

The Challenge of Pursuing a System Dynamics Approach in Analyzing Complex Natural Systems: Example of Solid Waste Landfills

Michael L. Shelley, W. Brent Nixon, and Charles A. Bleckmann

Air Force Institute of Technology

AFIT/ENV
2950 P street
Wright-Patterson AFB OH 45433-7765

(937) 255-3636 ext 4594
FAX (937) 656-4699

Michael.Shelley@afit.edu

Abstract

A system dynamics approach is attempted to determine the significant processes and appropriate level of detail required to capture dynamic behavior important in managing biodegradation in landfills. The approach used in analyzing complex natural (biochemical) processes in such systems is inherently different from that used in analysis of many management systems where influences and feedback may be more easily envisioned and represented at a higher level of aggregation. Successful aggregation of natural physical-chemical processes in search of a simpler (and useful) model structure is elusive and problematic. Yet, the simplest model structure achievable, without sacrificing relevant behavioral patterns and the accurate influence of potential engineering controls, must be pursued to enable broad implementation of a practical modeling tool in the field. This paper presents this struggle for an engineered system using complex naturally occurring biochemical processes (municipal solid waste landfill), with implications for confidence building in the model.

Key Words: system dynamics model, natural systems, ecological engineering, landfills

Introduction

System dynamics modeling has gradually developed into a well defined analysis discipline since its introduction as “industrial dynamics” by Jay Forrester in the 1960’s. Applications of the method have expanded beyond the management sciences to include the global environment, regional ecological dynamics, and applications of ecological engineering. However, the more definitive works which establish the foundational principles of the system dynamics approach generally arise from within the context of organizational or logistical process management.

These principles define the character of system dynamics and should (with reasonable, limited exceptions) universally apply to all contexts which claim to benefit from the system dynamics approach. The question that must be posed is to what extent some contexts (such as analysis of engineered or natural physical systems) necessarily exclude classical system dynamics principles and how does this impact the ultimate benefit of a rich system dynamics approach (intuitive understanding of system structure and behavior).

Foundational principles of the system dynamics approach include: 1) establishing a simple reference behavioral pattern of the system, either observed in the real system, intuitively hypothesized, or desired; 2) conceptualizing a simple system structure of influences which is consistent with reference behavior and which maximally aggregates system detail to represent only the primary system components that drive reference behavior; 3) formulating such structure to observe simulated behavior and explore required structural detail necessary to address the purpose of the analysis; and 4) performing a set of prescribed validation tests to gain confidence in the model structure as an implementation tool for system management or deeper system understanding (Legasto et al, 1980).

These classical iterative steps are well suited to the analysis of organizational behavior, for example, where ideal or observed undesirable behavior is easily expressed in simple patterns and system structure can be initially represented in terms of high level aggregate influences, such as a more stringent policy lowering morale which lowers performance which, in turn, induces an even more stringent policy. The highly complex details of psychological and social mechanisms which cause a policy to ultimately lower performance are ignored. The system can then be explored, through iterative simulation, to determine which influences dominate the behavior of interest and where more detail should be added to the model. Engineered systems, on the other hand, are generally less complex in underlying detail, and system structure is well understood, being designed and constructed beforehand. Furthermore, the optimized, cost effective design of such systems, to achieve desired behavior, promotes an initial assumption that the detailed system description is the simplest and most appropriate structure with which to explore conditions of optimum behavior. Therefore, with engineered systems, system behavior does not guide the modeler to system structure, but, rather, well defined system structure explores possible emergent behaviors through changing system parameter values. Analysis is thus reduced to a methodology for determining the specific combination of parameter values to be tested in answering the relevant questions about optimizing the system. This kind of analysis is much more simple and straightforward, falling short of the overall character of system dynamics.

The analysis of complex natural systems involving attempted engineering control falls between the two extremes above and presents unique challenges. Ecological systems, for example, are extremely complex, and the delicate yet stable balance largely depends on this complexity. The detailed sub-components of the system are often well understood in isolation (biochemical transformations, physical transport processes, etc), but aggregation of these processes into a meaningful higher order system structure is difficult. Such higher order structure is envisioned only at the highest levels (generalized nutrient pool fluxes and biomass production and decay rates). These generalizations appear useful for insight into disturbance thresholds causing significant decline in metrics of overall system health; but exploring means of adjusting subtle aspects of system performance (like improving a single species survival or reproduction rate

without degrading another) requires much more structural detail. It is difficult to find a starting point for simple, aggregate system structure which provides reasonable behavior. Part of the problem is a general lack of knowledge of how detailed system sub-components might be aggregated into higher level components which act as an entity to influence other components. In other words, we have a general understanding of the system at the highest level, good understanding of many micro-processes at the lowest level structure, but little insight how the structure hierarchically structures in between. This forces the systems modeler to start with a much more detailed structure than desired (that which can be mechanistically described at a low hierarchical level), use some criteria to place bounds on the breadth of detail to include, and then seek opportunities to aggregate into a simpler structure (a process opposite that advocated by most system dynamics modelers). As such, it becomes difficult to reach a level of confidence in the model structure, not knowing if the correct strategy of aggregation or initial boundaries on detail were sufficient to capture all relevant emergent behaviors of interest.

Here, we demonstrate the example of a municipal solid waste landfill, a system of natural degradation processes, both simultaneous and sequential, which ultimately bring organic solid wastes to stable forms such as carbon dioxide and methane. The objective is to develop a model that describes this degradation sufficient to explore engineering manipulations of the system to decrease stabilization time, limit environmental impact, or control the production of useful or harmful gases during the process.

General System Description

To comprehensively assess landfill performance, the microbiological, chemical, and physical degradation processes should be fully understood. However, the most significant process controlling decomposition is microbiological degradation (Murphy and Brennan, 1992). Understanding the causes and interactions among complex degradation processes and identifying the important variables are the initial steps in manipulation of the system to control or enhance the process.

