Numerical Modeling of Coupled Biochemical and Thermal Behavior of Municipal Solid Waste in Landfills

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ABSTRACT

A coupled bio-thermal (BT) model is proposed and validated for the prediction of long-term biochemical and thermal behavior of municipal solid waste (MSW) in landfills. The biochemical and thermal behavior of the waste was modeled using a two-stage anaerobic degradation model and diffusive heat transport model, respectively. A temperature function that accounts for the inhibitory effect of non-optimum temperatures on the microbial growth was proposed to simulate the coupled effects of biochemical and thermal behavior of waste in landfills. Six numerical simulation cases representing conventional and bioreactor landfill conditions were performed on a typical full-scale landfill cell model to determine the spatial and temporal variation in the long-term biochemical and thermal characteristics of waste in landfills. The results from the numerical analyses show that incorporating the effect of temperature of waste in the modeling of biodegradation of waste in landfills plays a significant role in realistically predicting the long-term biochemical and thermal regime in MSW landfills. The proposed BT model captures the key trends in the landfill gas (LFG) production and waste temperatures typically observed in actual full-scale landfills. Elevated waste temperatures were predicted especially in the bioreactor landfill cases suggesting that rapid decomposition of waste induces high heat generation rates; however, the elevated temperatures were short-lived.

Keywords: Biochemical processes; Bioreactor landfill; Coupled processes; Elevated temperatures; Heat generation; Landfill gas

1. INTRODUCTION

Municipal solid waste (MSW) in landfills, be it the conventional engineered landfills or the recently burgeoning bioreactor landfills, undergoes complex coupled interactions of various processes that mainly includes hydraulic (e.g. fluid flow, gas flow), mechanical (e.g. compression/settlement, shear), biochemical (e.g. biodegradation, leachate and gas production) and thermal (e.g. heat generation, heat transport) phenomena. In order to be able to reliably predict the long-term performance of MSW landfills, it is crucial to understand and interpret these major fundamental processes and their coupled interactions in a realistic sense. Of all the major phenomena, the biochemical behavior of waste in the landfills is what makes the prediction of waste behavior a unique and complex problem to solve.

In a conventional or a bioreactor landfill, prediction of the LFG production is an important aspect for the landfill owners/operators to help them design and install the gas extraction/collection systems, to evaluate the beneficial use of generated LFG for energy production, and also to control LFG emissions. Several researchers have proposed different biochemical models with varied complexity. In the 1980s, many models were developed based on simple first-order decay (FOD) kinetics to simulate the biodegradation and LFG generation in landfills. Vogt and Augenstein (1997) and El-Fadel et al. (1997) provide an excellent review of these simple models. Few studies have proposed models that essentially involve FOD kinetics but account for the variations in organic constituents that degrade at different rates by differentiating the organic content into readily, moderately, and slowly degradable components (e.g. IPCC 2006; Hettiarachchi et al. 2009). In recent years, some researchers proposed models that focus mainly on modeling the biochemical behavior of waste by rigorously considering the microbial dynamics with substrate depletion (e.g. Reichel and Haarstrick, 2008; Gawande et al. 2010). A few other researchers proposed complex coupled models that integrate the biochemical processes with other landfill processes (e.g. fluid flow, heat transport, mechanical compression) to simulate the coupled interactions within the waste on the biochemical reaction kinetics. These complex coupled models (e.g. McDougall 2007; De Cortázar et al. 2007; Gonzalorena et al. 2011; White and Beaven, 2013; Kowalsky et al. 2014; Hubert et al. 2016; Reddy et al. 2018a; Lu et al. 2019; Chen et al. 2020) include the transport of the various chemical constituents of the leachate and biogas within the pore space, settlement induced from conversion of degradable solids to gaseous compounds, and the contemporaneous changes in phase composition and waste properties that influence fluid flow and mechanical behavior. A good review of the some of these biochemical models is presented in Lamborn (2010) and Reddy et al. (2017a). Despite these developments in modeling the biochemical behavior of waste, there are a few important limitations associated with these models.

First, the empirical biodegradation models used in some of these coupled models are in most cases FOD models that lump all the complex kinetics of waste decomposition into a single parameter. These simplified empirical models are most suitable in cases where the waste composition is relatively homogeneous with more availability of readily degradable organics, and in cases where waste degrades under optimum environmental conditions. However, the actual waste decomposition behavior and LFG generation rates in landfills vary considerably based on site-specific factors (e.g. waste placement conditions, ambient temperature, precipitation) and involve complex interactions of different biochemical reactions influencing one another, which are not considered in the simple empirical models. Moreover, the model parameters used in the empirical models sometimes do not bear any physical significance other than to provide a better fit.

On the other hand, the complex multi-component biochemical models consider different physico-chemical and biological processes and their coupled interactions in the waste behavior, but naturally end up requiring numerous parameters to fully define the model. Most of the model parameters in such multi-component biochemical models are not generally recorded at landfills (e.g. determining molecular-level waste composition such as carbohydrate, protein, and lipid content, microbiological growth and death parameters for different microbial species considered in the model) and determining them on a regular basis would be practically not feasible. Due to these factors and also due to the lack of expertise on the use and interpretation of the complexity of the model by the end user, the general use and applicability of such highly parameter intensive models for predicting the LFG production and other long-term performance aspects of the MSW landfills has been limited.

With regard to modeling the thermal behavior of MSW landfills, many studies have proposed one-dimensional (1D) as well as multi-dimensional (i.e. 2D and 3D) models for the prediction of temperature within the waste in MSW landfills (e.g. El-Fadel et al. 1996; Yoshida et al. 1997, 1999; Houi et al. 1997; Lefebvre et al. 2000; Neusinger et al. 2005; Gholamifard et al. 2008; Garg and Achari 2010; Gawande et al. 2010; Hanson et al. 2013; Kutsyi 2015; Zambra and Moraga 2013; Kowalsky et al. 2014; Hubert et al. 2016; Hao et al. 2017). Few of these models (e.g. El-Fadel et al. 1996; Gholamifard et al. 2008; Hanson et al. 2013; Zambra and Moraga 2013; Hao et al. 2017) incorporate heat generation from biological waste decomposition to different degree while simultaneously accounting for the effect of temperature on the biodegradation and heat generation within the waste using different functions. As per the author's knowledge, White and Beaven (2013), Kowalsky et al. 2014, and Hubert et al. (2016) are the only studies that incorporated a thermal model in their respective thermo-hydro-bio-mechanical (THBM) models developed for modeling of all the major landfill processes. But Hubert et al. (2016) did not incorporate the effects of temperature on the biodegradation of waste in their THBM model. Likewise, White and Beaven (2013) in their LDAT model incorporated the effects of temperature on biodegradation and vice-versa, but the researchers did not discuss the significance of temperature on waste degradation nor did they present the possible thermal regime in MSW landfills using their model.

The authors in their previous studies developed a coupled hydro-bio-mechanical (CHBM) model to predict the long-term coupled hydro-bio-mechanical behavior of the waste and its influence on the performance of MSW landfills (Reddy et al. 2017b; Reddy et al. 2018a-c). The validation of the CHBM model was also performed (Reddy et al. 2018a). However, the biodegradation of waste in the CHBM model was modeled based on the LandGEM model (USEPA, 2005) which is a simplified FOD model developed by the United States Environmental Protection Agency (USEPA). The authors used the LandGEM model and incorporated the effect of moisture content of the waste onto the rate of waste decomposition. Since temperature of waste in a landfill plays a significant role in influencing the biodegradation of waste, recently the authors advanced their existing CHBM model by integrating it with a validated thermal model to incorporate the effect of waste temperatures in addition to the effect of moisture onto the biodegradation of waste and called it the CTHBM model (Kumar et al. 2018, 2020a). Though the approach adopted by the authors to model biodegradation of waste is better than assuming a single constant value for the decay rate parameter (which is the case in the original LandGEM model by USEPA), it still is based on simplification of the complex biochemical reaction kinetics within the waste that undermines the accurate and realistic simulation of the anaerobic decomposition of waste in landfills. For a practically reliable and realistic predictions about the biochemical characteristics of the waste in landfills (e.g. leachate chemistry, gas production rates and gas volumes), it is important that the complexity of the biochemical behavior is considered in the predictive model while maintaining fewer model parameters that aids in its practical use.

Incorporating the aforementioned limitations of the previous modeling efforts by the authors and other researchers, this study presents a bio-thermal (BT) model developed for realistic prediction of biochemical (e.g. waste degradation, gas production) and thermal behavior (e.g. heat generation, temperature distribution) of waste in landfills. The proposed BT model now replaces the old biodegradation model (based on the USEPA's LandGEM model) that was used in the old version of the CTHBM model developed by the first two authors (see Kumar et al. 2018, 2020a). The CTHBM model is implemented in Fast Lagrangian Analysis of Continua (FLAC), a finite-difference code with an explicit time marching solution approach (ICGI 2019). The focus of this study is to describe only the biodegradation and the thermal model that is embedded into the new version of the CTHBM model and any numerical analysis performed in this study does not incorporate the mechanical effects on the biochemical and thermal behavior of the waste. The mechanical model embedded into the new CTHBM model is presented in Kumar et al. (2020b) and the full description of the CTHBM model is presented in Kumar and Reddy (2020). The spatial and temporal changes in the moisture content of waste which is required as an input for the BT model is derived from the hydraulic model implemented in CTHBM model. For brevity, the description of the hydraulic model with the governing equations is not included in this study but can be found in Reddy et al. (2018a). The proposed BT model is validated using experimental data from six long-term laboratory experiments performed on waste samples from different landfills in the US and UK. Finally, the BT model is applied on a typical full-scale landfill cell geometry to predict the long-term spatial and temporal variations in biochemical and thermal behavior of waste in MSW landfills under both conventional and bioreactor landfill conditions. The implications of incorporating temperature effects on biodegradation of waste determined based on the numerical analyses performed are highlighted.

2. BIO-THERMAL MODEL

2.1. Biodegradation Model

2.1.1 Empirical Biodegradation Model

In the authors' previous work on modeling biodegradation of MSW in landfills, an empirical approach based on FOD kinetics was adopted. A brief description of the empirical model is presented here. Detailed description about the empirical model including the description on how temperature effects were incorporated and modeled is presented in Reddy et al. (2018a) and Kumar et al. (2018).

The empirical biodegradation model quantified the rate of methane (CH_4) gas produced based on the LandGEM model developed by USEPA as shown in Equation 1.

$$q(t)_{CH_4} = kL_oMe^{-kt} \tag{1}$$

where k is the decay rate constant (yr^{-1}), L_o is the biochemical methane potential (BMP) of the waste (m^3/kg), and M is the mass of MSW (kg). Since, the moisture content and the temperature of waste are among the two most influential factors that affect the rate of waste decomposition, the decay rate constant was formulated as a function of the degree of saturation of the waste and the temperature of the waste as shown in Equation 2.

$$k(S_w, T) = \frac{T(mf_w + n)}{C_N\left[1 + exp\left(\frac{T}{4} - 18\right)\right]} \quad (2)$$

where $f_w = (S_w - S_r)/(1 - S_r)$ is the water content factor, S_w is the degree of saturation of the waste, S_r is the residual degree of saturation, T is the temperature of the waste, m and n are linear constants based on the lower and upper bounds of k which were assumed to be 0.05 and 0.3, respectively based on USEPA (2005), and C_N is a normalization constant equal to 57.3 which was used to ensure that the peak degradation rate occurred at 60 °C based on Young (1989).

