adjust to fit T2LBM results with the results shown in Kasier (1996). These include the initial mass fraction of HAc in the liquid, and the single microbial growth rate for the breakdown of a single chemical species (HAc) as proxy for numerous microbial populations and substrates. It was found that a reasonable match could be obtained by setting the initial HAc mass fraction to 1.5 x 10⁻², and the microbial growth rate to 1.5 x 10⁻⁵ s⁻¹. Note that the specified saturation constant (K_s) is larger than the initial HAc mass

fraction, a relation that arises from maintaining consistency for some properties (e.g., K_s) while fitting others (X_{ii}^{HAc}). The input file for this sample problem is shown in Figure 2.

```

*SAMPLBM6* AEROBIC BIODEG. KAISER, J., Ecolog. Modelling 91, 25-37, 1996.
ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
FINE      2      1200.      .70  1.00E-12  1.00E-12  1.00E-12  0.0  132.
          3          .99      0.0
          1          0.e6      0.      1.
BDRY      2      1200.      .70  1.00E-22  1.00E-22  1.00E-22  0.0  1.e+5
          3          .99      0.0
          1          0.e6      0.      1.

START-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8

PARAM-----1-----*-----123456789012345678901--4-----*-----5-----*-----6-----*-----7-----*-----8
3900      9001 0 3 00 0231 4 0 1
          8.64e5      -1.      8.64e3      0.00000
          1.e+00
          1.E-05      1.E0
          100000.00      .5      0.00e-3      0.00e-5
          3.3e-2      10.500      20.
MULTI-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
6 7 2 8
TIMES-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
1
8.640e4
FE(25,33) yield coefficients, kg/kg substrate.
FE(26,34) maximum microbial growth rates, 1/s.
FE(27,35) maximum temperatures for microbes, C.
FE(28,36) saturation constants of microbes, kg/kg waste.
FE(29,37) microbial death rates, 1/s.
FE(30,38) initial biomass mass fractions
FE(31,39) enthalpies of reaction, J/kg substrate.
FE(41) critical oxygen mass fraction in the liquid.
FE(42) factor by which local Newton Raphson iteration
reduces substrate residual.
FE(43) factor by which local Newton Raphson iteration
reduces pH estimate residual.
FE(44) coefficient in arctan switching function.
FE(45) enthalpy modification factor for changing effective
heat capacity of aqueous phase.
FE(46) compaction coefficient.
SELEC-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
6 1 1 1
-1.e5
0.e-0 0.e-1
2.e-1 1.5e-5 80. 2.e-2 2.8e-7 1.3e-3 1.5e07
2.e-1 0.0e-5 60. 2.e-2 2.8e-7 5.e-5 1.0e06
1.0e-06 1.e-15 1.e-9 1.e10 0.024 0.
DIFFU-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
0.e-6 0.e-9
0.e-6 0.e-9
0.e-6 0.e-9
0.e-6 0.e-9
0.e-6 0.e-9
0.e-6 0.e-9
INCON-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
A11 1
100000.00 0.015e-0 0.00e-0 0.00e-0
3.3e-01 10.40 20.
A12 1
100000.00 1.e-6 0.00e-0 0.00e-0
3.3e-01 10.40 20.
FOFT -----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
A11 1

```

Figure 3. T2LBM input file for the aerobic biodegradation sample problem.

```

ELEME
A11 1          10.1000E+010.2000E+01          0.5000E+000.5000E+00-.5000E+00
A12 1          20.1000E+510.2000E+01          0.5000E+000.1500E+01-.5000E+00

```

```

CONNE
A11 1A12 1          20.5000E+000.5000E+000.1000E+010.0000E+00

```

```

GENER-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8

```

```

A11 1OXY01          21          COM51
      0.             4.32e4          8.64e4          1.296e5
      1.728e5        2.16e5          2.592e5          3.024e5
      3.456e5        3.888e5          4.32e5           4.752e5
      5.184e5        5.616e5          6.048e5          6.480e5
      6.912e5        7.344e5          7.776e5          8.208e5
      8.640e5
      1.40e-4         0.             1.40e-4          0.
      1.40e-4         0.             1.40e-4          0.
      1.40e-4         0.             1.40e-4          0.
      1.40e-4         0.             1.40e-4          0.
      1.40e-4         0.             1.40e-4          0.
      1.40e-4         0.             1.40e-4          0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.

```

```

A11 1INIT01        21          COM61
      0.             4.32e4          8.64e4          1.296e5
      1.728e5        2.16e5          2.592e5          3.024e5
      3.456e5        3.888e5          4.32e5           4.752e5
      5.184e5        5.616e5          6.048e5          6.480e5
      6.912e5        7.344e5          7.776e5          8.208e5
      8.640e5
      5.20e-4         0.             5.20e-4          0.
      5.20e-4         0.             5.20e-4          0.
      5.20e-4         0.             5.20e-4          0.
      5.20e-4         0.             5.20e-4          0.
      5.20e-4         0.             5.20e-4          0.
      5.20e-4         0.             5.20e-4          0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.          0.             20200.           0.
      20200.

```

```

A11 1H2O01        21          COM11
      0.             4.32e4          8.64e4          1.296e5
      1.728e5        2.16e5          2.592e5          3.024e5
      3.456e5        3.888e5          4.32e5           4.752e5
      5.184e5        5.616e5          6.048e5          6.480e5
      6.912e5        7.344e5          7.776e5          8.208e5
      8.640e5
      5.20e-6         0.             5.20e-6          0.
      5.20e-6         0.             5.20e-6          0.
      5.20e-6         0.             5.20e-6          0.
      5.20e-6         0.             5.20e-6          0.
      5.20e-6         0.             5.20e-6          0.
      5.20e-6         0.             5.20e-6          0.
      83680.          0.             83680.           0.
      83680.          0.             83680.           0.
      83680.          0.             83680.           0.
      83680.          0.             83680.           0.
      83680.          0.             83680.           0.
      83680.

```

```

A11 1BN201          COM6          1.e-6          20200.

```

```

ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8

```

Figure 3 cont'd. T2LBM input file for the aerobic biodegradation sample problem continued.

percent CO_2 and O_2 are plotted versus time along with H_2O . As shown, the volume percent of the sum of CO_2 and O_2 actually declines during the production of CO_2 . At the same time, as the temperature increases the amount of water in the gas phase goes up. Both the larger solubility of CO_2 in water and the increase in vapor pressure of the aqueous phase prevent the CO_2 in the gas from reaching the ideal volume percent (~21%) given by the initial O_2 volume percent and as shown in the experimental results. The kinetics of dissolution not considered in T2LBM may also play a role in this problem where time scales are relatively short. Future versions of T2LBM will employ more accurate solubility models for O_2 and N_2 which will lead to more accurate results in this problem. Also shown in Figure 6 is pH and $X^{\text{HAc}}_{\text{liq}}$, the values of which show predictable increase and decrease respectively, as the amount of CO_2 in the system decreases as HAc biodegrades.