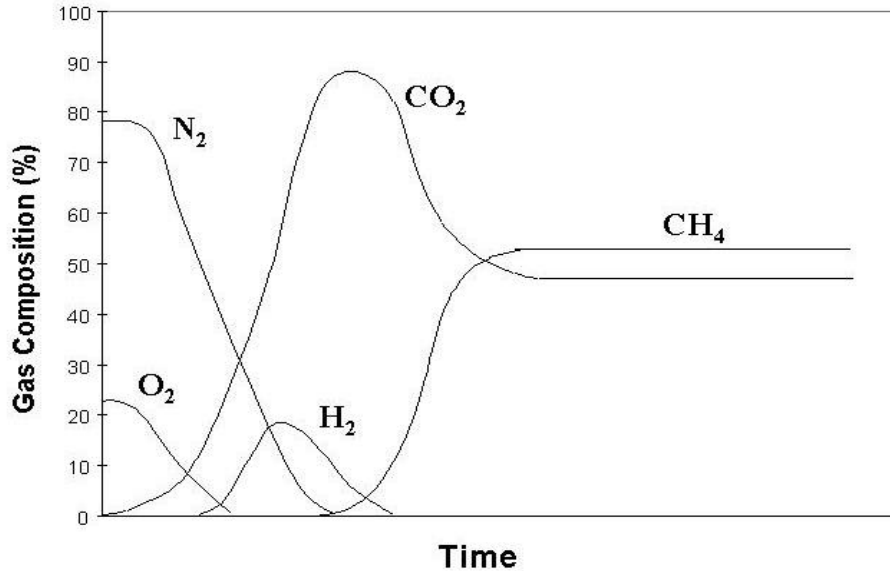
Realistic limits to the complexity of experimental biodegradation studies, as well as temporal and spatial limitations, limit the usefulness of such studies in ascertaining long-term microbial decomposition behavior (Moorhead et al, 1996). Various models simulate the underlying processes of degradation, most using analytical or numerical approaches (El Fadel et al, 1996). Although the fundamental processes of biodegradation associated with landfills have been aggressively studied by countless authors and modeled by a few others, landfill biodegradation remains an extremely complex subject.

Landfill models are typically limited either to general descriptions of the overall process or to intricate explanations or simulations of a particular reaction or bacterial phenomena associated with the process. Such efforts generally avoid a broad perspective and sometimes fail to question whether the entities chosen for modeling are *fundamental* to the process. Moreover, significant interrelationships within the system and indirect influences on system behavior from changing conditions may be ignored or their effects suppressed by focusing on a particular aspect of the process. By concentrating on the pieces of the system, without addressing how all the

pieces fit together, some modeling approaches fail to capture the essential mechanisms responsible for the degradation process and their interactions. However, biodegradation involves countless interactions among numerous individually complex entities and parameters: consortia of microbial populations, sequential appearance and disappearance of substrates, and continually changing environmental conditions. A comprehensive system structure is unreasonable to model and likely not required to capture relevant system behavior, but there is limited basis for simplified structural assumptions that still represent mechanistically understood system components which not only capture behavior patterns of interest but also respond to engineering intervention.

Observation of landfill gas production provides an empirical view of landfill system behavior, represented in general form by Tchobanoglous et al, 1993 (Figure 1). This serves as an excellent smooth, generalized reference behavioral pattern to begin the modeling process. However, this pattern, although each gas displays simple behavior, is not simple when all three of the generated gases (CH_4 , CO_2 , and H_2) are taken together. These gases are simultaneously produced by many microbial populations, but the gases have different behavioral patterns. All gases are also produced by reactions that degrade the products of other reactions, and there are no cause and effect relationships immediately apparent between the gases except that one of the many methane producing reactions depends on the availability of carbon dioxide and hydrogen. Therefore, it is difficult (not practically within reach) to propose a simple, high level model structure that produces the reference behavior pattern (relative amplitudes and phasing of gas curves over time) and that also represents biochemically understood real-world components. The modeler must therefore retreat to modeling the mechanistic detail of the various reactions known to exist while asserting some bounding criteria which limits the breadth of detail for practical modeling purposes. In general, solid waste is hydrolyzed at its surface, producing soluble monosaccharides which further degrade into lower carbon chains of organic acids and alcohols and, ultimately, to carbon dioxide and methane, with concurrent production of carbon dioxide and hydrogen throughout the sequence of reactions. The various reactions and reaction sequences produce different ratios of these gases. Hundreds or, perhaps, thousands of microbial populations are involved.

Figure 1. Conceptual representation of landfill gas formation over time derived from empirical data (after Tchobanoglous et al, 1993)



Model Description

The approach used here is to describe the breakdown of a specific volume of solid waste and to mechanistically follow the conversion of the solid material into soluble organic forms by sequential microbial processes. Solid material is assumed to initially exist as uniform spheres which are degraded from the outside by cleavage of a glucose molecule by hydrolysis. Glucose is the only monosaccharide modeled as a hydrolysis product and serves as a surrogate for all carbon chain molecules initially cleaved from the solid waste. This is a bounding assumption, considered reasonable because glucose is a dominant hydrolysis product, and most lower carbon organic molecules found within the system can be derived from glucose. Using the specific glucose molecule allows development of stoichiometrically balanced equations for the series of sequential breakdown reactions, eventually yielding methane and carbon dioxide (Conrad, 1999). The rate of hydrolysis is given as rate of glucose formed per surface area of solid organic waste. This abiotic reaction rate controls the disappearance of organic solid waste material in the landfill. Consumption (and subsequent production) of water is according to the stoichiometry in Table 1. All subsequent reactions, starting with the aerobic and anaerobic breakdown of glucose and ending with methane formation from carbon dioxide and hydrogen, are listed in Table 1. The reactions are derived by noting the predominant forms of organic carbon typically found in a landfill and employing all documented reactions known involving pathways from glucose, through these intermediate organic compounds, and, finally, to carbon dioxide and methane (Gottschalk, 1986). The nitrate pathway is provided to represent reactions yielding predominantly carbon dioxide in response to the presence of non-oxygen electron acceptors such

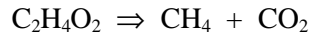
as nitrates, sulfates, and iron oxides. Again, these are all bounding assumptions intended to limit the amount of detail in the model. Together, these equations represent alternative pathways of degradation at the detailed reaction level, bounded in breadth of detail, and simple enough for practical simulation while, hopefully, providing enough detail to realize empirical behavioral patterns in the simulation results. Figure 2 is a schematic providing a visual flow diagram for the breakdown of solid waste, including all possible pathways considered in Table 1.

Table 1. Representative, simulated sequential and parallel reactions leading from organic solid waste material to methane and carbon dioxide stabilization within a landfill (Gottschalk, 1986).