2.1.2 Proposed Biodegradation Model

The biodegradation model proposed in this study is based on the two-stage anaerobic digestion model developed by McDougall (2007) but with some variations. The original model by McDougall (2007) describes a two-stage anaerobic degradation process in which the volatile fatty acids (VFA) represented by acetic acid, the methanogenic biomass (MB), and the solid degradable fraction (SDF) are the primary variables. The solids in the waste are divided into degradable and inert fractions. The degradable fraction of the solids is assumed to be composed entirely of cellulose as it is reported to account for most of the CH_4 generation potential of MSW (Barlaz et al. 1989). The depletion of cellulose is controlled by the VFA and MB concentrations, the moisture content in the waste. The first stage of anaerobic digestion is associated with hydrolysis of cellulose to glucose. Assuming that the fermentation of glucose involving acidogenesis/ acetogenesis is instantaneous, the second stage of anaerobic degradation is methanogenesis which involves the consumption of the VFA by MB to produce CH_4 and carbon dioxide (CO_2). It should be noted that the biodegradation model proposed by McDougall (2007) also simulates the advective and diffusive transport of the VFA and MB through the MSW pore spaces via fluid phase which is not simulated in this study. It is reasonable to assume that the fluid velocity in the pore spaces and the diffusion coefficient of the chemical species in the fluid are generally low enough, especially in cases where the hydraulic conductivity of the waste is low, that they do not affect the spatial distribution of the VFA and MB across the landfill considerably. However, higher hydraulic conductivity of waste which may induce higher fluid velocities can necessitate the inclusion of advective and diffusive transport as well. In any case, the spatial variation in the VFA and MB concentrations induced by the biochemical reactions is much more significant than the contribution of the advective and diffusive transport of those chemical species.

The overall stoichiometry of the degradation of cellulose to CH_4 and CO_2 considered in the biodegradation model proposed by McDougall (2007) is shown in Equation 3 below.

$$C_6H_{10}O_5 + H_2O \rightarrow CH_3COOH + 8H_2 + 4CO_2 \rightarrow 3CO_2 + 3CH_4 \quad (3)$$

The rate of hydrolysis of cellulose and its rapid transformation into VFA accounts for the influence of the changing digestibility of the solid degradable fraction, the inhibitory effects of high acid concentrations, and the availability of moisture and is given by Equation 4 below.

$$r_g = b\theta_e \left[1 - \left[\frac{S_0 - S}{S_0}\right]^n\right] exp(-k_{VFA} * c) \quad (4)$$

where, r_g is the rate of formation of VFA ($g_{[VFA]}$ $m^{-3}_{[aqueous]}$ day^{-1}), b is the maximum VFA growth rate ($g_{[VFA]}$ $m^{-3}_{[aqueous]}$ day^{-1}), $\theta_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ is the effective volumetric moisture content, θ is the volumetric moisture content, θ_s is the saturated volumetric moisture content, θ_r is the residual volumetric moisture content, S_0 is the initial solid degradable fraction (SDF) defined as the ratio of the initial mass of degradable solids per unit total volume of waste ($g_{[cellulose]}$ m^{-3}), S is the solid degradable fraction at any instant of time, n is the structural transformation parameter, k_{VFA} is the production inhibition rate constant ($m^{-3}_{[aqueous]}$ $g^{-1}_{[VFA]}$), c is the concentration of VFA in aqueous phase ($g_{[VFA]}$ $m^{-3}_{[aqueous]}$).

The MB production/growth rate (r_j) is calculated based on Monod kinetics using Equation 5 shown below.

$$r_j = \frac{k_0 c}{(k_{MC} + c)} m \tag{5}$$

where, k_0 is the specific growth rate (day^{-1}), m is the concentration of MB in aqueous phase ($g_{[MB]}$ $m^{-3}_{[aqueous]}$), k_{MC} is the half-saturation constant ($g_{[VFA]}$ $m^{-3}_{[aqueous]}$).

The VFA consumption rate r_h is directly linked to the MB growth rate through a substrate yield coefficient Y as shown in Equation 6 below. Further, the MB decay/death rate (r_k) is given by Equation 7.

$$r_h = \frac{r_j}{Y} \tag{6}$$

$$r_k = k_2 m \quad (7)$$

where, k_2 is the MB decay rate constant (day^{-1}).

Given the reaction rates for hydrolysis/acidogenesis and the methanogenesis including the formation and depletion rates of VFA and MB, the accumulation of VFA and MB over time (t) can be expressed by the ordinary differential equations shown in Equation 8 and 9, respectively.

$$\frac{\partial c}{\partial t} = \left[r_g - r_h\right] \quad (8)$$

$$\frac{\partial m}{\partial t} = \left[r_j - r_k\right] \quad (9)$$

The SDF is depleted as per the rate of hydrolysis reaction (Equation 4) and is given by Equation 10 as follows.

$$\frac{dS}{dt} = -\theta \frac{162}{60} r_g \quad (10)$$

The stoichiometric coefficient of 162/60 used in Equation 10 is obtained from the chemical equation (Equation 3), which indicates 60 g of acetic acid is a result of the hydrolysis of 162 g of cellulose. The stoichiometry of the hydrolysis step also shows that 162 g of cellulose consumes 18 g of water; hence the mass of water in the system is also decreased according to Equation 11 as follows.

$$dM_{H_2O} = \frac{18}{162} dM_{Cellulose} \tag{11}$$

where, M_{H_2O} is the mass of water, $M_{Cellulose}$ is the mass of degradable solids (i.e. cellulose).

Since both volumetric moisture content and the solid degradable fraction is reported per unit total volume of the waste, Equation 11 can be divided throughout by the total volume to determine the reduction in moisture content of the waste as follows.

$$d\theta = \frac{18}{162 \cdot \rho_{H_2O}} dS \tag{12}$$

where, ρ_{H_2O} is the density of water (1000 kg m^{-3}).

As mentioned earlier, the rate of VFA formation is same as the rate of hydrolysis assuming an instantaneous transformation of cellulose to acetic acid through fermentation. Similarly, it follows that the CH_4 is generated at the rate with which VFA is consumed by the microbial biomass with appropriate stoichiometry (i.e. one mole of cellulose produces 3 moles of CH_4 and 3 moles of CO_2) as shown in Equation 3 and the cumulative CH_4 produced is estimated.

Heat is one of the primary by-products of the waste decomposition process since the net enthalpy of the reactions involved in anaerobic decomposition of waste is exothermic. Although, the amount of heat released from anaerobic waste decomposition is substantially lower than the aerobic waste decomposition (El-Fadel et al. 1996b), the accumulation of the generated heat in the long-term can significantly increase the waste temperatures within the landfill. However, one of the limitations of the biochemical model proposed by McDougall (2007) is that it does not model the heat generation from waste decomposition nor does the model incorporate the effects of temperatures of waste on the waste decomposition. In order to address this very limitation, the following sections describe the thermal model incorporated into the BT model and how the temperature effect on waste degradation is modeled.

2.2. Thermal Model

The heat transport in the landfill mainly takes place by the means of heat conduction through waste constituents and convective heat transport from the liquid and gas flow through the pore spaces within the waste. It is reported that conduction is a major mechanism of heat transport in the landfills and that the fluid velocities within the waste are considerably low to affect the resulting temperature distribution (Yesiller et al. 2005). In cases where the fluid velocities are high enough to induce significant changes in the transient temperature distribution within the landfill, the convective heat transport can be easily incorporated into the thermal model proposed in this study. In this study, the heat transport in the BT model is described by the transient heat conduction equation (Equation 13) derived from the law of balance of energy (heat) and the Fourier's law of heat transport. The detailed description of the numerical implementation of heat conduction equation in FLAC is presented in ICGI (2019).

$$k_T \frac{\partial^2 T}{\partial {x_i}^2} + \dot{q} = C_T \frac{\partial T}{\partial t} \tag{13}$$

where, k_T is the coefficient of thermal conductivity (W/m-K), $\dot{q}$ is the rate of heat generation per unit volume (W m^{-3}), C_T is the volumetric heat capacity (J m^{-3} K^{-1}), T is the temperature (°C), x_i (i=1, 2) is distance in the two spatial dimensions.

To realistically simulate and predict the spatial and temporal distributions of temperature within the landfills, the seasonal temperature variations at the ground surface was incorporated and represented by a sinusoidal temperature function given by Equation 14.

$$T(t) = T_m - A_s \cos\left[\frac{2\pi}{365s}(t - t_0)\right] \quad (14)$$

where, $T(t)$ is the surface temperature at any time t, T_m is the mean temperature (°C), A_s is the amplitude of the ground surface temperature wave (°C), s is equal to one day expressed in seconds (86,400), t_0 is a phase constant.

2.2.1 Empirical Heat Generation Rate

In the authors' previous work on modeling thermal behavior of landfills, heat generation rate functions developed empirically from the field investigations of temperature data at different landfills by Hanson et al. (2013) were used in the thermal model. The heat generation rate functions accounted for the normal landfill operations (i.e. placement rate, placement moisture and placement waste density) and were based on the net heat gain from the waste decomposition in the landfills investigated. A heat generation rate function of the form of an exponential growth-decay curve was formulated by Hanson et al. (2013) to simulate the heat generation from biodegradation in landfills and is shown in Equation 15.

$$H = A\left[\frac{Bt}{B^2 + 2Bt + t^2}\right] e^{-\sqrt{\frac{t}{D}}} \quad (15)$$

where H is the heat generation rate (W/m^3), A is the peak heat generation factor (W/m^3), B is the shape factor (days), D is the decay rate factor (days), and t is the time (days).

The exponential growth and decay heat generation rate function (i.e. Equation 15) was scaled for temperature dependence to account for the sensitivity of the microbial activity to temperatures. In this regard, the peak heat generation, determined from Equation 15, was used when the waste temperatures were in the range of 30 to 50 °C. For waste temperatures between 50 °C and 80 °C and between 30 °C and 0 °C, the heat generation in the waste was scaled (i.e., ramped) from the peak heat generation value to zero. For waste temperatures below 0 °C and above 80 °C, zero heat generation was prescribed. A detailed explanation on the development of temperature dependent heat generation function is presented in Hanson et al. (2013) and the application of these heat generation functions to model thermal behavior of waste in the authors' previous modeling work is presented in Kumar et al. (2018, 2020a). Since, the heat generation rate functions were based on site-specific temperature data, the general applicability of the heat generation functions may be limited. Addressing this limitation, heat generation rates derived from the CH_4 gas generation rate as described below.

2.2.2 Biochemical Based Heat Generation Rate

In the BT model proposed in this study, the heat generation rate is determined based on the rate of CH_4 gas generation derived from the substrate (i.e. cellulose) depletion and the net enthalpy of the chemical reaction (Equation 3) as follows.

$$\dot{q} = R_{CH_4} H_C \tag{16}$$

where, H_C is the heat released from anaerobic decomposition of 1 kg of cellulose (i.e. to produce 3 moles of CH_4) which is equal to 1672 J $kg^{-1}{}_{[cellulose]}$ (Hao et al. 2017), and R_{CH_4} is the rate of CH_4 production per unit total volume determined from the biodegradation model. So, unlike the empirical heat generation rate functions that were derived from field temperature data, the heat generation rate in case of the proposed BT model is estimated based on the simultaneous progress in the biodegradation of waste. In order to truly simulate the coupled effects of thermal processes on biodegradation, a temperature feedback mechanism was formulated to simulate the effects of waste temperatures on the ensuing biochemical reaction kinetics as described below.

2.3. Temperature Feedback on Biodegradation

It is well-known that the microbial activity is susceptible to temperature changes and temperatures other than the optimum values could inhibit the microbial growth thereby influencing the decomposition of waste, heat production, and LFG production (Barlaz et al. 1989; El-Fadel 1999). In order to account for the effect of temperature on the microbial growth, a temperature function (f_T) was developed and used as a factor that influences the specific growth rate (k_0) of the microbes as shown in Equation 17.

$$k_0 = k_{0,max} * f_T \tag{17}$$

where, $k_{0,max}$ is the maximum specific growth rate of the microbes.