This relatively simple test problem reveals a number of complexities and sensitivities that will be important in any applications involving multiphase and multicomponent processes coupled with biodegradation processes.

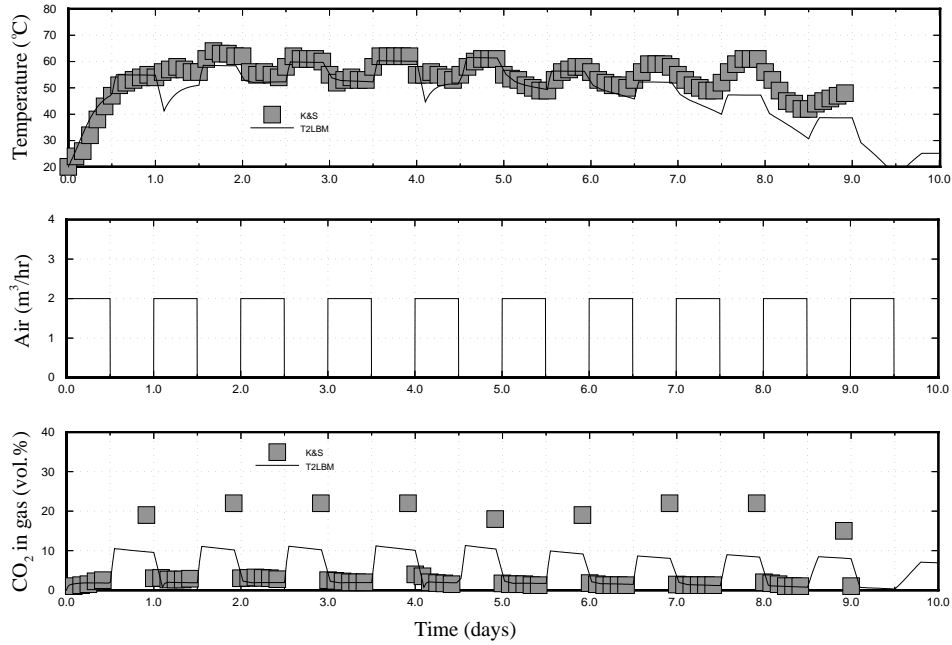


Figure 5. Temperature, air injection rate, and volume percent CO₂ in the gas from the Kasier and Soyez (1990) experiment (K&S) and from T2LBM.

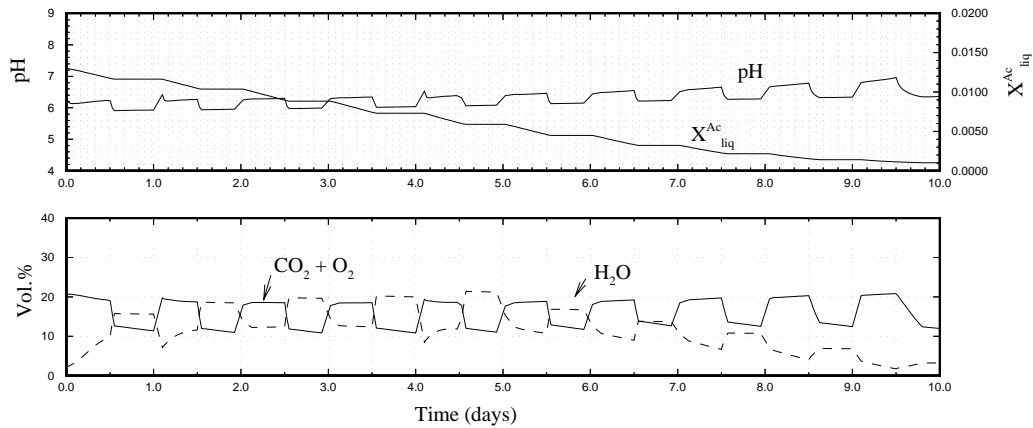


Figure 6. Evolution of pH and mass fraction of acetic acid in the liquid (X_{liq}^{HAc}), and gas phase volume percent CO₂ + O₂ and H₂O for aerobic biodegradation process.

5.2 Anaerobic Biodegradation (Methanogenesis)

In this sample problem, the methane production dynamics during anaerobic biodegradation of a small mass of waste mixed with acetate is compared to T2LBM simulation results. Test results for specific methane activity were given by Lay *et al.* (1998a). The system is sketched in Figure 7 and consists of a 120 mL vial filled with Organic Fraction of Municipal Solid Waste (OFMSW) and a solution of aqueous acetate below a nitrogen and carbon dioxide headspace. The vial batch reactor is incubated at 40 °C and the production rate of CH₄ is monitored. The system is modeled using one 120 mL gridblock connected to a large constant-pressure gridblock. The T2LBM simulation properties are given in Table 5 and Figure 8. The only constraints that could be imposed on the T2LBM simulation were the temperature, pressure, and headspace atmosphere composition. Other properties were chosen to fit the data reasonably closely, although no rigorous inverse model was employed. The values for the biodegradation properties appear reasonable and similar to those used for the aerobic test case of Kaiser (1996).

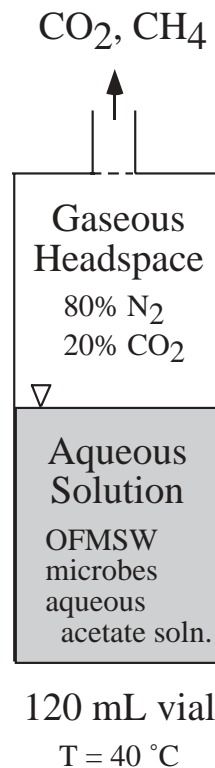


Figure 7. Schematic of the Lay *et al.* (1998a) vial in which the specific methane activity of acetate is measured.

Table 5. T2LBM properties for the Lay *et al.* (1998a) anaerobic biodegradation problem.

