

# Numerical simulation of waste landfill biodegradation: Fitting experimental data

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## Abstract

Landfill remains economically viable for the disposal of Municipal Solid Waste (MSW), however, experiences of failure in several Colombian and global locations, lead to soil, water, and air pollution, harming ecosystems, and biodiversity. Numerical models can help improve the design by considering biodegradation, hydraulic, thermal, and mechanical phenomena involved in landfills. This paper presents a simulation of the landfill biodegradation, calibrating parameters to make results match experimental data from previous references. COMSOL Multiphysics was used to implement McDougall's biodegradation model, tracking organic matter transformation into volatile fatty acids (VFA) and methane (CH<sub>4</sub>) production via acetogenesis. Parameters taken from previous references were recalibrated to fit data from six US landfills. The results for the concentration variation with time for organic matter, VFA and CH<sub>4</sub> successfully follows the expected behavior and fits the experimental data. McDougall's 2007 model, successfully implemented in COMSOL, can be calibrated for data from Colombian and global landfills.

**Keywords:** waste landfill, biodegradation; mathematical modeling; methane generation.

# Simulación numérica de la biodegradación en rellenos sanitarios: ajuste de datos experimentales

## Resumen

Los rellenos sanitarios siguen siendo económicamente viables para la disposición de Residuos Sólidos Urbanos (RSU), sin embargo, experiencias de fallas en varios lugares de Colombia y el mundo, conducen a la contaminación del suelo, agua y aire, perjudicando los ecosistemas, y la biodiversidad. Los modelos numéricos pueden ayudar a mejorar el diseño considerando los fenómenos de biodegradación, hidráulicos, térmicos y mecánicos involucrados en los rellenos sanitarios. Este trabajo presenta una simulación de la biodegradación en rellenos sanitarios, calibrando los parámetros para que los resultados coincidan con los datos experimentales de la literatura técnica. Se utilizó COMSOL Multiphysics para implementar el modelo de biodegradación de McDougall, siguiendo la transformación de la materia orgánica en ácidos grasos volátiles (AGV) y la producción de metano (CH<sub>4</sub>) vía acetogénesis. Los parámetros tomados de referencias anteriores se recalibraron para ajustarlos a los datos de seis vertederos estadounidenses. Los resultados de la variación de la concentración con el tiempo para la materia orgánica, los AGV y el CH<sub>4</sub> siguen satisfactoriamente el comportamiento esperado y se ajustan a los datos experimentales. El modelo de McDougall de 2007, implementado con éxito en COMSOL, puede calibrarse para datos de rellenos colombianos y mundiales.

**Palabras clave:** relleno sanitario; biodegradación; modelado matemática; generación de metano

## 1 Introduction

Utilizing stratified waste placement continues as an economically viable approach for the disposal of Municipal Solid Waste (MSW) in numerous countries. However,

experiences of failure in several Colombian locations, including Bucaramanga (Carrasco, 2017), Cali (2001), and Bogota (1998), have underscored the need for heightened scrutiny and research on MSW management within the country.

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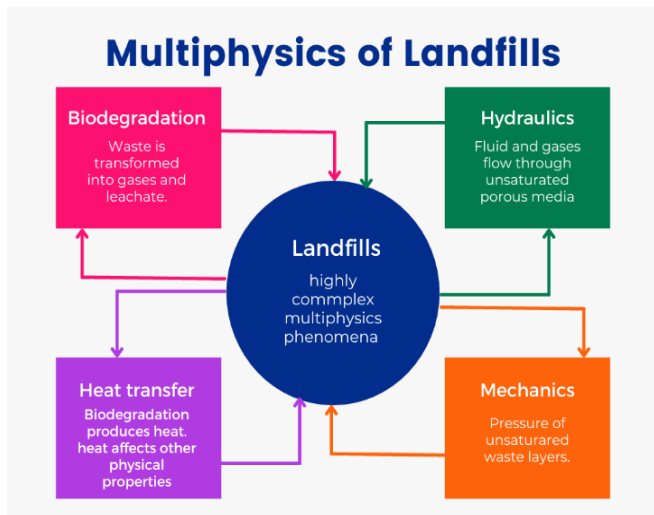


Figure 1. The Multiphysics phenomena influencing landfill design.  
Source: Own

One of the primary challenges in MSW landfill management revolves around the accurate estimation of settlement, given that landfills naturally undergo settling processes over time. The final settlement can amount around to 30% of the initial landfill height according to [1]. The intricate interplay of waste biodegradation significantly influences this settling phenomenon. As waste materials biodegrade, they generate byproducts such as gas and leachate, initiating a cascade of complex processes that involve biochemical, mechanical (settlement, stresses, etc.), hydraulic (flow, pressure), and thermal phenomena (temperature rise). Fig. 1 illustrates the multiphysics phenomena intricately interwoven in landfill design and performance [2].

Introducing a Multiphysics simulation of biodegradation in landfill waste is crucial for understanding the long-term behavior of municipal solid waste (MSW) and its environmental impact. Landfill settlement estimation and the complex processes involved are of significant concern in landfill management. To address these challenges, innovative models have been developed, such as hydro-mechanical [3-8], bio-mechanical [3-11], hydro-bio-mechanical [3-8,11], hydro-thermal [12,13], gas generation [3-5,9,11], and hydro-bio-thermal models [13-15].

The degradation model encompasses various stages, from organic matter coming from solid degradable fraction (SDF) transforming into volatile fatty acids (VFA) through hydrolysis and acidogenesis to the formation of methanogenic biomass (MB), which leads to methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>) production, Fig. 2 [2]. Methane generation is an environmental concern that further emphasizes the study of biodegradation in landfills [8].