A few studies previously investigated the inhibitory effect of non-optimal temperatures on the biodegradation of waste in landfills. Young (1989) studied the numerical modeling of biodegradation of waste in landfills and proposed a temperature function given by Equation 18 to account for the effect of temperature on microbial growth. Likewise, Hao et al. (2017) and Hao (2019) also proposed temperature functions, given by Equation 19 and 20 respectively, to account for the effect of temperature on LFG production.

$$f_T = \frac{(e^{-aT} - e^{-bT})}{(1 + e^{-c(T-d)})} \tag{18}$$

$$f_T = 4\frac{T^6}{(K_T^6 + T^6)}\frac{K_T^7}{(K_T^7 + T^7)} \tag{19}$$

$$f_T = \begin{cases} 1 & T < 37\ ^{\circ}\mathrm{C} \\ \dfrac{1}{\left\{e^{\left[-\left(\frac{36.4-47.5}{5.7}\right)^2\right]}+1\right\}}\left\{e^{\left[-\left(\frac{T-47.5}{5.7}\right)^2\right]} + e^{\left[-\left(\frac{T-36.4}{5.62}\right)^2\right]}\right\} & 37\ ^{\circ}\mathrm{C} \le T \le 47.5\ ^{\circ}\mathrm{C} \\ e^{\left[-\left(\frac{T-47.5}{12}\right)^2\right]} & T > 47.5\ ^{\circ}\mathrm{C} \end{cases} \tag{20}$$

where, a, b, c, d are curve fitting parameters equal to -0.08, -0.05, -0.45, 40 respectively, and K_T is a constant equal to 37 °C.

Further, the temperature function proposed by Hao (2019) assumed a maximum CH_4 yield potential of waste for all temperatures between 0 and 37 °C which is unlikely to happen due to the fact that methanogenesis is inhibited at temperatures lower than the optimum temperatures (i.e. less than 37 °C). Moreover, it is also reported in the literature that both mesophilic and thermophilic bacteria which have different optimum temperature ranges exist in MSW, and depending upon the waste temperatures, the mesophilic or thermophilic bacteria are active in anaerobic decomposition of waste (Pohland and Bloodgood 1963; Pfeffer 1974; Chen and Hashimoto 1978). Based on these observations from the literature and from the fitting of the reported experimental data of CH_4 yield for waste samples from actual landfills tested at different temperatures, a temperature function (f_T) as shown in Equation 21 is proposed in this study to realistically simulate the temperature effects on biodegradation of MSW in landfills.

$$f_T = \begin{cases} 4\dfrac{T^4}{(K_{TM}^4+T^4)}\dfrac{K_{TM}^4}{(K_{TM}^4+T^4)} & 0 \le T < 37\ ℃ \\[2ex] \dfrac{1}{\left\{e^{\left[-\left(\frac{K_{TM}-K_{TT}}{5.7}\right)^2\right]}+1\right\}}\left\{e^{\left[-\left(\frac{T-K_{TM}}{5.7}\right)^2\right]}+e^{\left[-\left(\frac{T-K_{TT}}{5.7}\right)^2\right]}\right\} & 37\ ℃ \le T \le 47.5\ ℃ \\[2ex] 4\dfrac{T^8}{(K_{TT}^8+T^8)}\dfrac{K_{TT}^8}{(K_{TT}^8+T^8)} & T > 47.5\ ℃ \end{cases} \quad (21)$$

where, K_{TM} and K_{TT} are constants equal to 37 °C and 47.5 °C, respectively.

Fig. 1 shows the graphical representation of the temperature functions proposed by different researchers and the present study. Now that the temperatures affect the growth rate of the microbes, the MB concentrations are influenced by temperature of the waste. As a result, all the other parameters which are directly or indirectly related to the MB concentrations, including the heat and gas production will also be affected. This way the temperature function acts as a link between the biochemical and the thermal model simulating the interdependency between the biochemical and thermal behavior of the waste.

3. VALIDATION OF THE BIO-THERMAL MODEL

3.1 Laboratory Experiments for Validation

The proposed BT model is validated with data obtained from six long-term laboratory experiments reported in two different studies (Ivanova et al. 2008 and Fei and Zekkos, 2018). Ivanova et al. (2008) reported the data on well-controlled laboratory experiments performed using two large-scale consolidating anaerobic reactors (CARs) on fresh MSW obtained from a landfill facility in Dorset, UK. The two CAR experiments differed in the amount of constant vertical pressure applied on the top of the waste sample during the entire course of the experiment (CAR1: 150 kPa and CAR2: 50 kPa) to simulate representative overburden stresses experienced in landfills. The two CAR experiments were run for a total of 919 days over the course of which the data on leachate chemistry, gas production, waste settlement was recorded. Detailed description about the CAR experiments and the recorded data is presented in Ivanova et al. (2008).

Fei and Zekkos (2018) reported data from a large-scale laboratory experiments performed using a 42-liter cylindrical column with a well-characterized MSW from four different landfills in four different states (i.e. Michigan, Texas, Arizona, and California) in the US. The four different waste samples used in the experiments represented different waste compositions and the authors also investigated its influence on the long-term biochemical and mechanical behavior of the waste. The experiments on the four different waste samples were run for different durations (MI – 1,100 days, TX – 1,500, AZ – 885, and CA – 850 days) and the data on leachate chemistry, gas evolution, and waste settlement was recorded during the course of the experiments. It should be noted that, unlike the CAR experiments, the experiments conducted by

Fei and Zekkos (2018) did not apply any external vertical pressure on the top of waste samples. This was done in order to determine the sole effect of biodegradation on hydro-bio-mechanical processes in the waste samples. Detailed description of the experimental investigation and the data recorded during the experiments is presented in Fei and Zekkos (2018). For convenience, the experimental data from the two CAR experiments will be referred to as CAR1 and CAR2. Likewise, the data for the experiments performed on waste samples from Michigan, Texas, Arizona, and California landfills will be referred to as MI, TX, AZ and CA, respectively.

3.2 Validation Modeling Methodology

Six simplified models with the same size (i.e. depth and diameter) as that of the waste samples used in the six experiments (i.e. CAR1, CAR2, MI, TX, AZ, CA) were modeled in FLAC. The proposed BT model was applied to the FLAC model in the six experimental cases with appropriate initial and boundary conditions. The initial values of the physical and biochemical properties of the waste samples used in the experiments and the values of the modeling parameters used to simulate the long-term biochemical behavior of the waste samples are presented in Table 1. The typical ranges of the values of the model parameters reported in McDougall (2007) was used while determining the model parameters for the six validation cases. Previous modeling studies (e.g. McDougall 2008; Datta et al. 2018) that used the two-stage anaerobic degradation model proposed by McDougall (2007) were also referred to while determining the model parameters. However, some changes had to be made in those parameters to obtain a better fit with the experimental data. It should be noted that all the six experiments were conducted by the corresponding researchers by maintaining a constant temperature (32 – 40 °C) close to the ideal temperatures required for biodegradation in the waste system for the entire duration of the experiments. However, the changes in temperature of the waste during the experiments were not monitored. Due to the lack of adequate data on waste temperature, the thermal model in the BT model could not be validated. The thermal model will be validated in the future developments of the BT model as appropriate experimental or field dataset with adequate input dataset becomes available. In the six experiments considered, the heat generated from the waste samples during the experiments was not substantial enough to change the temperature of the waste. Therefore, the thermal aspects of the experiments (e.g. heat generated and temperatures within the waste sample) are not discussed in this study. The FLAC numerical model simulations of the six experiments were run for the respective duration of the experiments reported earlier. The results obtained from the model are compared with the biochemical data during the experiments and are discussed in the following section.

3.3 Validation Results

Fig. 2a shows the comparison of the model predictions for the depletion of the SDF over time with the experimental data for the six experiments. The initial values of the SDF used in the model for the six experimental cases is presented in Table 1. The data with regard to the variation in the degradable solids was not available for CAR1 and CAR2. The data on the SDF for MI, TX, AZ and CA cases was not measured by Fei and Zekkos (2018) but estimated indirectly assuming that the consumption of degradable solids is proportional to the measured biogas (CH_4 + CO_2) considering the stoichiometry of the anaerobic decomposition process (Datta et al. 2018). For the four cases for which the SDF data is available (i.e. MI, TX, AZ and CA), except for the initial few days (5-20 days) where the concentration of the degradable solids varied due to recirculation of the leachate in those experiments, there is an excellent agreement in the model's predictions about the progress in the depletion of the degradable solids for the duration of the experiment.

Fig. 2b shows the comparison of the predictions of the concentration of the VFA by the BT model with the VFA data from the six laboratory experiments. It should be noted that the model considers acetic acid as a representative acid for all the other VFA (e.g. butyric acid, propionic acid) that may be present in the system. The model shows good agreement with the experimental data in all the cases with an excellent fit with the VFA data for MI and AZ cases. It can be seen from the experimental data that the generation of acids, although being dependent on the degradability of the waste and the microbial activity, is a relatively vigorous process. So, the assumption of instantaneous conversion of the hydrolyzed degradable solids into VFA is valid. A peak VFA concentration of approximately 11,493 mg/L, 12,362 mg/L, 3,058 mg/L, 3,558 mg/L, 13,444 mg/L, 474 mg/L was predicted for CAR1, CAR2, MI, TX, AZ and CA cases by the model which are close to the measured peak VFA values of 11,658 mg/L, 12,602 mg/L, 3033 mg/L, 4,772 mg/L, 13,444 mg/L, 475 mg/L respectively. Clearly, the AZ waste sample had the highest peak VFA concentrations in its system due to the high initial degradable organic fraction in the waste sample. In all the cases, the VFA concentrations were negligibly small after approximately 200 days of the duration of the experiments.

Fig. 2c shows the variation of MB concentration in the waste samples over the duration of the experiments as predicted by the BT model. The data on methanogenic microbial populations was not recorded in the experiments so, the model provides potential trends in the variation of the MB concentrations in the waste samples as they degraded. It can be seen that the rapid growth in the MB concentrations occurs as the accumulation of the VFA reaches its peak. The MB would then consume the VFA for their growth but at a declining rate until all the VFA is consumed and MB concentrations reaches a peak value. With no further availability of VFA in the system, the microbial growth is ceased and the MB continues to deplete at the specified decay rate (k_2). The model predicted peak MB concentrations of approximately 6,857 mg/L, 6,074 mg/L, 24,643 mg/L, 19,521 mg/L, 32,750 mg/L, 13,714 mg/L after approximately 158 days, 130 days, 127 days, 178 days, 130 days, and 223 days of the experiment for CAR1, CAR2, MI, TX, AZ and CA cases, respectively. The trends in the variation of the MB concentrations for CAR1, CAR2, MI and AZ cases were slightly different from the trends of TX and CA cases in that the former cases involved more rapid growth and decay compared to the latter cases. In the proposed model, the MB growth rate is influenced by the temperature of the waste. Since, the temperature of the system in all the six experiments were maintained at near optimum temperatures, the specific growth rate of the MB (k_0) was maintained close to its maximum value.

Fig. 2d shows the comparison of the prediction of cumulative biogas (CH_4 + CO_2) produced for CAR1 and CAR2 cases and the cumulative CH_4 produced for MI, TX, AZ, and CA cases with the measured gas volumes in the respective experiments. Except for the CA case, the model underpredicted the cumulative biogas or the CH_4 gas produced in all the cases to varying degree. It should be noted that the model was able to closely and, in some cases, accurately capture the typical sigmoidal (S-shape) curve of the cumulative biogas production for waste. The cumulative biogas predicted by the model for the CAR1 and CAR2 cases were approximately 4,574 L and 4,568 L whereas the actual measured value for the cumulative biogas were approximately 8,450 L and 6,929 L, respectively. Likewise, the cumulative CH_4 gas predicted by the model for MI, TX, AZ and CA cases were approximately 536 L, 381 L, 649 L and 307 L whereas the actual measured value for the cumulative CH_4 gas were approximately 570 L, 477 L, 1,117 and 189 L, respectively. The closest agreement with the measured data for cumulative CH_4 gas produced was obtained for the MI case, and in other cases, the model underpredicted the cumulative LFG/CH_4 produced in the experiment. The difference in the predicted total LFG/CH_4 gas volume and the actual measured volume could be attributed to two main reasons. One of the reasons for this difference could be inappropriate waste characterization. The percentage of degradable cellulosic constituents derived from the experimental studies and used in the models may not be reflective of the true cellulosic content in the waste samples. The difference in the predicted and the measured values can also be partially attributed to the fact that there could be degradable constituents (e.g. hemicellulose, lignin) other than cellulose in those waste samples that contributed to the total CH_4 gas produced which was not accounted by the model. In the CA case, Datta et al. (2018) reported that the waste was mostly composed of soil and had the lowest percentage of degradable fraction in the waste sample among the four waste samples. It could be possible that the availability of the biodegradable matter for degradation was hindered by the high soil content and other inorganic materials (e.g. metals, plastic) in the waste resulting in lower biogas production. In general, the predictions of the model with regard to the SDF, VFA and biogas production were in good agreement with the experimental data.