Model system property	Symbol	Value
Volume	V	$1.2 \times 10^{-4} \text{ m}^3$
Porosity	ϕ	0.99
Initial liquid saturation	S_{l0}	0.50
Anaerobic yield coefficient	Y	$0.5 \text{ kg microbe (kg waste)}^{-1}$
Anaerobic microbial growth rate	μ_{max}	$2.1 \times 10^{-5} \text{ s}^{-1}$
Maximum T for microbial growth	$T_{max,B}$	60 °C
Saturation constant	K_s	1.5×10^{-3}
Death rate of aerobic microbes	δ	$6.0 \times 10^{-7} \text{ s}^{-1}$
Initial biomass mass fraction	BNI	1.0×10^{-4}
Heat of reaction	ΔH_a	$0.0 \times 10^7 \text{ J (kg HAc)}^{-1}$
Incubation temperature	T_{intake}	40 °C
Initial CO ₂ mass fraction in the liquid	X_{liq}^{CO2}	1.65×10^{-4}
Initial HAc mass fraction in the liquid	X_{liq}^{HAc}	1.1×10^{-3}

```

*SAMPLBM7* ANAEROBIC BIODEG. Lay et al., 1998, Wat. Sci. Tech., 38(2), 177-184.
ROCKS---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
FINE 2 1200. .99 1.00E-12 1.00E-12 1.00E-12 0.0 1000.
      3 .99 0.0
      1 0.e6 0. 1.
BDRY 2 1200. .99 1.00E-12 1.00E-12 1.00E-12 0.0 1.e05
      3 .99 0.0
      1 0.e6 0. 1.
START---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
PARAM---1---*---123456789012345678901---4---*---5---*---6---*---7---*---8
      3900 9001 0 3 00 0231 4 0 1
      5.40e5 -1. 8.64e4 0.00000
      1.e+00
      1.E-05 1.E0
      100000.00 .5 0.00e-3 0.00e-5
      3.3e-2 10.500 20.
MULTI---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
      6 7 2 8
TIMES---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
      1
      8.640e4
      FE(25,33) yield coefficients, kg/kg substrate.
      FE(26,34) maximum microbial growth rates, 1/s.
      FE(27,35) maximum temperatures for microbes, C.
      FE(28,36) saturation constants of microbes, kg/kg waste.
      FE(29,37) microbial death rates, 1/s.
      FE(30,38) initial biomass mass fractions
      FE(31,39) enthalpies of reaction, J/kg substrate.
      FE(41) critical oxygen mass fraction in the liquid.
      FE(42) factor by which local Newton Raphson iteration
      reduces substrate residual.
      FE(43) factor by which local Newton Raphson iteration
      reduces pH estimate residual.
      FE(44) coefficient in arctan switching function.
      FE(45) enthalpy modification factor for changing effective
      heat capacity of aqueous phase.
      FE(46) compaction coefficient.
SELEC---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
      6 1 1 1
      -1.e5
      0.e-0 0.e-1
      2.e-1 0.0e-5 80. 2.e-2 2.8e-7 1.3e-3 1.5e07
      5.0e-1 2.10e-5 60. 1.50e-3 6.0e-7 1.e-4 0.0e06
      1.0e-00 1.e-15 1.e-9 1.e10 0.024 0.
DIFFU---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
      0.e-6 0.e-9
      0.e-6 0.e-9
      0.e-6 0.e-9
      0.e-6 0.e-9
      0.e-6 0.e-9
      0.e-6 0.e-9
GENER---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
INCON---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
A11 1
      100000.00 1.100e-3 0.165e-3 0.00e-0
      0.0e-01 10.50 40.
A12 1
      100000.00 0.e-0 0.165e-3 0.00e-0
      0.0e-01 10.50 40.
FOFT ---1---*---2---*---3---*---4---*---5---*---6---*---7---*---8
A11 1
A12 1
ELEME
A11 1 10.1200E-030.2000E-010.0000E+000.5000E+000.5000E-02-.6000E-02
A12 1 20.1200E+050.2000E-010.0000E+000.5000E+000.1500E-01-.6000E-02
CONNE
A11 1A12 1 20.5000E-020.5000E-020.1200E-010.0000E+000.0000E+00
ENDCY

```

Figure 8. T2LBM input file for the anaerobic biodegradation problem.

```

*SAMLB7* ANAEROBIC BIODEG. Lay et al., 1998, Wat. Sci. Tech., 38(2), 177-184.
      OUTPUT DATA AFTER ( 32, 3)-2-TIME STEPS
                                         THE TIME IS 0.625000E+01 DAYS
#####
TOTAL TIME      KCYC   ITER  ITERC   KON      DX1M      DX2M      DX3M      MAX. RES.   NER   KER   DELTEX
0.540000E+06   32     3     110     2      0.11184E-03 0.16187E-04 0.18519E-05 0.26415E-05  1     2     0.57165E+05
#####
ELEM.  INDEX    P          T          SL      XACETIC(LIQ) AEROFLAG   XCO2(LIQ) XCH4(LIQ)  XO2(LIQ)  XN2(LIQ)  DL
          (PA)      (DEG-C)
A11 1     1 0.10000E+06 0.38207E+02 0.49918E+00 0.21546E-04 0.31831E-10 0.32346E-03 0.49990E-05 0.00000E+00 0.52118E-05 0.99297E+03
A12 1     2 0.10000E+06 0.40000E+02 0.50000E+00 0.00000E+00 0.31831E-10 0.16500E-03 0.25414E-13 0.00000E+00 0.12216E-04 0.99229E+03
#####
ELEM.  INDEX  logkZ      pH      XBA      XBN      XH2O(GAS) XCO2(GAS) XCH4(GAS)  XO2(GAS)  XN2(GAS)  DG
          (log M**2)
A11 1     1 -.12000E+02 0.63137E+01 0.11167E-02 0.51499E-03 0.41548E-01 0.47287E+00 0.16302E+00 0.00000E+00 0.32256E+00 0.11247E+01
A12 1     2 -.12000E+02 0.65162E+01 0.11167E-02 0.72055E-04 0.43450E-01 0.23858E+00 0.80416E-09 0.00000E+00 0.71797E+00 0.11775E+01
#####
^L
      *SAMLB7* ANAEROBIC BIODEG. Lay et al., 1998, Wat. Sci. Tech., 38(2), 177-184.
                                         KCYC = 32 - ITER = 3 - TIME =0.540000E+06
ELEM1  ELEM2  INDEX  FLOH      FLOH/FLOF      FLOF      FLO(ACETIC)  FLO(GAS)  FLO(LIQ.)  VEL(GAS)  VEL(LIQ.)
          (W)      (J/KG)      (KG/S)      (KG/S)      (KG/S)      (M/S)      (M/S)
A11 1  A12 1     1 -.358768E-05 0.228256E+06 -.157178E-10 0.000000E+00 -.157178E-10 0.000000E+00 -.234891E-08 0.000000E+00
#####
^L
      *SAMLB7* ANAEROBIC BIODEG. Lay et al., 1998, Wat. Sci. Tech., 38(2), 177-184.
                                         KCYC = 32 - ITER = 3 - TIME =0.540000E+06
MASS FLOW RATES (KG/S) FROM DIFFUSION
ELEM1  ELEM2  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP  PHASE COMP
          all -1-  all -2-  all -3-  all -4-  all -5-  all -6-
A11 1  A12 1 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
#####
^L
      *SAMLB7* ANAEROBIC BIODEG. Lay et al., 1998, Wat. Sci. Tech., 38(2), 177-184.
                                         KCYC = 32 - ITER = 3 - TIME =0.540000E+06
ELEM.  INDEX    X1      X2      X3      DX1      DX2      DX3      PCAP      K(GAS)  K(LIQ.)  VIS(LIQ.)
A11 1     1 0.10000E+06 0.21546E-04 0.32346E-03 -.11184E-03 -.16187E-04 0.18519E-05 0.00000E+00 0.10000E+01 0.00000E+00 0.67428E-03
A12 1     2 0.10000E+06 0.00000E+00 0.16500E-03 0.10909E-04 0.00000E+00 0.26520E-13 0.00000E+00 0.10000E+01 0.00000E+00 0.65143E-03
#####
^L
***** VOLUME- AND MASS-BALANCES *****
***** [KCYC,ITER] = [ 32, 3] *****
                                         THE TIME IS 0.540000E+06 SECONDS, OR 0.625000E+01 DAYS

      PHASES PRESENT
*****
PHASES *      GAS      AQUEOUS
*****
VOLUME (M^3) * 0.59497717E-04 0.59302283E-04
MASS (KG) * 0.66915125E-04 0.58885380E-01
*****

      COMPONENT MASS IN PLACE (KG)
*****
PHASES *      GAS      AQUEOUS      ADSORBED      TOTAL
*****
COMPONENTS *
WATER * 0.27801956E-05 0.58864463E-01 0.00000000E+00 0.58867243E-01
ACETIC ACID* 0.00000000E+00 0.12687310E-05 0.00000000E+00 0.12687310E-05
CO2 * 0.31642455E-04 0.19046999E-04 0.00000000E+00 0.50689453E-04
CH4 * 0.10908184E-04 0.29436586E-06 0.00000000E+00 0.11202550E-04
O2 * 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
N2 * 0.21584291E-04 0.30689829E-06 0.00000000E+00 0.21891190E-04
*****