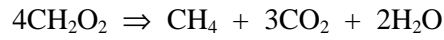
Hydrolysis of Solid Organics:	1 mole of glucose cleaved consumes 1 mole of water (one molecule of water cleaves one polysaccharide bond)
Aerobic Degradation of Glucose:	$C_6H_{12}O_6 + 6O_2 \Rightarrow 6CO_2 + 6H_2O$
Nitrate Anaerobic Pathway: ^a	$C_6H_{12}O_6 + 3NO_3^- + 6H^+ \Rightarrow 3NH_4^+ + 6CO_2 + 3H_2O$
Other Anaerobic Degradation Pathways of Glucose:	
direct to acetate ^b	$C_6H_{12}O_6 \Rightarrow 3C_2H_4O_2$
butyrate forming ^b	$C_6H_{12}O_6 \Rightarrow C_4H_8O_2 + 2CO_2 + 2H_2$
propionate & acetate ^b	$3C_6H_{12}O_6 \Rightarrow 4C_3H_6O_2 + 2C_2H_4O_2 + 2CO_2 + 2H_2O$
Lactate	$C_6H_{12}O_6 \Rightarrow 2C_3H_6O_3$
Lactate & ethanol	$C_6H_{12}O_6 \Rightarrow C_3H_6O_3 + C_2H_6O + CO_2$
Lactate & acetate (bifidum)	$2C_6H_{12}O_6 \Rightarrow 2C_3H_6O_3 + 3C_2H_4O_2$
Ethanol	$C_6H_{12}O_6 \Rightarrow 2C_2H_6O + 2CO_2$
clostridial fermentation	$C_6H_{12}O_6 + 6H_2O \Rightarrow 6CO_2 + 12H_2$
Mixed acid	$10C_6H_{12}O_6 + 7H_2O \Rightarrow 7C_3H_6O_3 + 4C_2H_4O_2 + 8C_2H_6O + CH_2O_2 + 14CO_2 + 13H_2$
Other Acetogenic Reactions:	
from butyrate	$C_4H_8O_2 + 2H_2O \Rightarrow 2C_2H_4O_2 + 2H^+ + H_2$
from lactate	$3C_3H_6O_3 \Rightarrow 2C_3H_6O_2 + C_2H_4O_2 + CO_2 + H_2O$
from propionate	$C_3H_6O_2 + 3H_2O \Rightarrow C_2H_4O_2 + HCO_3^- + H^+ + 3H_2$
from ethanol	$C_2H_6O + H_2O \Rightarrow C_2H_4O_2 + 2H_2$

Methanogenic Reactions:

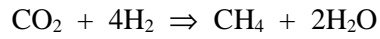
from acetate



from formate



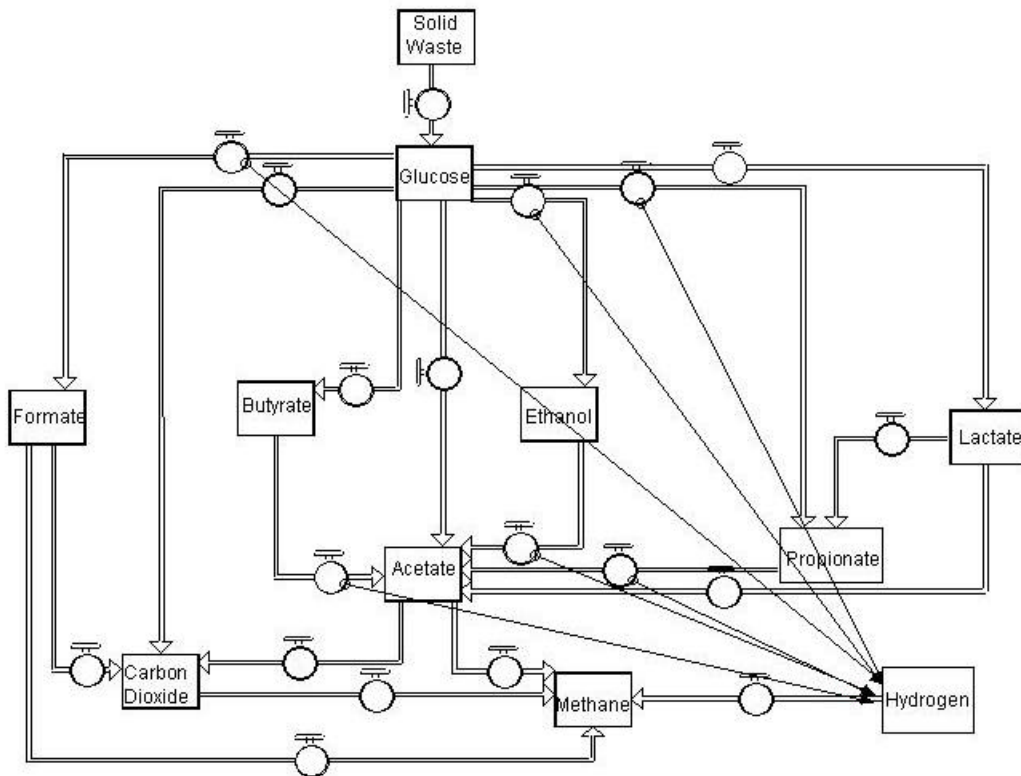
from carbon dioxide
& hydrogen



^aStumm and Morgan, 1996

^bMajor Pathways (Voolapalli and Stuckey, 1999)

Figure2. Schematic of the alternative breakdown pathways of landfill solid waste to the ultimate degradation products of carbon dioxide and methane at complete stabilization.



The rate of each of the reactions, beyond hydrolysis, is determined by the mass of the microbial population responsible for the reaction, the amount of reactant (biological substrate) in the system, and the intrinsic growth rate of the population in accordance with the classical Monod formulation:

$$\frac{dX}{dt} = \frac{\mathbf{m}_{\max} C}{k + C} X - fX$$

where X = biomass
 C = substrate concentration
 \mathbf{i}_{\max} = intrinsic population growth rate constant
 k = Monod half saturation constant
and f = population death rate coefficient.

The equation couples Monod growth with a first-order death term. In the case of population growth depending on two substrates (for example, CO₂ and H₂ for CO₂ methanogens), the Monod growth term is given as:

$$\frac{dX}{dt} = \frac{\mathbf{m}_{\max} C_1 C_2}{(k_1 + C_1)(k_2 + C_2)} X - fX$$

A biomass “yield” constant is applied to the Monod growth term to determine the substrate degradation rate with the appropriate fraction (determined by the Monod growth term) going to new biomass and the complementary fraction yielding the products of respiration according to the balanced equations in Table 1.