4. APPLICATION OF BIO-THERMAL MODEL TO FULL-SCALE LANDFILL CELL

This section presents the application of the BT model to a typical full-scale landfill cell model to predict the long-term biochemical and thermal behavior of waste in landfills. In particular, the long-term spatial and temporal variations in biochemical characteristics (e.g. solid degradable fraction, volatile fatty acids concentrations, methanogenic biomass concentrations, CH_4 gas volume produced) and the thermal characteristics (e.g. temperature of waste) were examined. The predictions of the BT model will be compared with the predictions from a simplified empirical modeling approach previously developed by the authors to assess the relative advantages of the proposed model in predicting the biochemical and thermal behavior of MSW in landfills.

4.1. Model Geometry

A two-dimensional (2D) model of a full-scale landfill cell was selected for demonstrating the application of the proposed BT model presented in this study. The landfill cell model spanned a length of 125 m and had a maximum height of 106 m which included the final cover, the waste thickness and the subgrade. A schematic of the simulated landfill geometry is presented in Fig. 3. The model consists of a 75-m thick layer of subgrade soil extending below the bottom liner. This depth of subgrade was required in order to establish a far-field boundary condition for the thermal model which corresponded to the mean annual earth temperature. The bottom liner was 1 m thick silty clay soil. The bottom liner and the subgrade had identical material properties. The bottom liner is overlain by geosynthetics consisting of a HDPE geomembrane overlain by a nonwoven geotextile. The mechanical interaction between the waste and the geosynthetic interfaces in the liner system were not simulated as it is out of the scope of this study which is focused mainly on the biochemical and thermal aspects of the landfill. The liner system is comprised of a 5 m flat runout length at the crest of the slope, a 2 (H): 1 (V) side slope portion of length 33.5 m, and a 90 m wide base portion. The liner system was overlain by waste, which was assumed to be placed in ten 3-m thick layers, to reach a total waste height of 30 m. Finally, a 1-m thick soil layer of same soil properties as that of the compacted clay liner was placed overlying the waste to simulate the final cover. The final cover consists of a 3-m long flat portion at the base of the exposed slope, a 3 (H): 1 (V) of length 47.4 m, and a 70-m long horizontal portion. For the bioreactor landfill scenario, four horizontal trenches (HTs) were simulated within each of the shallow and deep layers of the landfill model representing a leachate injection system and were laid out as presented in Fig. 3. The horizontal and vertical spacing between the successive HTs was 30 m and 10 m, respectively, representing a typical spacing of HTs in bioreactor landfills (Haydar and Khire, 2005; Giri and Reddy, 2015).

4.2. Initial, Boundary and Interior Conditions

The mechanical boundary conditions applied in the model include restraining the movement of the base of the subgrade in the model in both vertical and horizontal directions. The horizontal deformations along the vertical far-field boundaries of the model are restrained, and only vertical deformations are allowed. The hydraulic model in the CTHBM model that describes the fluid flow is based on the Darcy's law and the relative permeability of the liquid through the unsaturated waste is given by van Genuchten model (van Genuchten 1980). In regard to the hydraulic boundary conditions, all the boundaries except the bottom of the waste are considered impermeable (i.e. pore pressures and degree of saturation varied freely as per the fluid flow internally). Seepage was allowed along the top of the bottom liner (at the immediate bottom of the waste) to simulate leachate collection and removal system (LCRS). The interpretation of different hydraulic boundary conditions used in FLAC are described in ICGI (2019). Interior hydraulic conditions were applied to simulate the injection of leachate at the location of HTs shown in Fig. 3. Continuous leachate injection was simulated through all four HTs at an injection pressure of 50 kPa. The injection pressures selected were based on the reported values in the previous studies on modeling of leachate injection systems (Townsend and Miller, 1998; Xu et al. 2011; Giri and Reddy, 2015). The thermal boundary conditions include fixing a far-field temperature boundary at 75 m below the bottom of the waste, to the mean annual earth temperature of 12.8 °C determined based on field measurements and data on groundwater temperatures reported in the literature (Hanson et al. 2013; ORNL, 1981). In addition, a sinusoidal surface temperature boundary condition defined by Equation 14 with a mean surface temperature and a surface temperature amplitude was applied to simulate seasonal temperature variations at the ground surface.

The general methodology employed for the model setup includes generating the subgrade layer with appropriate hydraulic, mechanical, and thermal boundary conditions and progressing towards the full-scale landfill cell model with sequential placement of waste layers and the final cover. First, the subgrade along with the bottom liner system without any waste above it is solved with the applied thermal boundary conditions for ten years to establish the representative initial temperatures under the influence of ground surface temperature fluctuations in the subgrade. Thereafter, the waste is placed in 3-m thick layers at a waste placement rate of 22 m/year (Liu 2007; Hanson et al. 2013) sequentially and the temperatures within the subgrade layer and the waste layers are determined with appropriate boundary conditions, initial conditions, and interior heat generation source conditions derived from the biothermal model or the site-specific heat generation functions applied (depending upon the case being simulated) to arrive at the temperature distributions across the full-scale landfill cell model. Meanwhile, biochemical degradation of waste occurs as per the proposed BT model or empirical biodegradation model (depending upon the case being simulated) and contemporaneous variations in the biochemical parameters (e.g. SDF, VFA, MB) of waste and the thermal parameters (e.g. heat, temperature) is obtained. After the placement of the ten lifts of waste and the 1-m thick final cover, the model is run for a total of 50 years in all the six cases simulated.

The mesh size varied across the model with certain regions of the model, where stress concentrations and high thermal gradients were anticipated, having a finer mesh size. In general, the mesh size varied between 0.4 m × 0.5 m and 2.8 m × 3.75 m. The mesh size used was determined to be appropriate for the convergence to the numerical solution. Since, the numerical scheme is based on an explicit approach, a stable timestep is determined based on the stability criteria for different phenomena (fluid flow and heat transfer). The final timestep used for the three simulations was 1000 seconds which is much lower than the minimum stable timestep suggested through FLAC guidelines (ICGI 2019) for numerical stability.

4.3. Material Properties

Wherever relevant, the hydraulic, biochemical, and thermal properties were assigned to the final cover, MSW, bottom liner and subgrade materials in the landfill cell model. The density of the final cover soil, compacted clay and subgrade soil were assumed to be 2,000 kg/m^3 and the initial value of density (i.e. placement density) for the MSW was assumed to be 500 kg/m^3. The initial geotechnical mass-volume properties relevant for the hydraulic model, namely the degree of saturation and the porosity of the waste were determined to be 36% and 56 % respectively, based on phase relationships. The vertical and horizontal saturated hydraulic conductivity of the MSW was assumed to be 1×10^{-8} m/s and 1×10^{-7} m/s, with an assumed anisotropy of 10 in the hydraulic conductivity of the waste based on Singh et al. (2014). The van Genuchten model parameters to simulate the water retention curve of MSW for the fluid-flow computations were taken from McDougall (2007) (α = 1.4 m^{-1}, n_{vG} = 1.6). The biochemical properties of waste used for the full-scale landfill cell simulation cases which are described in the next section are presented in Table 1. It can be seen that the biochemical model parameters used for validation cases are substantially different from those used for the application cases. This was due to the different time scales at which a laboratory simulation and a full-scale landfill operates. The values of the model parameters obtained from the laboratory batch experiments on waste samples are not suitable for the full-scale landfill cell simulation. In order to obtain the values of the model parameters that are reflective of a full-scale landfill cell operations, the heat generation rate curve obtained from the proposed BT model was fitted with the heat generation rate curve proposed by Hanson et al. (2013) for a conventional landfill cell (called Cell B) in Michigan, USA. The model parameters that gave the best fit with the heat generation rate curve for the Cell B were used for the BT model application in this study. The values of the thermal properties for the waste and the soil including the values of the heat generation rate function parameters required for the empirical thermal model are presented in Table 2 and were derived from Hanson et al. (2013). The thermal properties of waste vary for different regions; hence, the values of the thermal properties were relevant to the typical soils found in Illinois, USA.

4.4. Simulation Cases

Six numerical simulation cases (Case C1, B1, C2, B2, C3, B3) were examined on a typical landfill cell geometry described earlier. The alphabets C and B in the case terminology represents that those cases simulated conventional and bioreactor landfill conditions, respectively. The only difference between the conventional and bioreactor cases was the injection of leachate in the bioreactor cases through the four HTs as indicated in Fig. 3. The bioreactor landfill simulations were conducted to examine how leachate injection can influence the long-term spatial and temporal variations in biochemical and thermal characteristics of the waste. Case C1 and B1 used the BT model proposed in this study with the temperature function (f_T) to incorporate the effects of temperature on biodegradation and vice-versa representing the most realistic case of the coupled biochemical and thermal behavior of waste in landfills. Case C2 and B2 were examined to investigate the implications of not incorporating the effects of temperature on the biochemical behavior of waste. Case C2 and B2 used the BT model similar to Case C1 and B1 but did not incorporate the temperature function into the BT model. The heat generation rate in these cases was derived from the biodegradation model (Equation 16) and used in the thermal model to determine the waste temperatures. The remaining two simulations, Case C3 and B3, were carried out to investigate the relative advantages of using a more fundamental biochemical reaction kinetics-based model (i.e. the BT model) over the simple empirical biodegradation model (Equation 1) proposed in the authors' previous modeling investigations and predict the long-term biochemical and thermal behavior of waste. The empirical model incorporated the temperature effects on the rate of waste degradation (see Equation 2), but the waste degradation did not in any way contribute to the heat generation. The heat generation for the thermal model in Cases C3 and B3 was derived from empirical heat generation functions (Equation 15). All the six cases were carried out on the same model geometry, used the same waste properties, and same boundary, initial, and interior conditions.

5. RESULTS AND DISCUSSION

5.1. Moisture Distribution

Fig. 4 shows the comparison of the saturation contours for the conventional and bioreactor landfill simulation cases at the end of waste and final cover placement (EWP), and after 1 year

(1Y), 5 years (5Y), 10 years (10Y), 15 years (15Y), 20 years (20Y), 30 years (30Y) and 40 years (40Y). The pressurized injection of leachate (i.e. water) in the bioreactor cases distributed the injected leachate both vertically downward and laterally within the landfill thereby increasing the degree of saturation of the waste. After the injected leachate reached the bottom of the waste, the flow of the leachate in the lateral direction was limited as the leachate seeped out through the bottom LCRS. For the applied leachate injection pressure (i.e. 50 kPa) and for the given hydraulic properties (e.g. hydraulic conductivity, van Genuchten parameters) of the waste, approximately 60% of the cross-sectional area of the waste in the landfill cell model reached a minimum degree of saturation of at least 80%. It should be noted that the areal extent to which the injected leachate is distributed may vary based on the positioning and spacing of the HT locations and the injection pressure employed.

In case of the conventional landfill simulations, the leachate flow was mainly dictated by gravity. Moreover, the consumption of moisture by the waste during hydrolysis/acidogenesis, further reduced the moisture content within the waste but by a very low percent. In general, the moisture content of the waste remained in the same range as the initial conditions of the waste for conventional landfill simulations. Considering the precipitation events (based on the site-specific precipitation records) onto the exposed waste during the waste filling period may alter the moisture regime within the landfills.