```

Figure 9. Portion of T2LBM output file for the anaerobic biodegradation problem.

T2LBM simulation results are shown in Figure 9 with graphical comparison to Lay *et al.* (1998a) in Figure 10 where the cumulative production (mL) of CH₄ is plotted against time. While agreement is good, it is acknowledged that there are many free parameters in T2LBM that can be changed to match the experimental result. The important confirmation of the model is simply that the observed dynamics of production of methane can be matched with T2LBM.

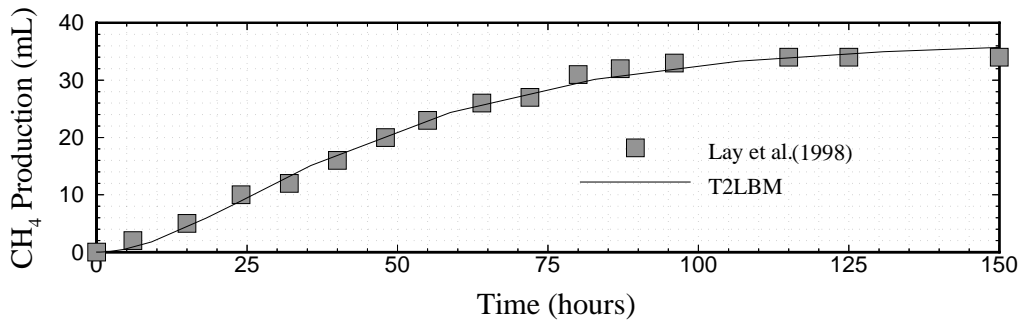


Figure 10. Results of the evolution of methane production over time from Lay *et al.* (1998a) and T2LBM.

5.3 Landfill Sample Problem

In this sample problem, a relatively complex two-dimensional landfill system in which air is injected at the bottom and leachate is injected at the top is simulated to demonstrate code capabilities. The system consists of a two-dimensional 10 m thick landfill pile 20 m across. The permeability field and boundary conditions are shown in Figure 11 where the heavy lines are gridblock boundaries and the dotted lines are the connections in the interior of the domain. The top boundary models the ground surface by specification of constant temperature and pressure (i.e., an atmospheric boundary condition), while the bottom models a leachate collection system (constant temperature, pressure) where liquid water is collected and removed. During the first 10 days, the system receives only leachate recirculation (constant injection of water at the top at a rate of 2 cm day⁻¹). For the final 10 days, the system receives 2 cm day⁻¹ of water injection at the

top as well as $20 \text{ m}^3 \text{ hour}^{-1}$ of dry air injected at the bottom ($1 \text{ m}^3 \text{ hour}^{-1} \text{ m}^{-1}$). Over the course of the 20 days of simulation, the landfill pile compacts by approximately 10%. The system starts out aerobic, becomes anaerobic as O_2 is used up by aerobic biodegradation, and then returns to aerobic conditions as air injection occurs during the final 10 days.

Properties of the system are presented in Tables 6 and 7. The initial acetic acid mass fraction and the biodegradation parameters were either chosen arbitrarily or borrowed from the prior sample problems. For lack of better data, the landfill material is specified to have capillary pressure and relative permeability properties similar to that of sand. The heterogeneous permeability field was generated using simulated annealing techniques and imported into the MESH file using permeability modifiers (see Pruess *et al.*, 1999). The initial saturation and flow field was generated using EOS7 and read into T2LBM using the NKIN feature (see Pruess *et al.*, 1999).

Table 6. Aerobic and anaerobic biodegradation properties for the landfill sample problem.

Model System Property	Symbol	Aerobic	Anaerobic	Units
Yield coefficient	Y	0.2	0.2	$\text{kg microbe (kg waste)}^{-1}$
Microbial growth rate	μ_{max}	5.0×10^{-7}	5.0×10^{-7}	s^{-1}
Maximum T for microbial growth	$T_{max,B}$	80.	60.	$^{\circ}\text{C}$
Saturation constant	K_s	1.0×10^{-3}	1.0×10^{-3}	-
Death rate of microbes	δ	3.0×10^{-8}	3.0×10^{-8}	s^{-1}
Heat of reaction	ΔH_a	1.5×10^7	1.0×10^6	J (kg HAc)^{-1}

Table 7. General properties for the landfill sample problem.

Property	Symbol	Value	Units
Initial mass fraction HAc	X_{liq}^{HAc}	2.5×10^{-3}	-
Compaction ratio	cr	0.10	-
Heat capacity of matrix	C_p	132.	$J\ kg^{-1}\ K^{-1}$
Thermal conductivity	λ	2.1	$J\ m^{-1}\ s^{-1}\ K^{-1}$
O ₂ injection rate	q_{O_2}	1.4×10^{-4}	$kg\ s^{-1}$
N ₂ injection rate	q_{N_2}	5.2×10^{-4}	$kg\ s^{-1}$
Air injection temperature	T_{intake}	20.	°C
Water injection rate	q_{H_2O}	2.3×10^{-4}	$kg\ s^{-1}$
Water injection temperature	T_{intake}	20.	°C
Critical oxygen mass fraction	$X_{crit}^{O_2}$	1.8×10^{-6}	-
Porosity	ϕ	0.7	-
Permeability	k	mean $\log_{10}(k) = -12$ $\sigma = 0.7$	$\log(m^2)$
Relative permeability $S_{gr} = 0.005$	γ, S_{lr}, S_{ls}	0.59, 0.21, 1.0	-, -, -
Capillary pressure $\alpha/\rho g = 8.4 \times 10^{-4}\ Pa^{-1}$ $P_{max} = 1.0 \times 10^5\ Pa$	γ, S_{lr}, S_{ls}	0.59, 0.20, 1.0	-, -, -