Anaerobic reactions are inhibited until oxygen is depleted in the system. The production and consumption rate of gases controls the transport rate to and from the atmosphere in accordance with prevailing molar gas fractions. All forms of waste, gases, and biomass are tracked to conserve mass throughout model simulations. A more detailed description of the model can be found in a separate work (Shelley et al, 2001).

The model was formulated and executed with the numerical integration software STELLA[®] version 6.0.1 Research (High Performance Systems, Inc.) using the 4th-order Runge-Kutta integration algorithm with a time step of 0.01 day.

Results

Model output for all simulations reported achieved a mass balance within 1% of initial mass in the system by the end of the simulation without exceeding that value at any time during the simulation. Figure 3 shows initial output of the model with all populations characterized by identical kinetic parameter values (Table 2). The model in this initial state allows all populations to respond with equal potential, limited only by available substrate. As such, methanogenesis competes well with earlier reactions as the products of these reactions become available as energy sources. Early carbon dioxide formation, along with abundant hydrogen, enables CO₂ methanogens to proliferate, consuming CO₂ (limiting its peak). This early dominance of CO₂ methanogens may also explain the higher methane to carbon dioxide ratio in the final stabilization stage compared the reference behavior of Figure 1. This simulation verifies the mechanistic mass balance model by behaving smoothly and providing reasonable results, with all

organic matter eventually yielding CO_2 and CH_4 . However, the time appearance of the gases is not properly phased nor do the gases reach similar amplitudes when compared to empirical data (Figure 1).

Figure 3. Initial simulation output with all populations as described in Table 1 with identical kinetic parameter values, limited only by the concentration of substrate upon which the population depends.

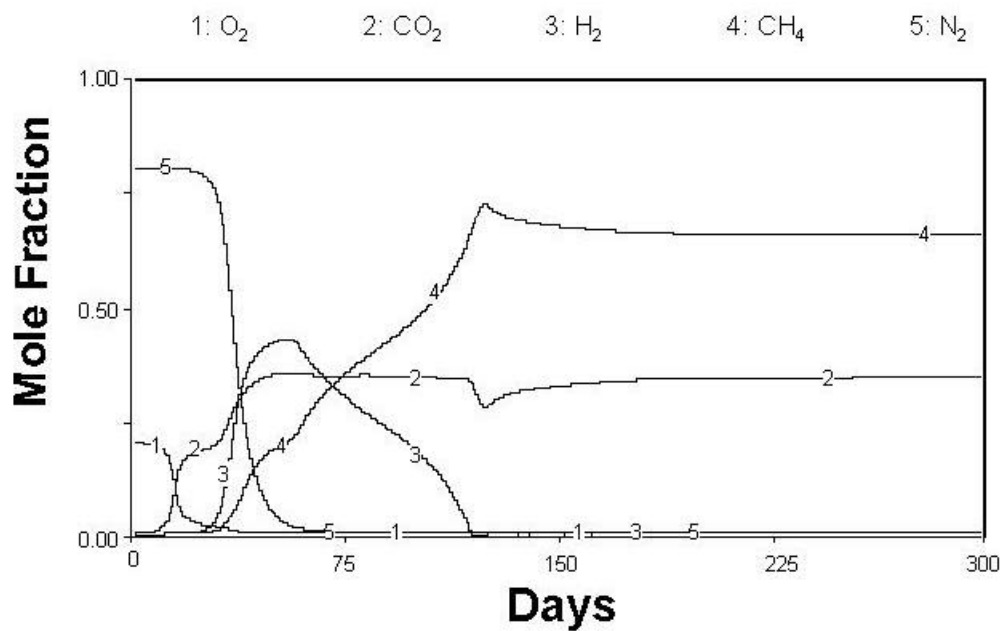


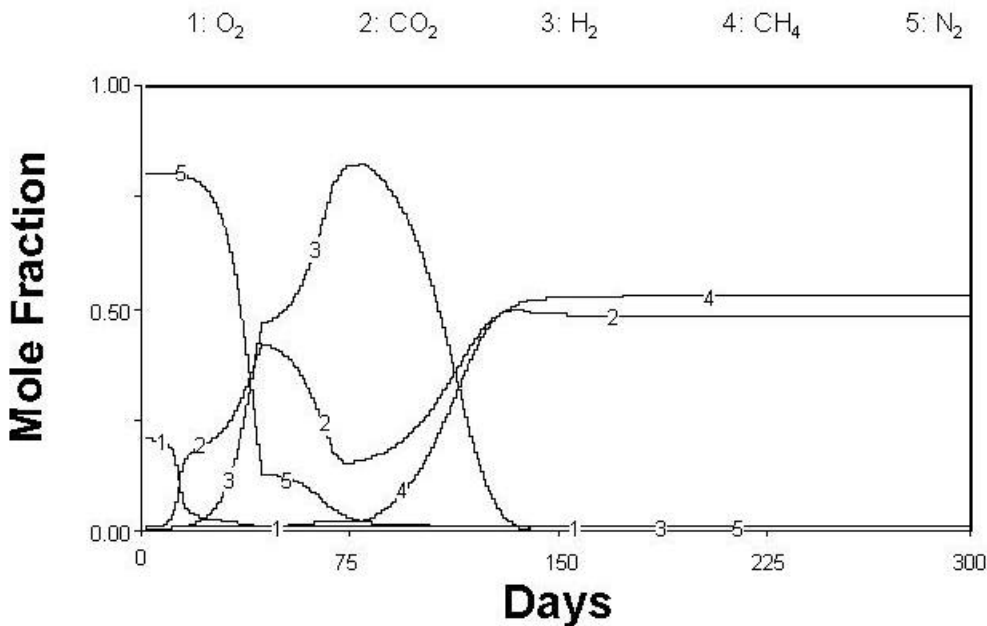
Table 2. Initial baseline model parameter values resulting in the output of Figure 3 (all populations use identical kinetic parameter values).