5.2. Solid Degradable Fraction, Volatile Fatty Acid and Methanogenic Biomass

Fig. 5 shows the spatial variation in SDF, VFA and MB concentrations along the vertical section BB' (see Fig. 3) at EWP and after 1Y, 5Y, 10Y, 15Y, 20Y, 30Y, 40Y for the cases C1, B1, C2 and B2. The full spatial variation of SDF, VFA and MB concentrations across the entire landfill cell for cases C1, B1, C2, and B2 at different time intervals is shown in Fig. S1, S2, and S3, respectively. The maximum initial value of the SDF in each case was approximately 200 kg/m^3. In case C1, the reduction in the SDF with degradation was more prominent in the central region of the landfill due to the high waste temperatures that were established within that region. These relatively higher waste temperatures in the central region promoted relatively higher rates of microbial growth in the central region compared to the surrounding regions (see case C1 in Fig. 5c). In case B1, the depletion of SDF was rapid and more pronounced in the regions around the leachate injection locations (see case B1 in Fig. 5a) due to enhanced rate of hydrolysis from increased moisture content of the waste. By the end of 40 years, most of the degradable solids (i.e. SDF) along the section BB' had depleted in case C1. The same amount of depletion in SDF took place in approximately 15 years in case B1 because of the high rate of hydrolysis.

In the top few meters of the waste depth in the landfill (i.e. approximately the top 8 m of the waste), the SDF had only partially reduced suggesting that the waste was not completely degraded in that region (see Fig. S1). This is due to the influence of the ground temperature fluctuations (i.e. periodic colder and warmer temperatures due to seasonal variations) that resulted in unfavorable conditions for the microbial growth. With time, the death rate of the microbial biomass in the top few meters of waste exceeded the low growth rate from periodic exposure to unfavorable cold temperatures thus leading to undepleted degradable solids in that region. This also agrees well with rapid decrease in the MB concentrations with time in the top 8 m compared to the rest of the waste depth as shown in Fig. 5c for case C1 and B1. The MB concentrations decreased in the bottom region of the landfill similarly, but this was due to the depletion of the degradable solids itself. It should be noted that the variation in the SDF, VFA and MB presented in Fig. 5, Fig. S1, S2, and S3 is specific to the simulated waste conditions (e.g. initial MB concentrations, MB growth and death rates, initial moisture and temperature of waste) and simulated landfill cell conditions (e.g. the leachate injection system layout and operation). Different initial conditions can have a significant influence on the resulting biochemical and thermal behavior of waste in landfills as demonstrated by McDougall and Philip (2001) in their parametric study.

The variation in VFA concentrations along section BB' for case C1 and B1 (see Fig. 5b) is a result of the dynamic influences of the hydrolysis of SDF and the consumption of the generated VFA by the MB which is immanently influenced by waste temperature. Since the formation of acids (i.e. acidogenesis) is a relatively vigorous process, despite starting from an initial VFA concentration of zero, the VFA concentrations in all the cases rose quickly. To a large extent, the variation in VFA followed similar trends as that of SDF. The VFA concentrations in case B1 reduced rapidly due to the favorable conditions for depletion of VFA established by an increase in both moisture and the temperature of waste at very early stages after EWP. However, in regions along the section that experienced relatively colder temperatures (i.e. approximately the top 8 m of the waste), the lack of MB concentrations led to the accumulation of acids which impeded the microbial growth. In general, Case C1 showed a slower rate of depletion of acids and had a larger proportion of waste with undepleted VFA compared to the Case B1.

When compared to case C1 and B1, case C2 and B2 showed a uniform and a much rapid rate of depletion in the SDF and VFA across the entire section BB' (see case C2 and B2 in Fig. 5a and 5b). This is because the microbial growth was not affected by the temperatures within the waste, which resulted in high MB concentrations to be established all across the landfill that rapidly depleted the SDF and thereby the generated VFA in the waste (see case C2 in Fig. 5c). It can also be noticed that the SDF along the entire depth of the section BB' was depleted which is highly unrealistic given that the rate of waste degradation is quite variable across a landfill and waste is never completely degraded across the entire landfill. Such unrealistic outcomes bolster the fact that temperature is an important factor that determines the course of depletion of degradable constituents within the waste in landfills.

5.3. Degree of Degradation

Degree of degradation is a parameter that is indicative of the extent of waste degradation that has occurred in the landfill. In this study, the degree of degradation (DOD) is defined as the ratio of the difference between the initial mass of degradable solids and the mass of degradable solids at any other time to the initial mass of degradable solids (Equation 22). An alternate definition of DOD that was used for the cases B3 and C3 which used empirical biodegradation model is the ratio of the volume of the cumulative CH_4 gas produced from a specific mass of waste to the maximum CH_4 generation potential of that specific mass of waste (Equation 23).

$$DOD = \frac{M_{D0} - M_{Dt}}{M_{D0}} \times 100\% \tag{22}$$

$$DOD = \frac{Cumulative\ CH_4\ gas\ produced}{L_0 \times Total\ mass\ of\ waste} \times 100\% \tag{23}$$

where, M_{D0} is the initial mass of the degradable solids (kg), M_{Dt} is the mass of degradable solids (kg) at any time t (seconds).

Fig. 6 shows the spatial variation in the DOD along the vertical section BB' at EWP and after 1Y, 5Y, 10Y, 15Y, 20Y, 30Y, 40Y for the cases C1, B1, C2, B2, C3, and B3. The full spatial variation in DOD across the entire landfill cell for the six cases at different time intervals is shown in Fig. S4. Since DOD depends on the mass of SDF (see Equation 22), the variation in DOD along section BB' for cases C1, B1, C2 and B2 were similar to the trends in the variation of SDF as seen in Fig. 5a. In this regard, for Case C1, the DOD is higher in the central region compared to the top and bottom regions of the landfill for the same reasons discussed for the SDF variation in the previous section. The areal extent of degradation of waste for case B1 was higher than case C1 because of the availability of moisture even in those regions that remained undegraded in the Case C1.

In case C2 and B2, the SDF depletion occurs much faster due to the temperature independent microbial growth, thus readily consuming the VFA generated from the depletion of SDF. As a result, nearly all the waste in the landfill is completely degraded for case C2 and B2. Such a behavior is practically not possible in a landfill which suggests that incorporating temperature effects in modeling of biodegradation is crucial for reliable and realistic predictions of the biochemical behavior of waste in landfills. Since Case C3 and B3 also incorporates the effect of temperature on the rate of waste degradation, the variation in DOD along section BB' for these cases showed similar trends as that of case C1 and B1, respectively. However, the empirical biodegradation model does not influence the thermal behavior of the waste which may lead to unrealistic predictions of temperatures within the landfills as will be discussed in a later section. It should be noticed that a relatively higher amount of waste was degraded in cases C3 and B3 when compared to cases C1 and B1. This will have an implication on the total amount of CH_4 gas produced which is discussed in the next section.

5.4. Landfill Gas Production

Fig. 7 shows the variation of cumulative CH_4 gas production with time for the six cases (i.e. C1, B1, C2, B2, C3, B3). Although the total amount of waste and the CH_4 generation potential of the waste was kept the same in all the six cases, the total cumulative CH_4 gas volume produced was different. This is due to the difference in the amount of waste that was degraded in the landfill cell for the six cases. In Case C1 and B1, until approximately 5 years, the rate of CH_4 generation was similar in both the cases and was uninfluenced by the leachate injection in the bioreactor case (see Fig. 7). During this time, the temperatures within the waste were also similar with a slightly higher temperatures around the leachate injection locations in the Case B1. In later years, with higher waste temperatures across most of the landfill and with the increased degree of saturation of the waste from leachate injection, larger extent of waste was degraded resulting in higher amounts of CH_4 gas production in case B1 compared to case C1. The CH_4 gas production did rise after 5 years in case C1 but at a much slower rate. The time to reach the total cumulative CH_4 gas of ~74,142 m^3 in case C1 was approximately 30 years and the time taken to reach the total cumulative CH_4 gas of ~82,145 m^3 in case B1 was approximately 22 years. It should be noted that the volume of LFG produced, and the corresponding timelines to reach the cessation of CH_4 production could vary considerably based on the simulated leachate injection system operation (e.g. injection locations/layout, injection pressures/volumes) and also on the simulated initial waste conditions (e.g. initial MB concentrations, MB growth and death rates).

In case C2 and B2, the lack of temperature effects on microbial growth had established favorable conditions all across the landfill for enhanced degradation of waste to occur. This resulted in a significantly faster and higher rates of CH_4 gas production in the two cases with practically no difference between case C2 and B2 which is not realistic. The total CH_4 gas produced was similar (~93,200 m^3) in case C2 and B2 but it is widely reported that bioreactor landfills have enhanced gas production rates and gas production volumes compared to the conventional landfills (Benson et al. 2007; Bareither et al. 2010). The cumulative CH_4 gas production results for Case C2 and B2 suggest that ignoring the effects of temperature in modeling of biodegradation in landfills overpredict the CH_4 gas production rates and CH_4 gas production volumes, and the results from such analysis may not be reliable for the planning of LFG management systems.

In case C3 and B3, the total cumulative CH_4 gas produced in the Case C3 and B3 were ~86,859 m^3 and ~89,490 m^3, respectively. The total cumulative CH_4 gas production in the empirical model depends upon the maximum BMP of the waste which is assumed to be equal to 0.06 m^3/kg of dry waste in this study based on Grellier et al. (2007). There was no initial phase of microbial acclimatization as observed in case B1 or C1 suggesting that the empirical model considers well established microbiological conditions from the very beginning of waste placement which is not realistic. Unlike the Case C2 and B2, the CH_4 production rate was substantially different between Case C3 and B3 due to the inclusion of the moisture and temperature effects on the rate of waste degradation. Although the prediction of CH_4 gas production by the empirical model my not follow a realistic trend as done by the proposed BT model, the empirical model could still be used to estimate the total LFG produced reasonably well for conventional and bioreactor landfills given some initial data regarding the progress in LFG production.

5.5. Temperatures

Fig. 8 shows the variation in waste temperatures along the vertical section BB' at EWP, and after 1Y, 5Y, 10Y, 15Y, 20Y, 30Y, 40Y for cases C1, B1, C2, B2, C3, and B3. The full spatial distribution of temperatures across the entire landfill for the six cases at different time intervals is shown in Fig. S5. Temperatures in the top 8 m of waste which was closer to the ground surface were influenced by the ground surface temperature fluctuations. In all the cases, the temperature profile along the waste depth had a convex shaped curve with high temperatures in the center compared to the top and bottom waste regions which is a typical variation in temperature along the waste depth observed in landfills (Yesiller et al. 2005).

In case C1 and B1, the initial 3 years did not show any significant increase in the waste temperatures due to the lack of favorable temperatures for the microbial concentrations to degrade the organic substrate and produce heat. In case C1, the temperatures in the waste increased and reached about 40 °C after approximately 15 years and temperatures continued to increase gradually to peak values close to 45 °C and later subsided to steady state temperatures after approximately 35 years. These temperatures predicted for Case C1 are well within the typical temperatures measured in the conventional landfills (Yesiller et al. 2005; Hanson et al. 2010). In case B1, the enhanced moisture from the leachate injection triggered rapid waste decomposition thereby promoting high heat generation rates. As a result, temperatures in the waste reached peak values in the range of 60 – 63 °C in the central region of the landfill after 10 years but quickly subsided to temperatures less than 40 °C after 15 years. Such high temperatures have been measured in MSW landfills, but they are not persistent for a long period of time (Yesiller et al. 2005). Co-disposal of high organic and high moisture content municipal sludges are reported to stimulate higher rates of biological reactions and thereby inducing higher heat generation rates (Khire et al. 2020).

Case C2 and B2 predicted the waste temperatures well above 55 °C in the landfill and Case B2 predicted temperatures as high as 75 °C. Such elevated waste temperatures are observed in a few MSW landfills, but those landfills had other sources of heat from inorganic reactions (e.g. aluminum dross, ash hydration, pyrolysis, aerobic degradation) which are highly exothermic (Jafari et al. 2017). Hence, the lack of temperature effects on waste degradation resulted in unusually high heat generation rates which lead to predicting unrealistically high elevated temperatures in case C2 and B2.