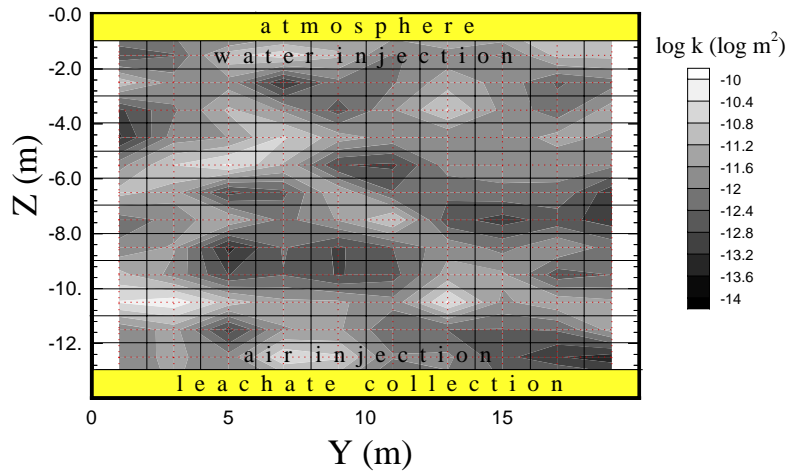


Figure 11. Permeability field, numerical grid, and boundary conditions for the landfill sample problem.

Results are shown in Figures 12–15 at $t = 1$ day, 2 days, 10.1 days, and 15 days. In the figures, the first four frames show liquid saturation, temperature, liquid mass fraction of acetic acid, and aerobicity fields with superimposed liquid velocity vectors. (Recall that aerobicity is equal to one for aerobic conditions and equal to zero for anaerobic conditions). The second four frames show gas mass fractions of CH_4 and CO_2 with gas velocity vectors superimposed, followed by anaerobic and aerobic mass fractions with liquid velocity vectors. As shown, the system starts out with variable liquid saturation and downward flow of water as controlled by the effective permeability and capillary pressure fields. Note the higher temperatures in the upper region, reflecting the aerobic reactions that are occurring there. The anaerobic regions coincide with the low-permeability regions (*cf.* Figure 11) due to the relative inability of air to replenish oxygen in these regions following the initial aerobic reactions therein. As these areas become anaerobic, methane forms as shown in Figure 12. At $t = 2$ days (Figure 13), more of the system has become anaerobic. The temperature field reflects higher temperatures where aerobicity is

equal to one, and where acetic acid concentrations are still relatively high. At this time, significant CH₄ and CO₂ have formed as has aerobic biomass. At $t = 10$ days, the air injection at the bottom begins. Results at $t = 10.1$ days are shown in Figure 14. Note that some air flows downwards into the leachate collection system due to the low effective permeability of the refuse mass. At $t = 10.1$ days, the air injection at the bottom is causing aerobic conditions to migrate upward from the bottom perturbing the anaerobic state that had developed prior to air injection. The gas flow velocity vectors show gas flow along the high-permeability pathways and corresponding dilution of CH₄ and CO₂. The aerobic biomass continues to increase as it is produced in high-permeability regions where air circulation is highest. The anaerobic biomass tends to be more uniform. By $t = 15$ days (Figure 15), the system is becoming more aerobic and temperatures have increased to approximately 30 °C even though 20 °C water and air are being injected. The CO₂ concentrations are large in the upper regions of the domain and in low-permeability regions where concentrations resist dilution. By $t = 20$ days, nearly the entire system becomes aerobic and the acetic acid mass fraction is reduced to very low values. The progressive compaction of the system can be seen by the decreasing heights of the various fields plotted in Figures 12–15.