Parameter	Value
<i>Microbial Population Parameters:</i>	
Monod μ_{\max} (intrinsic growth rate without substrate limitation)	0.5 (kg new biomass per kg biomass per day)
Monod Half Saturation Constant	1 (mg/l)
Minimum Death Rate Coefficient	0.1 (kg lost biomass per kg biomass per day)
Cell Yield	0.5 (kg new biomass per kg substrate utilized)
Initial Biomass	100,000 (kilograms)
<i>Landfill Physical Parameters:</i>	
Initial N ₂ Fraction	0.8 (mole fraction)
Initial O ₂ Fraction	0.2 (mole fraction)
Gas Diffusion Rate Coefficient (Rate of gas seepage into or out of landfill in moles per day per moles of excess gas)	1.0 (moles per day per mole departure from landfill molar capacity at standard temperature and pressure)
Initial Percent Moisture	25 (%)
Landfill Cell Length	1000 (meters)
Landfill Cell Width	1000 (meters)
Landfill Cell Depth	3 (meters)
Initial Solid Waste Sphere Radius	0.07 (meters)
Average Solid Waste Density ^a	1350 (kg/m ³)
Initial Nitrate Concentration in Landfill	100 (mg/l)
Hydrolysis Rate (rate of glucose formation per surface area of solid organic waste)	0.5 (kg glucose per day per square meter organic solid waste surface)

^aShelley et al, 2001

Refinement of the output is achieved by differentiating the behavior of the populations in a manner supported by the literature. For example, populations adapted to lower energy-yielding electron acceptors have a lower intrinsic population growth rate (Schink, 1997). This is initially represented in the model by different λ_{max} values for the aerobic population, anaerobic populations using glucose as substrate, other acetogens, and methanogens (0.6, -0.4, 0.3, and 0.25, respectively). Biomass yield per substrate consumed is also expected to be lower (Tchobanoglous and Burton, 1991), particularly for anaerobic populations (Thauer et al, 1989) (cell yields of 0.6, 0.05, 0.04, and 0.03, respectively, as above). Initial biomass model values for later stage populations (acetogens and methanogens) are also lowered from 10^5 to 10^4 kilograms (assuming that acetogenic and methanogenic conditions are not well developed until the waste is landfilled). This results in the output of Figure 4, which shows a better sequencing of gas production over time with delayed CO_2 methanogenesis, yielding a better methane to carbon dioxide ending ratio but allowing abnormally large hydrogen buildup. This hydrogen peak distorts the amplitude of carbon dioxide as well as the initial development of methane on a graph of gas mole fraction, compared to the reference behavior of Figure 1. Further experimentation with the λ_{max} values of individual populations could not yield improved results, and any such specific differentiation of intrinsic growth rates is not well supported in the literature. It was found that λ_{max} values affect the trajectories or slopes of the associated gas product curves (and, thus, the relative phasing of gas peaks) but cannot significantly alter the amplitude proportions.

Figure 4. Simulation output as in Figure 3 with differentiated λ_{max} and cell yield values for aerobic, anaerobic glucose degraders, acetogens, and methanogens.



In order to achieve correct gas volume proportions (particularly CO₂ vs. H₂), a mechanism (or mechanisms) must be inserted (or given competitive advantage) in the model which either inhibit hydrogen formation or enhance carbon dioxide formation during initial anaerobic phases. Arbitrarily experimenting with inhibiting specific populations in varying combinations yielded poor results. Selective inhibition of individual populations which allow production of hydrogen at some point in the degradation sequence simply allows other hydrogen producing pathways to compete better, resulting in very little change in the relative production of H₂ vs. CO₂ compared to the results of Figure 4. Only the aerobic pathway, the nitrate pathway, and the direct acetate pathway do not form hydrogen, and the direct acetate path does not form CO₂ until later in the methanogenic phase. Even inhibiting all hydrogen producing pathways, no combination of parameter values within the model produce sufficient CO₂ to give over 80% CO₂ gas fraction within the landfill at any time. The aerobic pathway appears to have potential but cannot significantly affect the CO₂ peak due to quick oxygen depletion. In fact, as shown later, in any simulation starting with 20% O₂, aerobic activity has almost no effect on the phasing and amplitude of percentage gas formation in the landfill. The nitrate pathway would equally have potential to produce a large CO₂ peak, but not without providing an unreasonably large pool of nitrate within the system. Repeated experimentation with model simulation reveals that, under the assumptions of this model, the reference mode behavior of Figure 1 can be achieved under very specific conditions: 1) all populations are initially only substrate limited, 2) a glucose depleting reaction exists that produces CO₂ as the only gas and continues to be limited only by substrate (no other nutrient limitation such as nitrate), and 3) other anaerobic pathways are environmentally inhibited during the time when hydrogen production would otherwise be at its peak. Although temperature, pH, and moisture conditions are possible inhibiting environmental factors, the coincidence of the required inhibition with the formation of hydrogen suggests an end-product inhibition in response to H₂ buildup, a concept well supported in the literature (Hoh and Cord-Ruwisch, 1996).

Figure 5 is model output, as in Figure 4, with the addition of an unlimited CO₂ producing pathway, simulated by providing a large initial nitrate pool for the nitrate population. In order to achieve a substantial early CO₂ peak, the model is further modified to add a hydrogen growth inhibition factor applied to all anaerobic populations except the nitrate population and CO₂ methanogens (Figure 6). The inhibition factor is a linear function of hydrogen concentration (no inhibition at zero hydrogen; 50% inhibition at 1 kg or more of hydrogen per cubic meter of landfill volume). Figure 6 is annotated to identify key events describing the state of the system at various times. These results now match the empirically observed gas production behavioral pattern of a landfill as represented by Tchobanoglous et al (1993) in Figure 1.

Figure 5. Simulation output as in Figure 4 with unlimited nitrate availability for the nitrate population.