Case C3 and B3 also predicted unrealistically high waste temperatures similar to case C2 and B2 due to the high heat generation rates applied by the empirical heat generation rate functions used in case C3 and B3. These elevated temperatures suggest that the heat generation rate functions cannot be generally applicable to any waste conditions and they must to be developed specifically to the waste conditions simulated. This also suggests that a thermal model used to predict thermal regime in landfills should incorporate heat generation rates derived from a biodegradation model itself for realistic predictions of the thermal regime in landfills.

6. CONCLUSIONS

A coupled BT model is proposed which was developed by building upon the limitations of the previous efforts by the authors and other researchers in modeling the coupled biochemical and thermal processes in landfills. The proposed BT model integrates a two-stage anaerobic digestion biochemical model with a heat conduction based thermal model to incorporate the effects of temperature on microbial growth and subsequently on the degradation of waste. Further, the thermal model in turn is dependent on the biodegradation model to derive the amount of heat generated as a result of substrate depletion and thereby predicts the temperatures within the landfill. The proposed BT model is validated with the biochemical data recorded during six long-term laboratory-scale experiments conducted on waste samples from actual MSW landfills in US and UK. The proposed BT model was further applied to a typical landfill cell geometry to understand the long-term spatial and temporal variation in biochemical and thermal characteristics of waste under typical conventional and bioreactor landfill conditions. Additional simulations were performed on the same landfill cell geometry to evaluate the significance of incorporating the coupled effects of temperature on the biodegradation of waste and also to evaluate the relative advantages of a more mechanistic-based biodegradation model over a simplified empirical FOD-based model in predicting the biochemical behavior of waste in landfills. Based on the numerical simulations performed, following conclusions can be drawn from this study.

- The predictions of the proposed BT model show a good agreement with the simulated long-term large-scale laboratory experimental data on the variations in the biochemical parameters such as volatile fatty acids and degradable solids in the waste samples during the course of the experiments. Although, the model underpredicted the CH_4/LFG gas production when compared to the actual measured data in most cases, it was able to accurately capture the trend in the progress in gas production over the duration of the experiment.
- The results from the numerical simulations of the full-scale landfill cell model, especially the Case C1 and B1, show that the dynamic interactions between the thermal aspects (e.g. heat generation and temperature) and the biochemical aspects (e.g. SDF, VFA, MB) are

well captured by the BT model in the predicted trends for the evolution of SDF, VFA, MB, the LFG production, and the temperatures within the landfill. For the specific waste and leachate injection conditions simulated, elevated temperatures (>55°C) were predicted as a result of leachate injection in the bioreactor landfill case (case B1).

- The results from Case C2 and B2 suggest that ignoring the temperature effects on waste degradation would result in a uniform and a complete degradation of waste across the entire landfill which is practically not possible given that the environmental conditions vary considerably across the landfill. Therefore, it is imperative that the biochemical models developed for MSW should incorporate temperature effects for realistic and reliable predictions of the biochemical behavior in MSW landfills.
- The use of simplified FOD-based biodegradation model and an empirical heat generation function as in the Case C3 and B3 resulted in unrealistically high gas generation rates and waste temperatures at the early stages of landfill operation itself. These results clearly suggest that simplification of microbially mediated biochemical reactions within the waste into a lumped FOD model and empirical heat generation rate function with no consideration to microbial dynamics can significantly undermine the actual biochemical and thermal behavior of waste in landfills.
- The proposed BT model can be easily integrated with any coupled fluid-flow and mechanical model to realistically simulate and predict the long-term coupled hydraulic, mechanical, biochemical, thermal behavior of MSW landfills.
- Future developments of the BT model will include validating the biochemical model with a more comprehensive dataset consisting of both biochemical and thermal aspects, addition of advective and diffusive transport mechanisms for biochemical constituents

(e.g. VFA, MB) and heat in the model formulation, and inclusion of other major pathways for methanogenesis to accurately predict the LFG production in landfills.

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Table 1: Initial values of the biodegradation model parameters used for the validation and application cases

Parameter	Value						
	CAR1	**CAR2**	**MI**	**TX**	**AZ**	**CA**	**Application Cases**
Initial volumetric moisture content (%)	56.3	64.3	27.0	49.0	38.0	42.0	20.0
Volumetric residual moisture content (%)	11.0	11.0	7.7	15.0	11.6	16.0	12.5
Percentage of degradable solids (%)	55.0	55.0	30.2	11.7	24.0	9.0	40.0
Degradable solids density (kg m^{-3})	745.0	745.0	882.0	1,044.0	955.0	1,338.0	745.0
Inert solids phase density (kg m^{-3})	1,735.0	1,735.0	895.0	1,727.0	1,716.0	1,660.0	1,735.0
Initial SDF concentration (kg m^{-3})	240.6	196.6	93.4	70.1	111.6	57.4	200.0
Initial VFA concentration ($g_{[VFA]}\ m^{-3}{}_{[aqueous]}$)	300.0	300.0	0.0	0.0	8,500.0	0.0	0.0
Initial MB concentration ($g_{[VFA]}\ m^{-3}{}_{[aqueous]}$)	1,000.0	1,000.0	300.0	100.0	1,200.0	10.0	1,500.0
Maximum hydrolysis rate ($g_{[VFA]}\ m^{-3}{}_{[aqueous]}\ day^{-1}$)	18,000.0	24,000.0	9,000.0	2,000.0	5,200.0	2,000.0	2,500.0
Product inhibition factor ($m^3 g^{-1}$)	1×10^{-4}	1×10^{-4}	8.5×10^{-4}	4.2×10^{-4}	1.2×10^{-4}	6.3×10^{-3}	2×10^{-4}
Structural transformation parameter (-)	0.06	0.06	1.00	0.75	1.00	0.70	0.70
Maximum specific growth rate for MB (day^{-1})	0.047	0.047	0.128	0.250	0.075	1.000	0.005
Methanogen death rate (day^{-1})	0.0040	0.0040	0.0050	0.0005	0.0040	0.0005	0.0008
Half saturation constant (g m^{-3} aq.)	4,000.0	4,000.0	1,000.0	1,000.0	3,500.0	700.0	20,000.0
Cell to substrate yield coefficient (-)	0.08	0.08	0.3	0.4	0.4	0.3	0.017

Table 2: Initial values of the thermal properties of soil and waste and heat generation function parameters

Property	Application Cases	
Thermal conductivity of waste (W/m K)	1.0	
Heat capacity of waste (kJ/kg K)	2000.0	
Density of subgrade soil (kg/m^3)	2000.0	
Thermal conductivity of subgrade soil (W/m K)	2.4	
Heat capacity of subgrade soil (kJ/kg K)	1,300.0	
Mean subgrade soil surface temperature (°C)	12.8	
Amplitude of subgrade soil surface temperatures (°C)	16.6	
Mean waste surface temperature (°C)	13.0	
Amplitude for waste surface temperature (°C)	19.4	
	Case B3	**Case C3**
Parameter A (W/m^3)	104.5	130.0
Parameter B (days)	5,000.0	2,000.0
Parameter D (days)	120.0	80.0

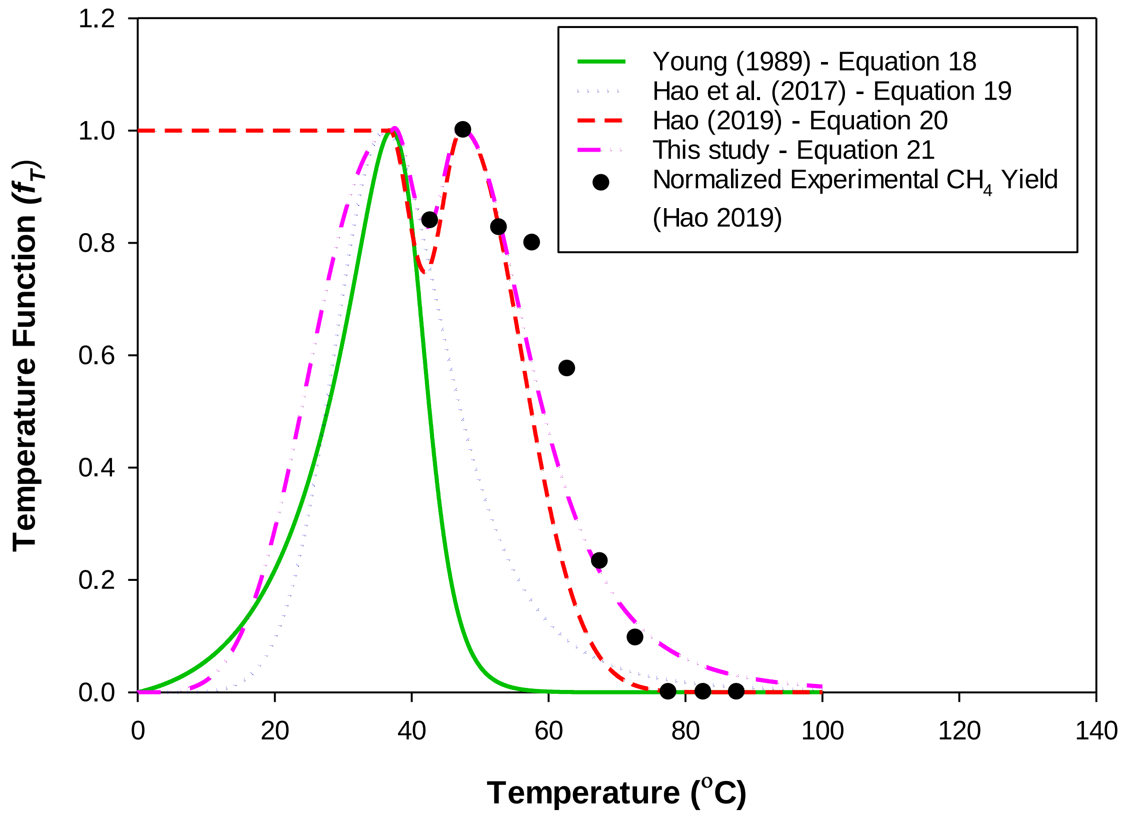

Fig. 1: Temperature functions proposed by different researchers and in this study