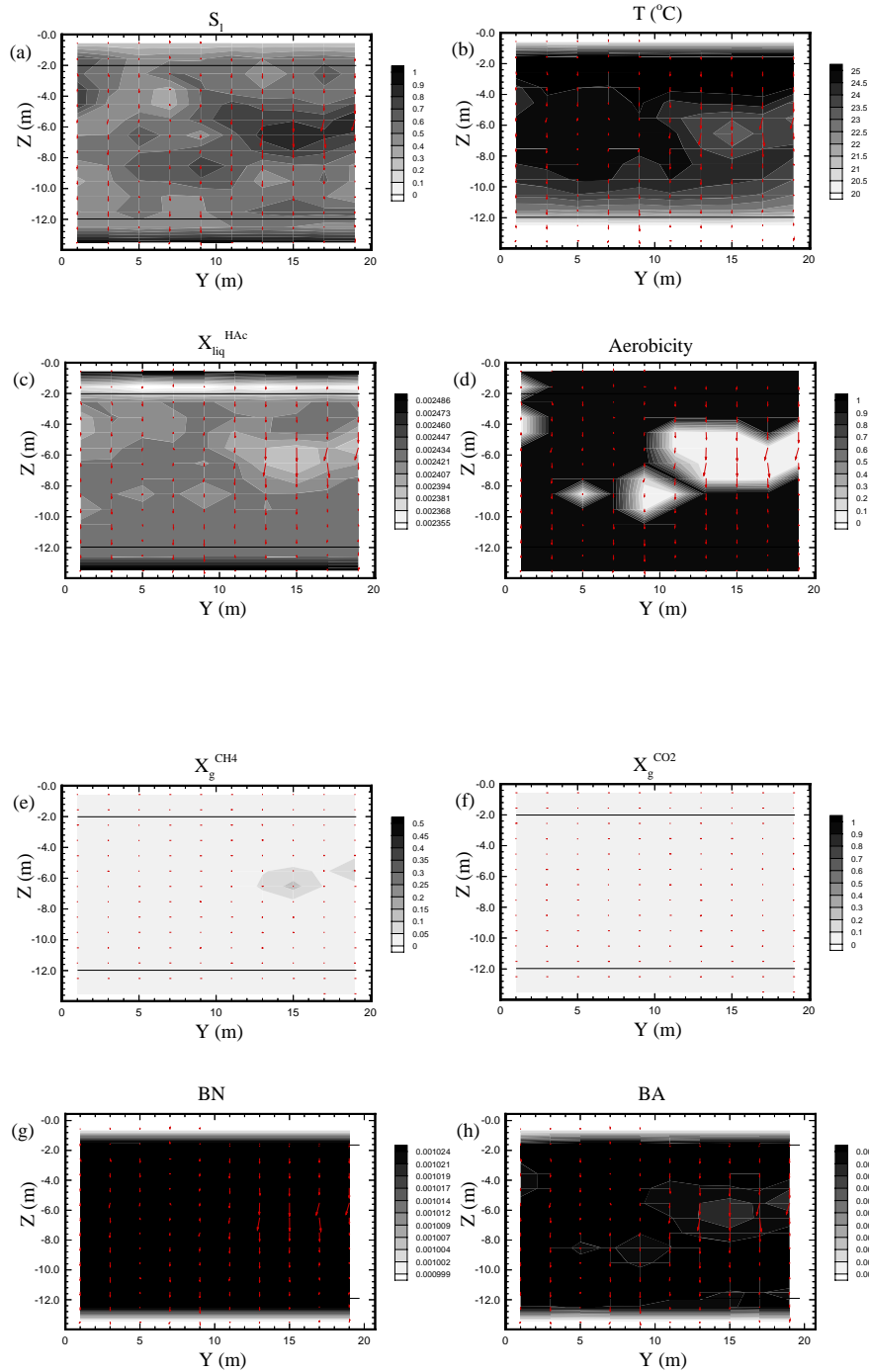


Figure 12. Liquid saturation (S_l), temperature (T), mass fraction acetic acid ($X_{\text{liq}}^{\text{HAc}}$), and aerobicity with liquid velocity vectors, along with CH_4 and CO_2 mass fractions with gas velocity vectors ($X_g^{\text{CH}_4}$, $X_g^{\text{CO}_2}$), and anaerobic and aerobic biomass fractions at $t = 1$ day.

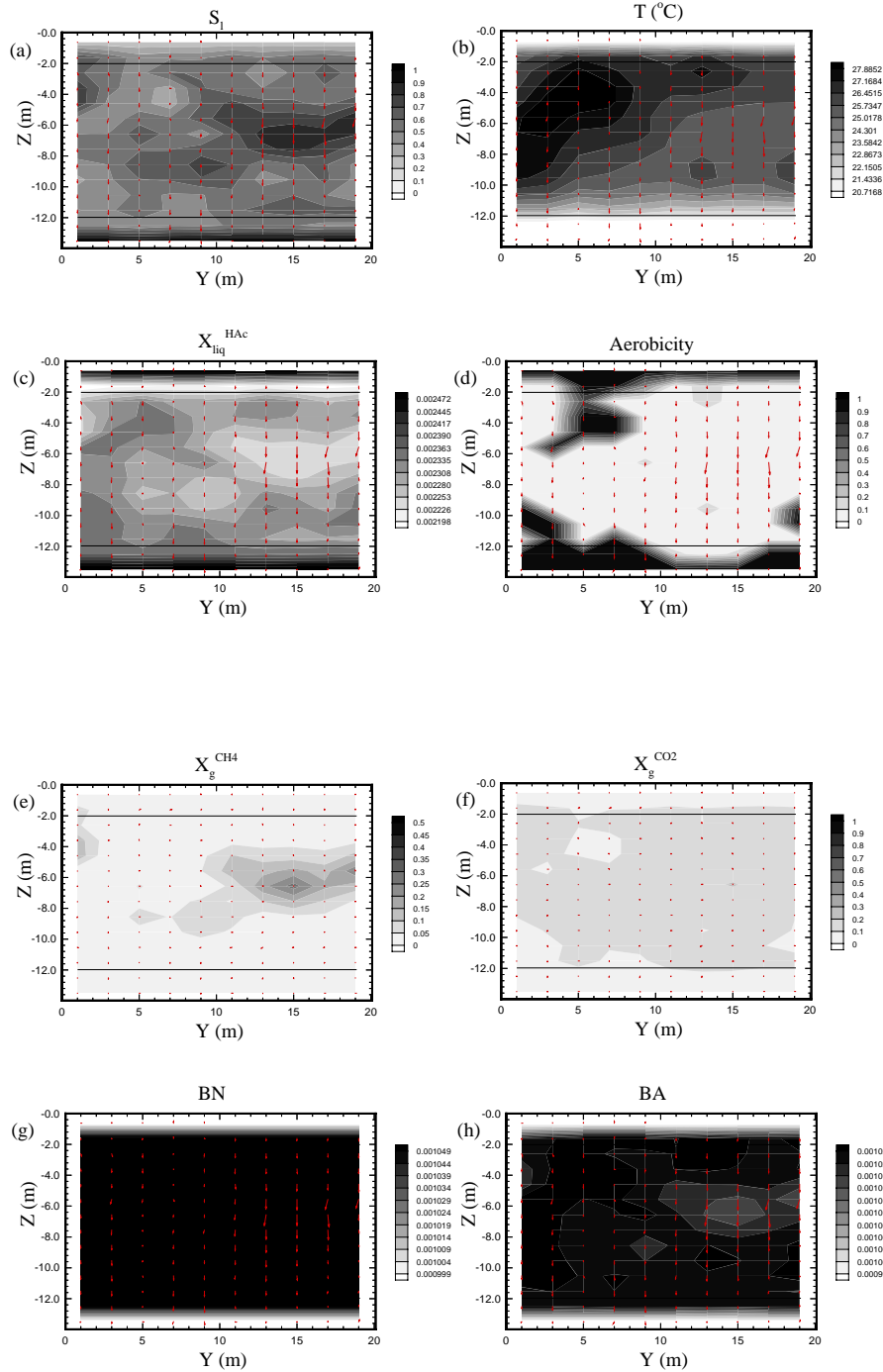


Figure 13. Liquid saturation (S_l), temperature (T), mass fraction acetic acid ($X_{\text{liq}}^{\text{HAc}}$), and aerobicity with liquid velocity vectors, along with CH_4 and CO_2 mass fractions with gas velocity vectors ($X_g^{\text{CH}_4}$, $X_g^{\text{CO}_2}$), and anaerobic and aerobic biomass fractions at $t = 2$ days.