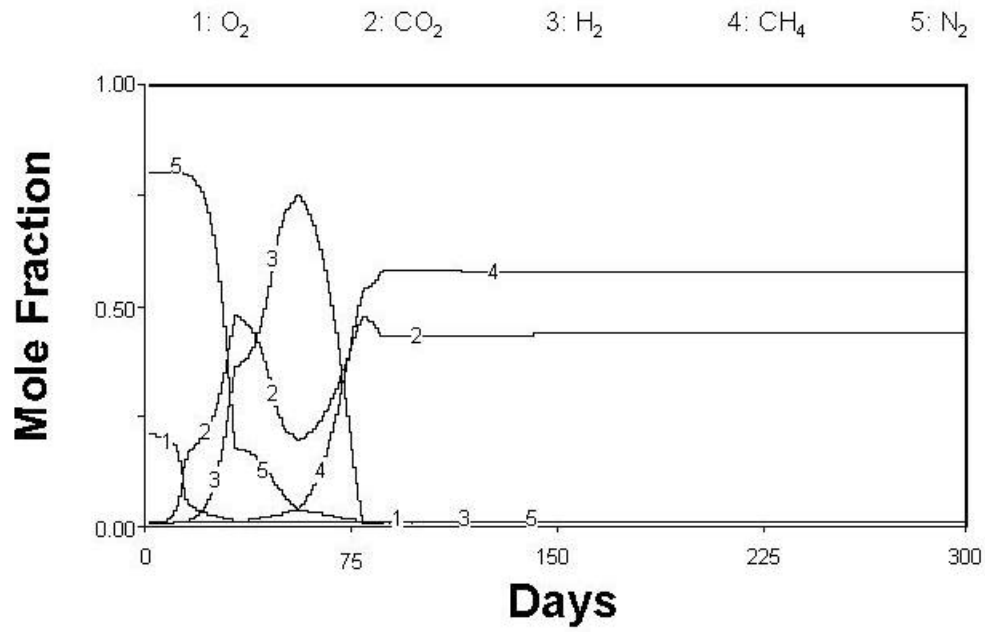
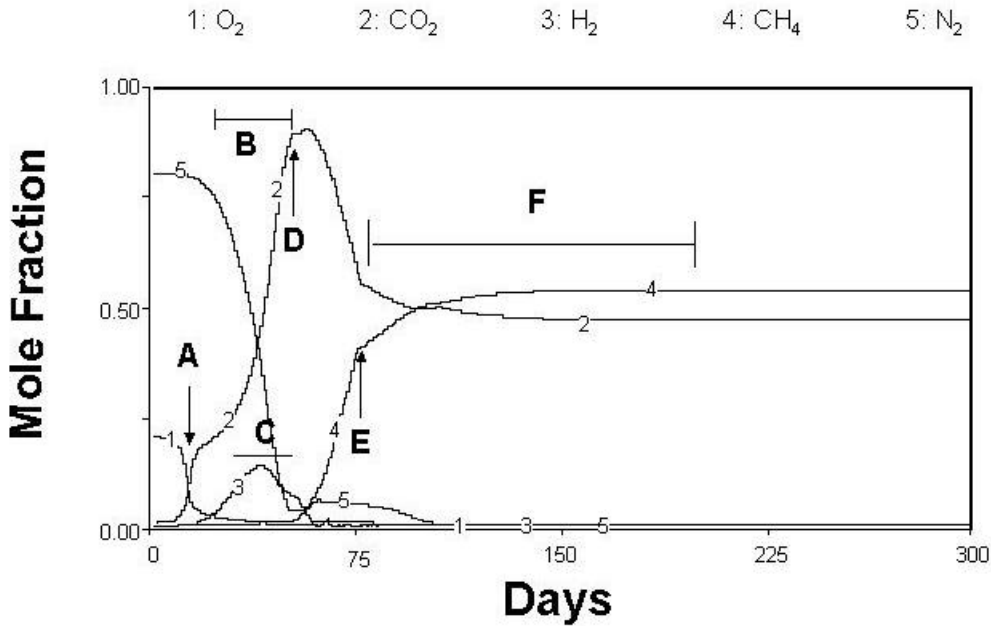


Figure 6. Simulation output as in Figure 5 with H₂ inhibition of the growth rate of all anaerobic populations except the nitrate population and CO₂ methanogens.

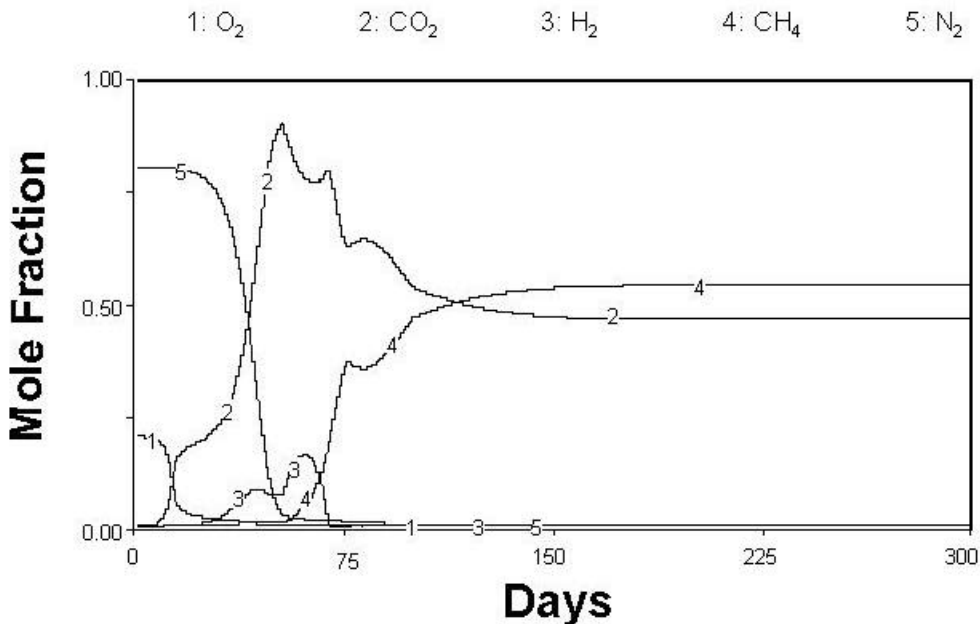


- A. Aerobic peak activity
- B. Anaerobic, glucose-depleting population dominance
- C. Hydrogen inhibition of anaerobic populations except nitrate and CO₂ methanogens
- D. Initial glucose wave depleted; glucose now limited by hydrolysis rate; all glucose-depleting populations declining; acetogen populations and CO₂ methanogens rapidly increasing
- E. CO₂ methanogen population hydrogen limited (low activity level); acetate methanogen population at maximum activity
- F. Long acetate tail; acetate methanogens producing both methane and carbon dioxide; CO₂ methanogens maintain low activity; all processes hydrolysis limited

Although the model produces a desired behavioral pattern, the behavior has not been achieved by proposing a simple model structure related to the pattern and matching that structure to known elements within the higher order structure of the system. Instead, a set of specific reactions has been selected from the hundreds that are available at a lower order, highly detailed level of the system. A set of reasonable parameter values and an inhibition feedback loop consistent with the literature, along with an additional “unknown” but plausible reaction, provide a simulation case with desired behavior. This does not instill confidence that the model structure sufficiently characterizes the real system to produce reasonable, expected behavior across a practical range of imposed conditions. Therefore, organizing criteria are sought to aggregate reactions into sets in order to simplify the model and search for a possible higher order structure which might be more clearly related to reference behavior (thus validating the model to a much greater extent).