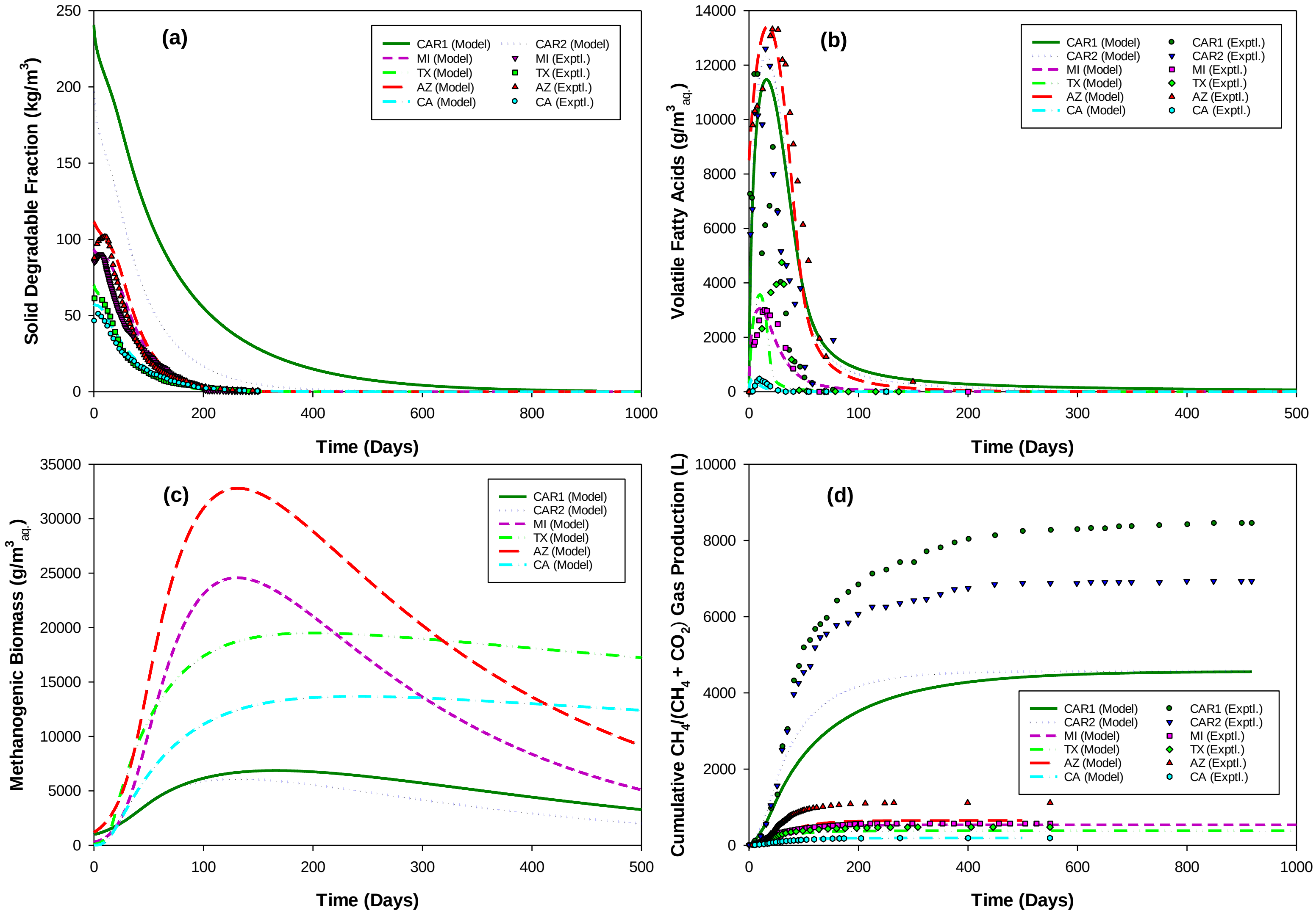

Fig. 2: Comparison of the model predictions with the six different experimental dataset for (a) SDF concentration, (b) VFA concentration, (c) MB concentration, and(d) cumulative LFG/CH_4 gas

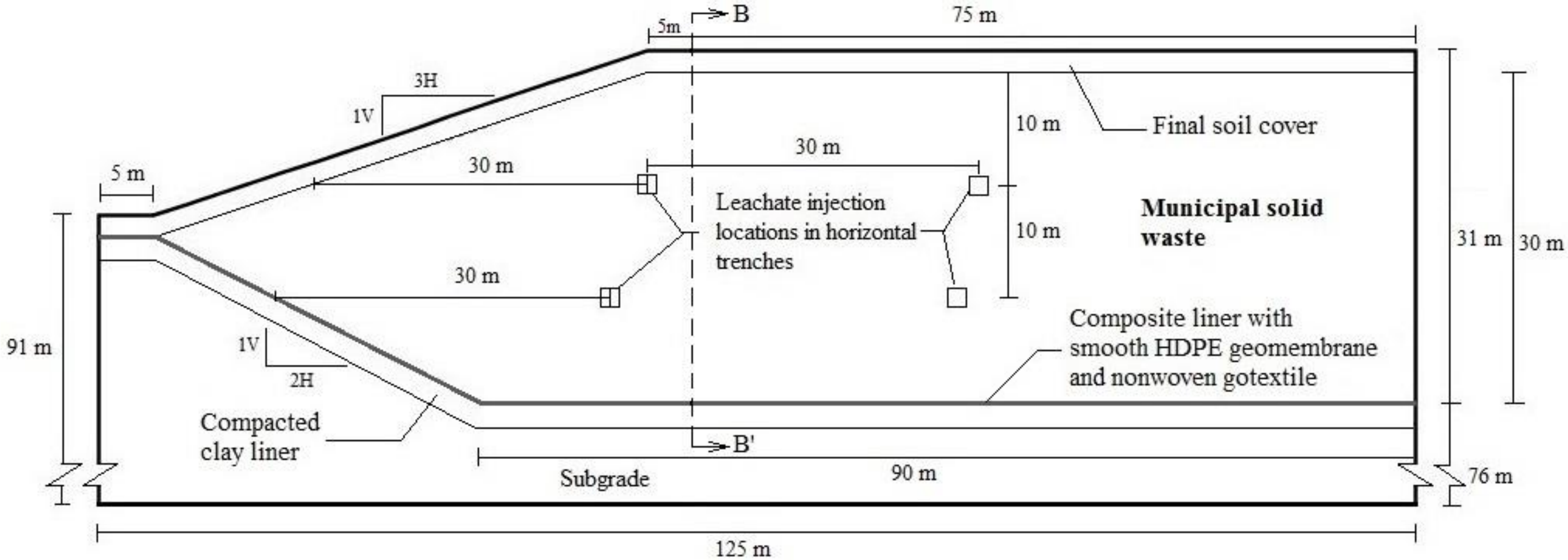

Fig. 3: Schematic of the landfill model used for the numerical simulations (Note: horizontal trenches shown are used for leachate injection in bioreactor landfill simulations)

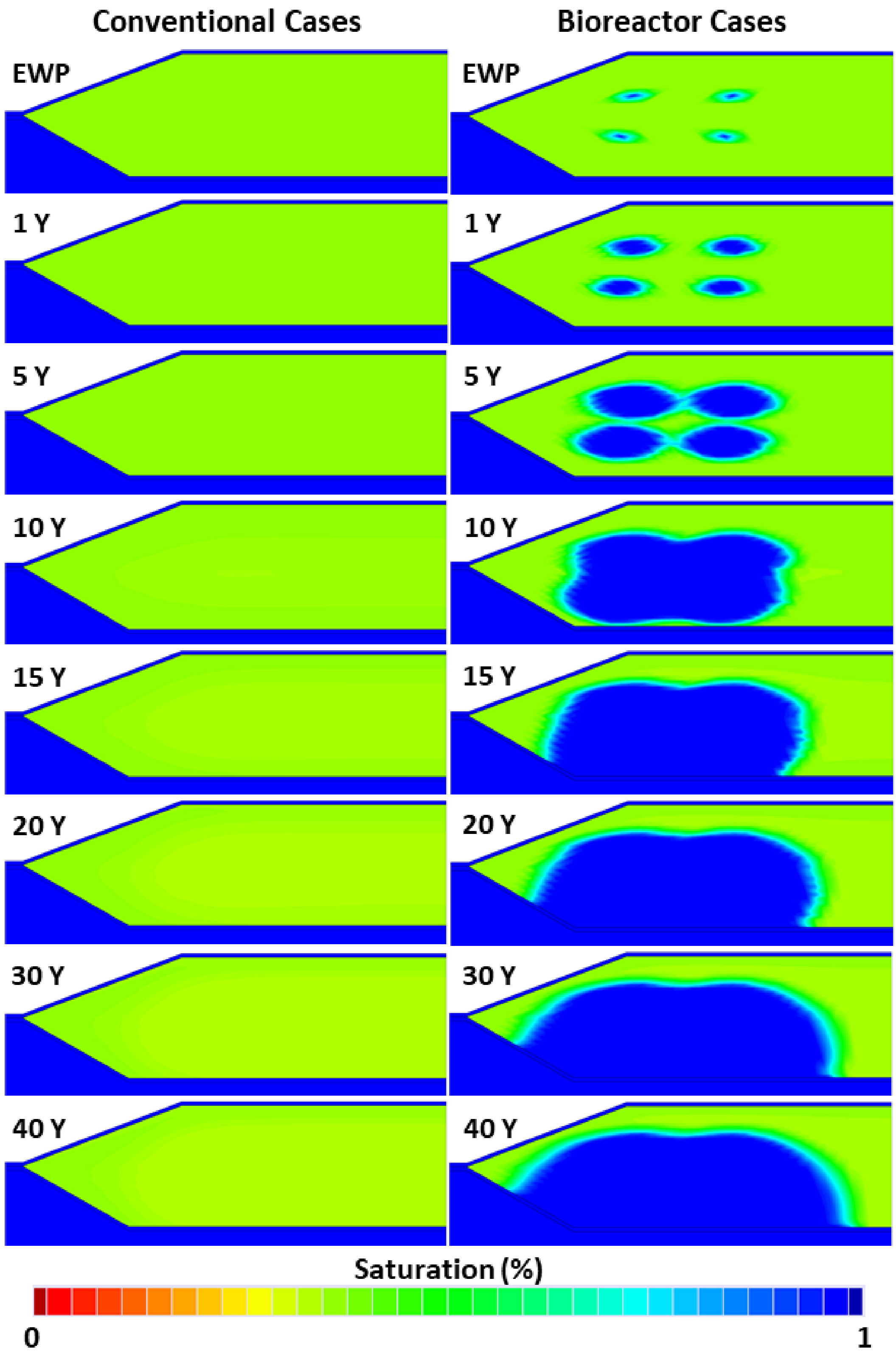

Fig. 4: Spatial and temporal variation in saturation of waste for bioreactor and conventional landfill cases

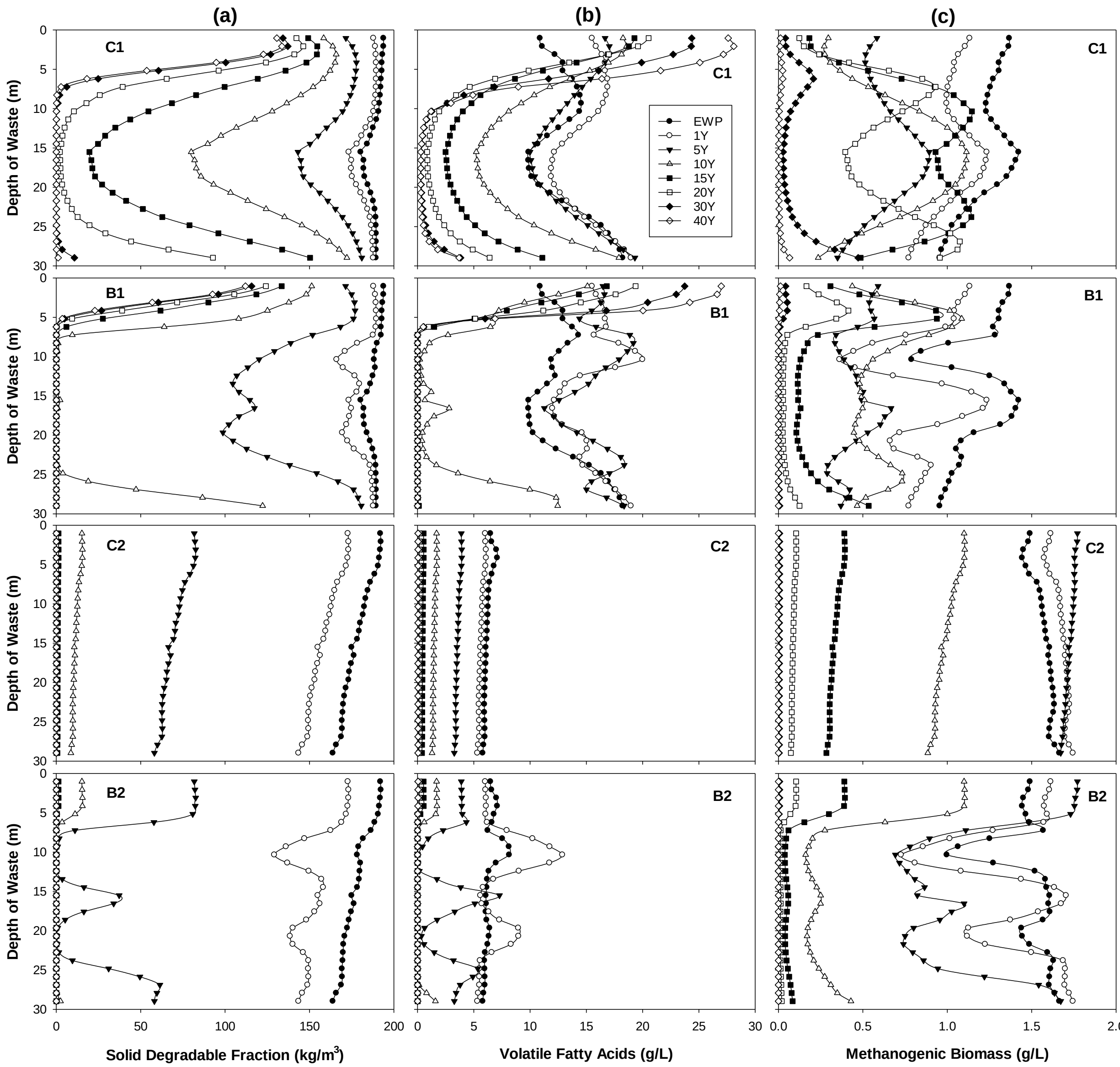

Fig. 5: Variation in (a) solid degradable fraction, (b) volatile fatty acids concentration, (c) methanogenic biomass concentration along the vertical section BB' for Cases C1, B1, C2, B2