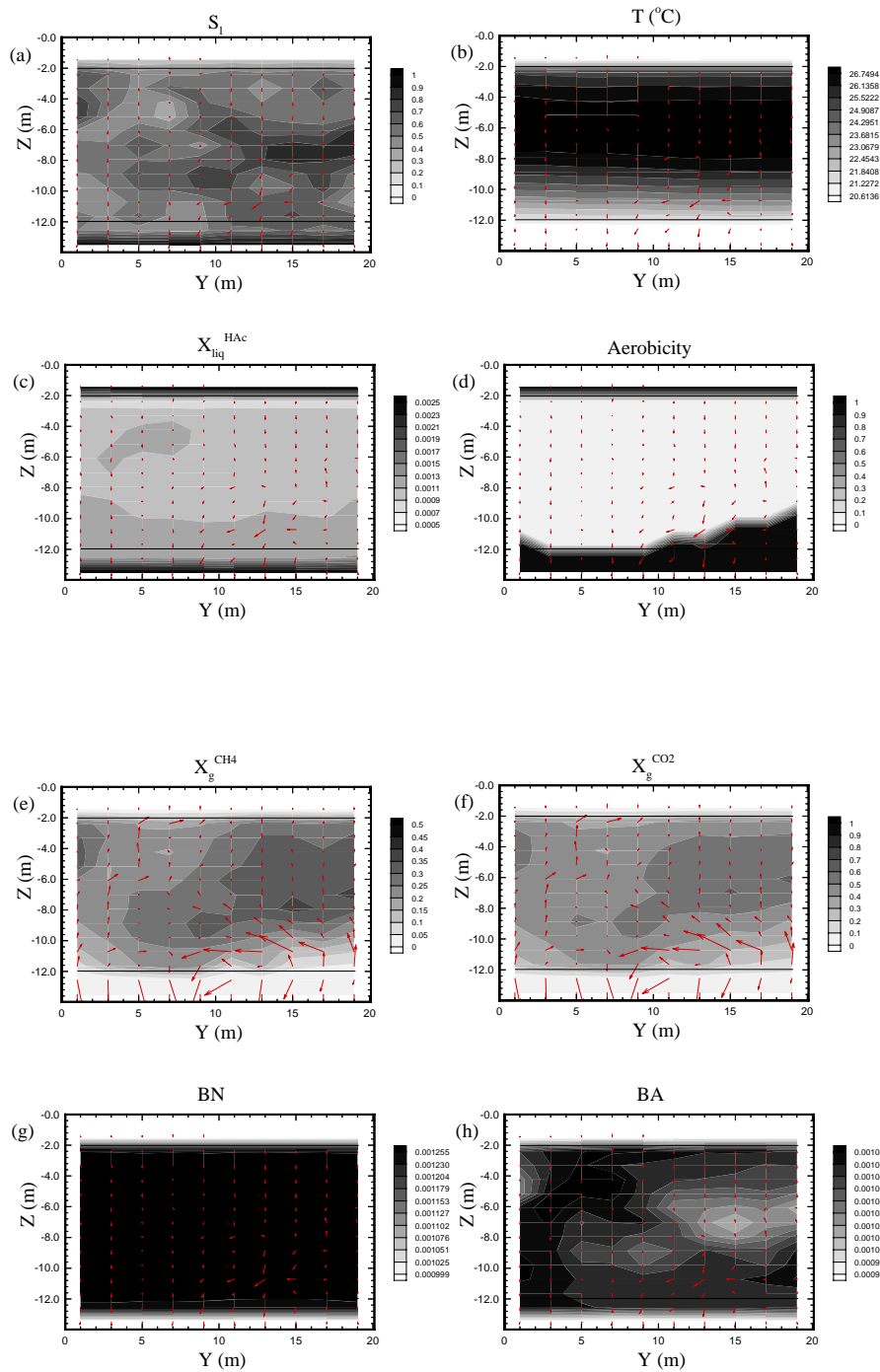


Figure 14. Liquid saturation (S_l), temperature (T), mass fraction acetic acid ($X_{\text{liq}}^{\text{HAc}}$), and aerobicity with liquid velocity vectors, along with CH_4 and CO_2 mass fractions with gas velocity vectors ($X_g^{\text{CH}_4}$, $X_g^{\text{CO}_2}$), and anaerobic and aerobic biomass fractions at $t = 10.1$ days.

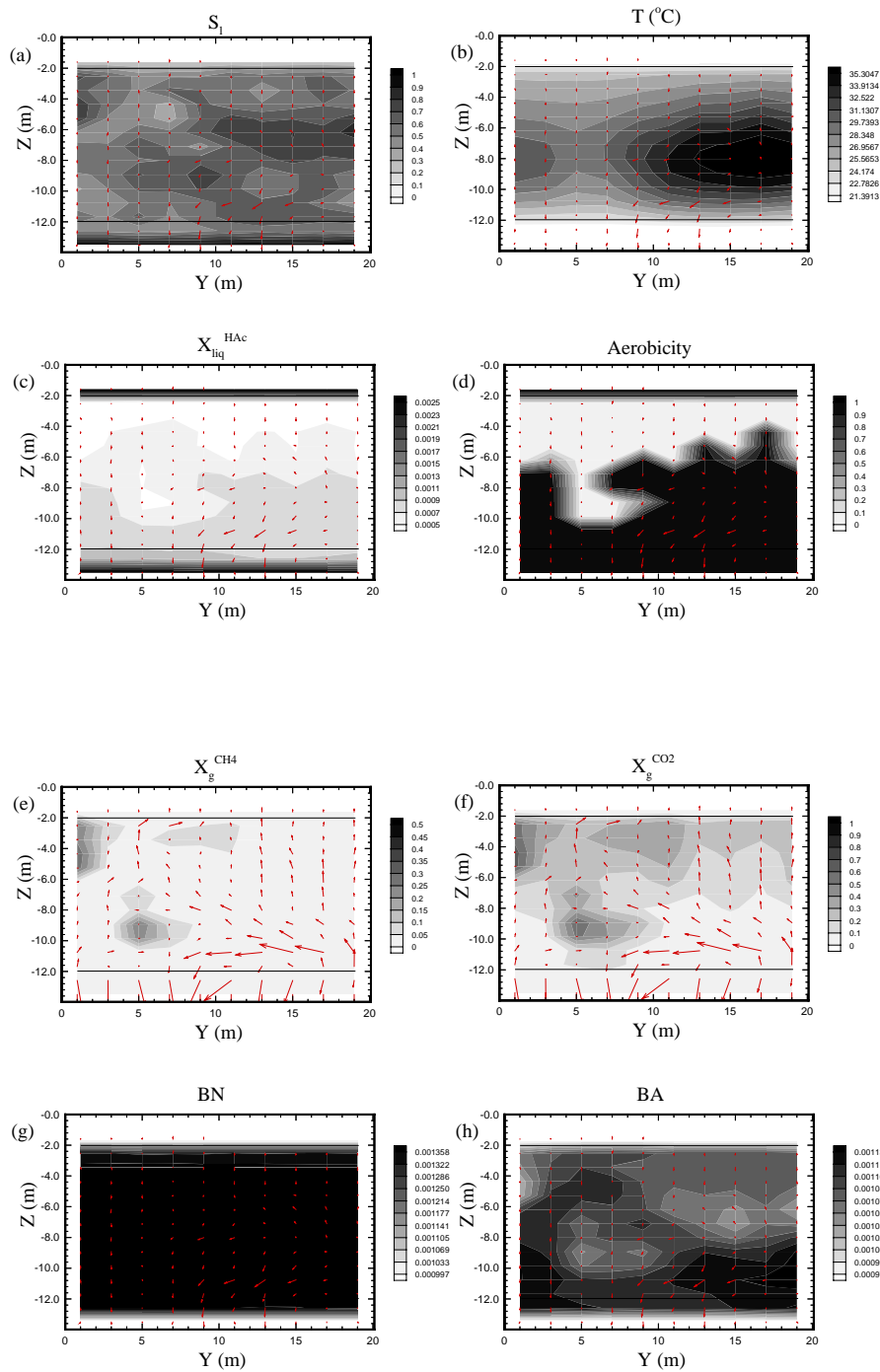


Figure 15. Liquid saturation (S_l), temperature (T), mass fraction acetic acid ($X_{\text{liq}}^{\text{HAc}}$), and aerobicity with liquid velocity vectors, along with CH_4 and CO_2 mass fractions with gas velocity vectors ($X_g^{\text{CH}_4}$, $X_g^{\text{CO}_2}$), and anaerobic and aerobic biomass fractions at $t = 15$ days.