A good model simplification would represent the system behavior well, would aggregate model components that do not contribute significantly to the behavior individually, and would better communicate the important aspects of the system relevant to management concerns. For example, should future exploration reveal that temperature, pH, moisture, etc., have similar effects on all anaerobic populations, then a single anaerobic pathway representing total glucose degradation (beyond the strong CO₂ producing pathway) could be used as a simplification which yields similar results. Figure 7 is model output as in Figure 6 with only the unlimited nitrate and mixed acid pathways representing glucose depletion along with subsequent acetogenesis and methanogenesis pathways relying on mixed acid products. This simplification gives a similar behavioral pattern with minor qualitative differences. The single mixed acid pathway more clearly distinguishes between initial glucose depleting and later acetogenesis phases with the dominant hydrogen peak appearing later, reflecting a shift in overall hydrogen production which is now more dominant during acetogenesis. This is a divergence from the reference mode of Figure 1 which could be significant depending on the question being asked and casts doubt on this simplification as an appropriate aggregation. The final ratio of methane to carbon dioxide, however, is not discernibly different.

Figure 7. Simulation output as in Figure 6 with only the nitrate and mixed acid pathways representing anaerobic glucose depletion (exploring potential model structure simplification).



A number of simulations of intermediate simplification were performed to test whether or not the simplification of Figure 7 was an extreme departure from the reference behavior, such that eliminating less pathways would sequentially draw closer to the behavior of the original model in Figure 6. Results were inconclusive, in that each simulation qualitatively and quantitatively departed from the reference mode in different ways depending on the number of pathways eliminated and the specific pathways chosen for system representation. Figures 8 and 9 are examples of simplifications employing 5 of the 9 original anaerobic glucose depleting pathways beyond the unlimited nitrate pathway as indicated.

Figure 8. Model structure simplification using an unlimited nitrate pathway and using only clostridial, butyrate, lactate, acetate, and mixed acid pathways to represent anaerobic glucose depletion.

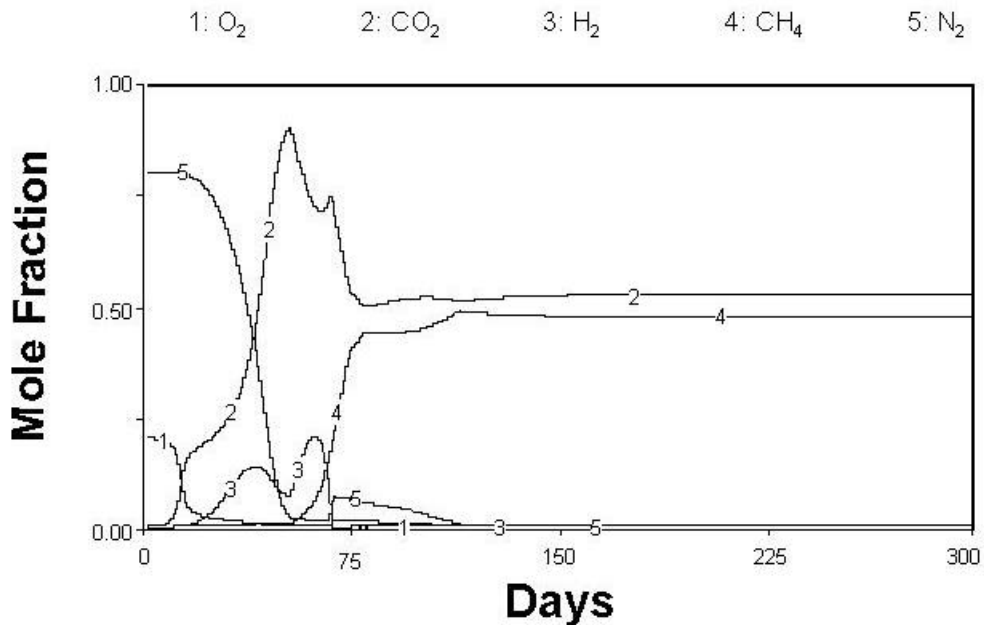
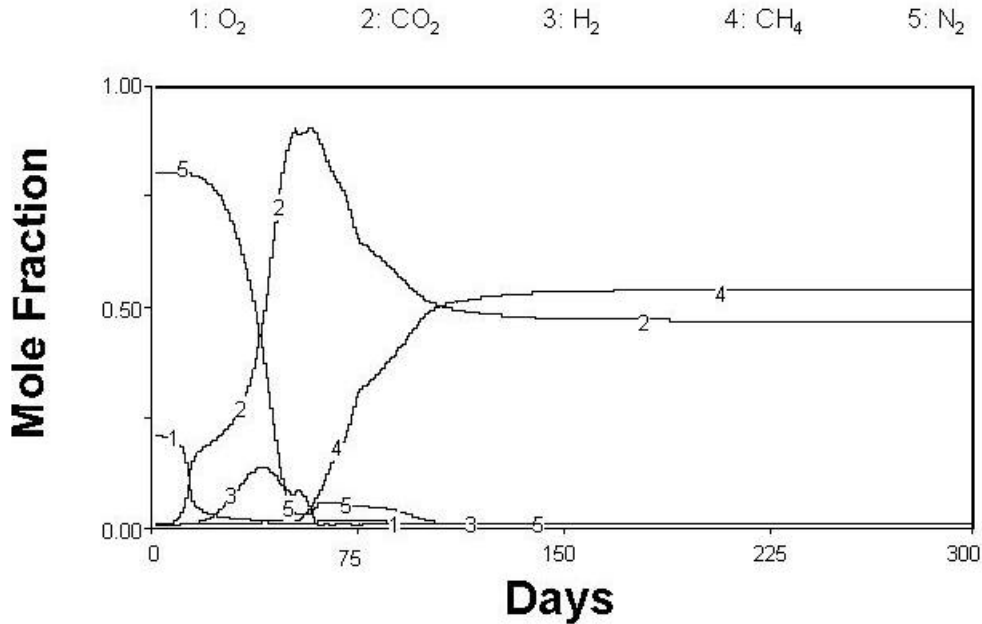


Figure 9. Model structure simplification using an unlimited nitrate pathway and using only clostridial, bifidum, lactate & ethanol, acetate, and mixed acid pathways to represent anaerobic glucose depletion.