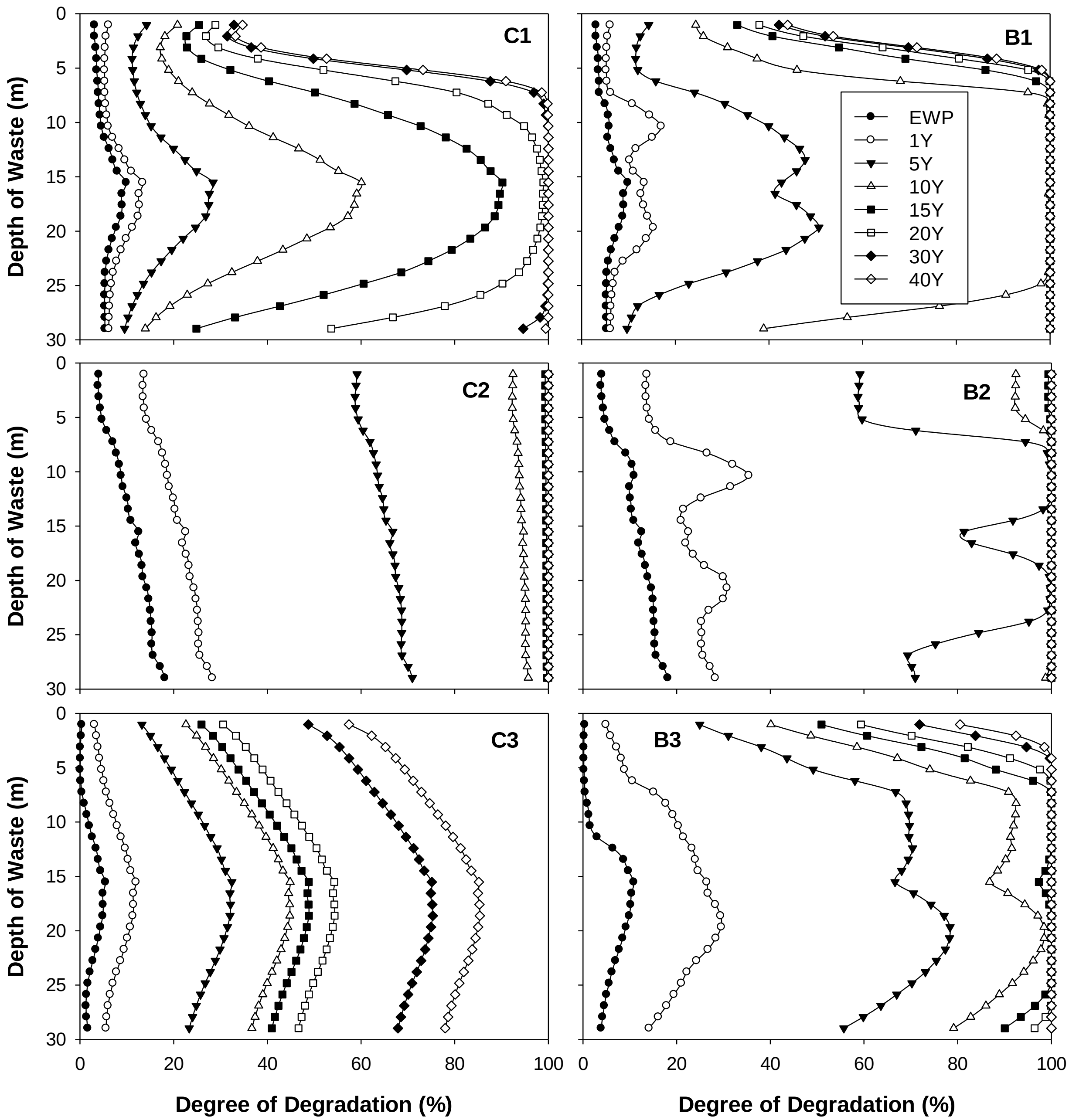

Fig. 6: Variation of degree of degradation along the vertical section BB' for the cases C1, B1, C2, B2, C3, and B3

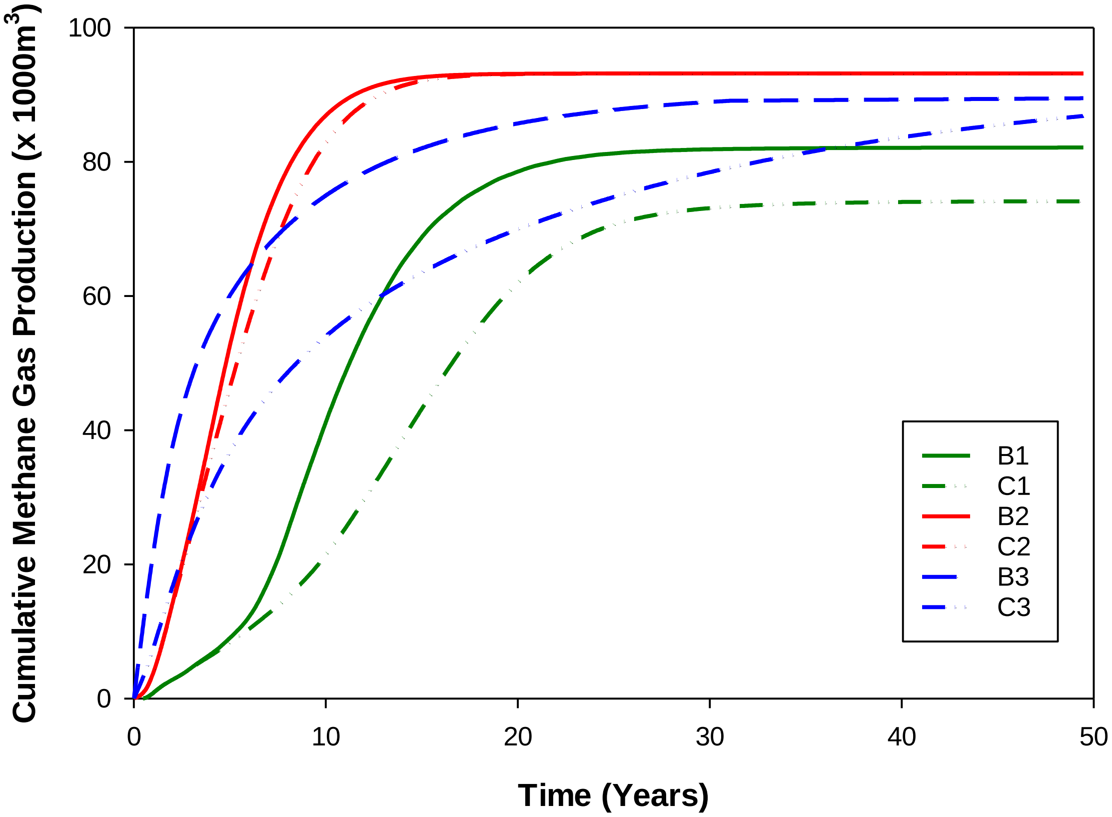

Fig. 7: Variation of cumulative methane gas production with time for the cases C1, B1, C2, B2, C3 and B3

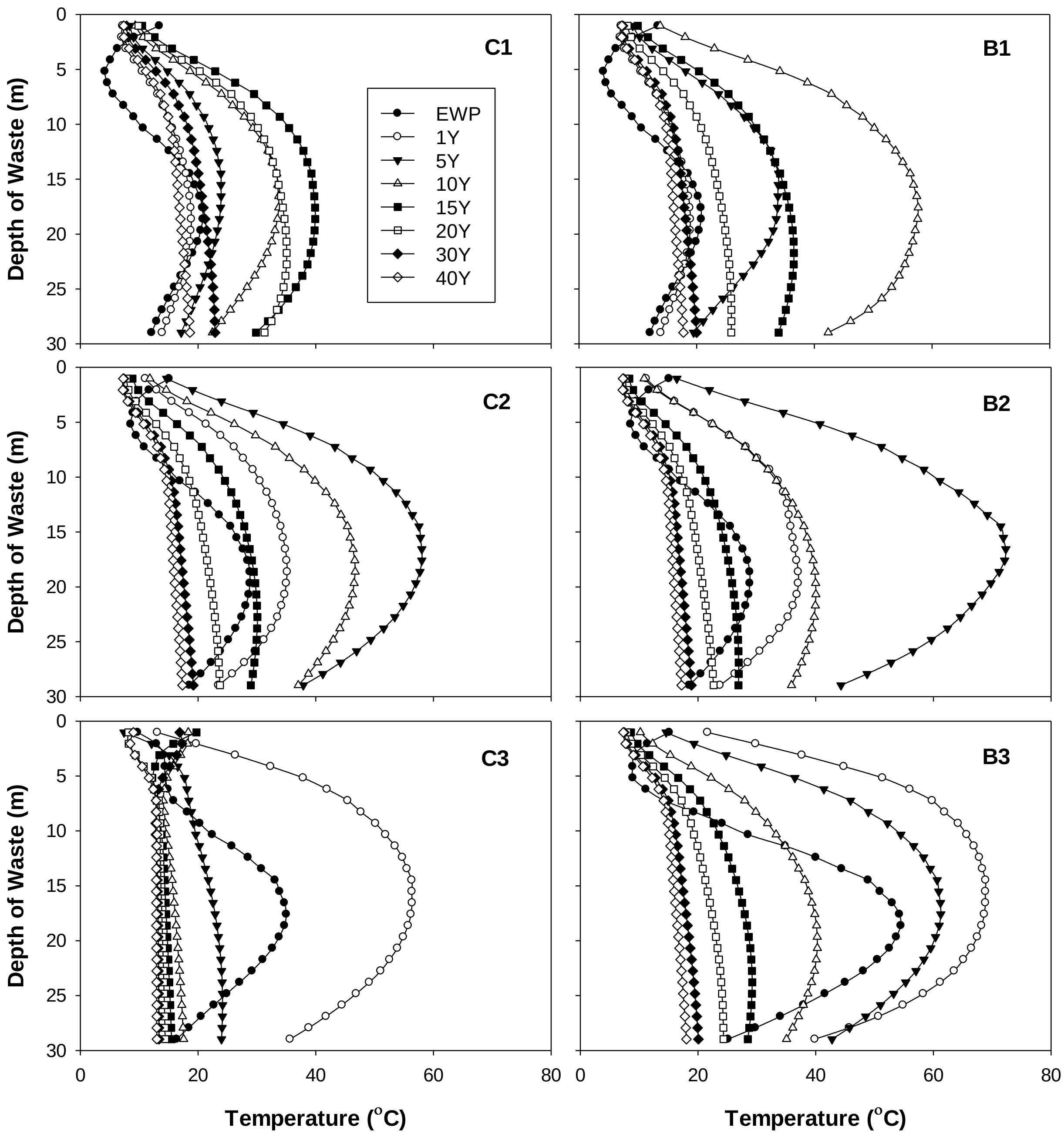

Fig. 8: Variation in temperature of waste along the vertical section BB' for cases C1, B1, C2, B2, C3 and B3