6. Final Notes

T2LBM implements a simple Monod kinetic model for biodegradation of landfill materials. The model is built on the TOUGH2 model, which by itself embodies complex coupled flow and transport processes. The coupling of biodegradation to flow and transport along with the additional chemical components of T2LBM create new processes and complexities that may be challenging to simulate and interpret. In addition, long simulation times can be expected for problems with many gridblocks. Along with experience in the use of TOUGH2, the requirements for successful use of T2LBM are a significant motivation and sufficient time for learning and experimenting.

Acknowledgments

I thank Karsten Pruess, Terry Hazen, and Alfredo Battistelli for advice and useful comments during the course of this work. This work was supported by the Office of Science, U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Nomenclature

a	arctan switching function	-
B	microbial concentration	kg microbes (kg aqueous phase) ⁻¹
BA	aerobic biomass concentration	kg microbes (kg aqueous phase) ⁻¹
BN	anaerobic biomass concentration	kg microbes (kg aqueous phase) ⁻¹
cr	compaction ratio	-
Cp	heat capacity	J kg ⁻¹ °C ⁻¹

d	molecular diffusivity	$\text{m}^2 \text{s}^{-1}$
f	function to be minimized	kg
f_B^T	coefficient of T-dependent growth	-
F	Darcy flux vector	$\text{kg m}^2 \text{s}^{-1}$
g	acceleration of gravity vector	m s^{-2}
ΔH_B	enthalpy of biodegradation reaction	J kg^{-1}
hr	refuse height ratio	-
k	permeability, time-step index	$\text{m}^2, -$
K	equilibrium constant	-
K_H	Henry's Law coefficient	Pa^{-1}
$K_{S,B}$	saturation constant	$\text{kg substrate (kg aqueous phase)}^{-1}$
M	mass accumulation term	kg m^{-3}
MW	molecular weight	g mole^{-1}
n	inward unit normal vector	
NEQ	number of equations per grid block	
NK	number of mass components (species)	
NPH	maximum number of phases present	
p	iteration index	
P	pressure	Pa
P_c	capillary pressure	Pa
q	source term	$\text{kg m}^{-3} \text{s}^{-1}$
S_β	phase saturation	-
S	substrate (acetic acid) concentration	$\text{kg substrate (kg aqueous phase)}^{-1}$
t	time	s, days
T	temperature	$^\circ\text{C}$
V	volume	m^3
x	mole fraction	-

X	mass fraction	-
Y	yield coefficient	kg microbes (kg substrate) ⁻¹
Y	Y-coordinate	m
z_c	compaction factor	-
Z	Z-coordinate	m

Greek symbols

α_1, α_2	coefficients of Stumm and Morgan (1996)	
γ	van Genuchten (1980) parameter	
δ	microbial death rate	s ⁻¹
Γ	surface area	m ²
λ	thermal conductivity	J m ⁻¹ K ⁻¹ s ⁻¹
μ	dynamic viscosity	kg m ⁻¹ s ⁻¹
μ_B	microbial growth rate	s ⁻¹
$\mu_{max,B}$	maximum microbial growth rate	s ⁻¹
ϕ	porosity	—
ρ	density	kg m ⁻³
θ	moisture content	—
τ	tortuosity	—

Subscripts and superscripts

a	air
aq	aqueous
B	biomass, microbes
crit	critical
g	gas
l	liquid

<i>l_s</i>	liquid satiated
<i>max</i>	maximum
<i>R</i>	rock
0	reference value, initial value
β	phase index
κ	mass components

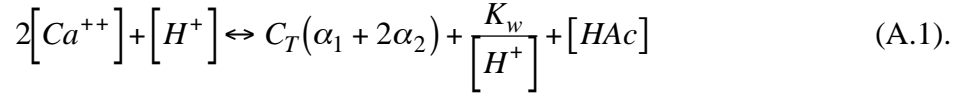
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Appendix A. pH Calculation

The pH of the aqueous phase is estimated by the method of Stumm and Morgan 1996), p. 386. Starting with the dissociation reaction,



and introducing the charge balance relations,

$$\alpha_o = \left(1 + \frac{K_{a1}}{[H^+]} + \frac{K_{a1}K_{a2}}{[H^+]^2} \right)^{-1} \quad (A.2)$$

$$\alpha_1 = \left(\frac{[H^+]}{K_{a1}} + 1 + \frac{K_{a2}}{[H^+]} \right)^{-1} \quad (A.3)$$

$$\alpha_2 = \left(\frac{[H^+]^2}{K_{a1}K_{a2}} + \frac{[H^+]}{K_{a2}} + 1 \right)^{-1} \quad (A.4)$$

$$[Ca^{++}] = \frac{\left(\frac{K_{SO}}{K_H P_{CO_2}} \right) \alpha_o}{\alpha_2} \quad (A.5)$$

$$C_T = \frac{K_H P_{CO_2}}{\alpha_o} \quad (A.6)$$

and the values of the equilibrium constants at 40°C,

$$K_{a1} = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} = 4.467 \times 10^{-7} \quad (A.7)$$

$$K_{a2} = \frac{[H^+][CO_3^{--}]}{[HCO_3^-]} = 6.026 \times 10^{-11} \quad (\text{A.8})$$

$$K_w = [H^+][OH^-] = 2.951 \times 10^{-14} \quad (\text{A.9})$$

$$K_{SO} = [Ca^{++}][CO_3^{--}] = 2.951 \times 10^{-9} \quad (\text{A.10})$$

(see Stumm and Morgan, 1996, Table 4.3), the only unknown in Equation A.1 is $[H^+]$ in units of moles L^{-1} which can be solved by Newton-Raphson iteration.

Appendix B. T2LBM Program Units

Table B1. Summary of program units in T2LBM.

Program unit	Basic changes for biodegradation.
MAIN	Added new common blocks for biodegradation.
CYCIT	Changed to call subroutine COMPACT after each time step.
INPUT	Reads and assigns initial biomass fractions.
RFILE	Reads local biomass fractions from INCON file.
WRIFI	Writes local biomass fractions to SAVE file.
CONVER	Updates biomass mass fractions at end of time step.
COMPACT	Computes compaction and writes new MESH files with updated geometry, permeability, and porosity after each time step.
EOS	Changed to handle HAc, CO ₂ , CH ₄ , O ₂ , and N ₂ components.
MULTI	Changed to call subroutine BIOREACT.
BIOREACT	Computes biodegradation reactions.
HENRYINV	Computes Henry coefficients as a function of temperature.
ESTPH	Estimates pH of the aqueous phase.
BALLA	Writes out total masses of components and phases.
VISGAS	Calculates viscosity of gas mixtures.
OUT	Writes output file.