Although Figure 9 compares very well to the original (unsimplified) model of Figure 6, the model appears quite sensitive to the precise combination of pathways used in the structure. There is very little confidence that the specific combination of Figure 9 would always behave like the original model in any realistic scenario which might be explored. Therefore, simplification of the model by elimination of selected pathways identified in the original model is considered inappropriate. In fact, it has already been demonstrated that *expansion* of the structure to include a strong unlimited CO₂ producing pathway is required. Thus, confidence in the model must rest on the fact that the structure is a mechanistic mass conservation model employing representative biochemical pathways known to exist in such environments, with key parameter values and feedback influences consistent with the literature. The single exception is the suggested existence of a strong unlimited pathway producing CO₂ from the initial hydrolysis product (glucose in the model).

This model, with its assumptions, now expresses a “dynamic hypothesis” within the system dynamics paradigm and might be used to explore questions about landfill management practices. However, given the method of development, the question remains open as to how much more the model behavior could be improved (more robustly reflect expected behavior) with additional structural detail. Since only a small (but representative) set of reactions were chosen to represent

the system, it is reasonable to assume that a much larger set of known reactions would refine model behavior and cause the model to be less sensitive to changing parameter values. However, the model is near the practical limits of size, and it is difficult to establish criteria for how much detail is enough. Moreover, there is no criteria to guide the modeler in a specific direction for adding detail. Therefore, from a system dynamics point of view, the next reasonable step would be to enter the implementation phase of the analysis by exploring management scenarios with the existing structure and looking for opportunities to test the model's structural boundary when specific additional system detail relevant to the management context becomes apparent.

Conclusions

Although a landfill is thought of as an engineered structure, its operating components are collections of complex natural microbial processes acting within a complex web of interactions and influences. It is therefore typical of complex natural environmental systems. These systems are often reduced to their basic detailed components for in-depth study, but interaction of these components within a systems context is poorly understood. Identifying higher order organization of these components into aggregate entities whose broader, more clearly envisioned interactions explain system behavior is difficult. In fact, such higher order organization may not exist. It may be that the breadth of intricate system detail may be the essential characteristic which keeps these systems in balance and resilient to normal fluctuations in environmental conditions.

This presents problems for the modeler in developing a simplified representation of the system relevant to specific objectives. The multitude of non-linear feedback loops which characterize natural systems lends itself to a system dynamics modeling view; but these systems do not appear well suited to the central features of the system dynamics approach. Smoothed, generalized observed behavioral patterns are often too complex to relate to simple model influence structure. Even if a structure could be derived, it likely cannot be related to the real system to identify the components of the structure. Therefore, the modeler must resort to a bottom-up approach rather than top-down, starting with what is known about detailed subcomponents. Rationale must be derived for selecting a practical set of detailed components which is sufficient to capture system behavior important to the modeler's purpose. The higher order (simpler, more elegant) system structure can then be sought by trying to identify aggregate groups of components which exert system influence in an aggregate way, but such attempts are rarely successful.

Modelers attempting to model natural environmental systems should be aware of these limitations and recognize the implications for building confidence in their model structure. Such models must be continually tested for validation in each application to ensure the model structure used is appropriate in the context of the model objective and initial conditions.

REFERENCES

- Conrad, R. 1999. Contribution of hydrogen to methane production and control of hydrogen concentrations in methanogenic soils and sediments. *FEMS Microbiology Ecology* 28:193-202.
- El Fadel, M., A.N. Findikakis, and J.O. Leckie. 1996. Numerical Modeling of Generation and Transport of Gas and Heat in Landfills I: Model Formulation. *Waste Management & Research* 14: 483-504.
- Gottschalk, G. 1986. *Bacterial Metabolism* (2nd ed). Springer-Verlag. New York.
- Hoh, C.Y. and R. Cord-Ruwisch. 1996. A Practical Kinetic Model that Considers Endproduct Inhibition in Anaerobic Digestion Processes by Including the Equilibrium Constant. *Biotechnology and Bioengineering* 51: 597-604.
- Legasto, A.A., J.W. Forrester, and J.M. Lynes (editors). 1980. *System Dynamics*. Vol 14 of *TIMS Studies in the Management Sciences*.
- Moorhead, D.L., R.L. Sinsabaugh, A.E. Linkins, J.F. Reynolds. 1996. Decomposition Processes: Modelling Approaches and Applications. *The Science of the Total Environment* 183: 137-149.
- Murphy, R.J. and T.J. Brennan. 1992. Aerobic Degradation of Municipal Solid Waste. 92-21.01. Proceedings of the 85th Annual Meeting and Exhibition of the Air & Waste Management Association, Kansas City, MO.
- Schink, B. 1997. Energetics of Syntrophic Cooperation in Methanogenic Degradation. *Microbiology and Molecular Biology Reviews* 61: 262-280.
- Shelley, Nixon, Bleckmann, Colborn, and Benter. 2001. A Dynamic Simulation of Landfill Waste Stabilization. Submitted to the *ASCE Journal of Environmental Engineering*.
- Stumm, W. and J.J. Morgan. 1996. *Aquatic Chemistry* 3rd Ed. John Wiley & Sons, Inc. New York.
- Tchobanoglous, G., H. Theisen, and S. Vigil. 1993. *Integrated Solid Waste Management*. McGraw-Hill. New York.
- Tchobanoglous, G. and F. L. Burton. 1991. *Wastewater Engineering: Treatment, Disposal, and Reuse*, 3rd Ed., McGraw-Hill, Inc. New York.
- Thauer, R.K., D. Moller-Zinkhan, A. M. Sporemann. 1989. Biochemistry of Acetate Catabolism in Anaerobic Chemotrophic Bacteria. In *Annual Review of Microbiology*. L.N. Ornston (Ed.) 43: 43-67.
- Voolapalli, R.K. and D.C. Stuckey. 1999. Relative Importance of Trophic Group Concentrations during Anaerobic Degradation of Volatile Fatty Acids. *Applied and Environmental Microbiology* 65: 5009-5016.