Different methods, such as one-state, two-state, and multi-state, can be used to classify anaerobic biodegradation models based on the number of chemical and bacterial reaction paths. The two-state method is the most widely used and relies on variables such as Solid Degradable Fraction (SDF), VFA, and MB.

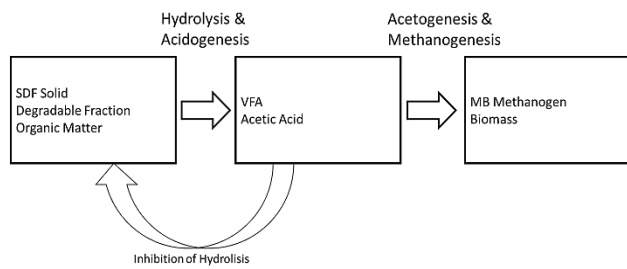


Figure 2. Biodegradation process.  
Source: Own

Several mathematical models have been proposed to describe the depletion rate of SDF in MSW. A mathematical model proposed by McDougall [3] based on a chemical equation has served as a foundation for subsequent studies. [16] proposed a bio-thermal (BT) model validated through six laboratory experiments conducted by [5] and [17]. As a result of calibrating the model, the author applied it to a typical full-scale landfill cell geometry to examine the long-term spatial and temporal variation over time. A laboratory test performed by [18] achieved similar results using a biodegradation model based on McDougall of approach.

Estimating MSW properties for numerical modeling requires empirical measurements. Studies by [5] and [17] conducted laboratory tests to characterize biodegradation potential and measure key byproducts such as VFA and MB. These studies provide valuable insights into the behavior of MSW under different conditions.

A series of laboratory tests were performed and carried out to characterize anaerobic biodegradation potential of fresh MSW, using two large-scale Consolidating Anaerobic Reactors (CARs). The CARs contained waste material of the same composition as that used in BMP tests in other laboratory test performance by the authors. Two levels of constant vertical overburden pressures were 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 [5].

[17] run out laboratory tests to investigate the biochemical and physical characteristics of MSW under leachate recirculation-enhanced conditions. Waste samples were extracted from different waste landfills around USA, with duration ranging approximately 850 to 1500 days (namely, Michigan MI – 1,100 days, Texas TX – 1,500, Arizona AZ – 885, and California CA – 850 days).

Correlations of Methane generation potential (L<sub>0</sub>) and a percentage of biodegradable waste prior to degradation, parameter B<sub>0</sub>, were obtained. In the same way, correlations of methane generation rate (r<sub>CH<sub>4</sub></sub>), L<sub>0</sub> and maximum soluble chemical oxygen demand in leachate were developed.

The articles by [19] and [4] present mathematical models for predicting the biodegradation of organic matter in landfills. [19] model considered factors like moisture content, temperature, and pH levels, accurately predicting degradation rates. [4] focused on biochemical processes, including hydrolysis, acidogenesis, acetogenesis, and methanogenesis, validating the model with empirical data and using it to predict waste degradation rates and methane production.

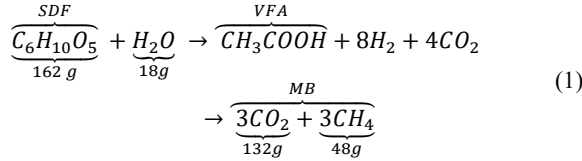
Understanding biodegradation processes and modeling them is crucial for landfill management and reducing greenhouse gas emissions. The processes can provide valuable insights and optimization strategies.

This paper presents the modeling and simulation of landfill biodegradation using the mechanistic biodegradation model [3], widely used in technical literature. The analysis is based on model parameter values reported in the literature [5,17,20,21]. In addition, the basis is laid for future comparison with laboratory measurements to corroborate the theory and calibrate the model parameters.

## 2 Methodology

### 2.1 Mathematical Model

The most used model for biodegradation in landfills is that of [3], which was implemented in this study by means of COMSOL Multiphysics software. According to the McDougall model, the three main mechanisms involved in biodegradation (Fig 1) can be simplified by eq. (1).



The Solid Degradable Fraction (SDF), Volatile Fatty Acids (VFA) and Methanogenic Biomass (MB) are represented chemically in eq. (1) by cellulose, acetic acid, and carbon dioxide plus methane, respectively. The VFA accumulation rate  $r_g$  in gVFA m<sup>-3</sup>aqueous day<sup>-1</sup>, is expressed mathematically by eq. (2). where  $k_{VFA}$  is the production inhibition rate constant,  $c$  is the concentration of VFA in the aqueous phase in gVFA m<sup>-3</sup>aqueous,  $S$  is the solid degradable fraction at any instant of time,  $S_0$  is the initial solid degradable fraction (SDF)  $b$  is the maximum VFA growth rate (gVFA m<sup>-3</sup>aqueous day<sup>-1</sup>),  $n$  is the structural transformation parameter,  $\theta_e = \frac{\beta_s - \theta_r}{\theta_r^2}$  is the effective volumetric moisture content, and  $\theta$ ,  $\theta_r$  and  $\theta_s$  are respectively the volumetric, residual and saturation moisture contents.

$$r_g = \theta_e b \left[ 1 - \left[ \frac{S_0 - S}{S_0} \right]^n \right] * e^{-k_{VFA}(c)} \quad (2)$$

The MB production/growth rate ( $r_j$ ) represents methanogenic substrate depletion and methanogen growth, which are described by Monod kinetics according to eq. (3). Where  $k_0$  is the specific growth rate (day<sup>-1</sup>),  $m$  is the concentration of MB in aqueous phase (g[VFA] m<sup>-3</sup>aqueous) and  $k_{MC}$  is the half-saturation constant (g[VFA] m<sup>-3</sup>aqueous).

$$r_j = \frac{k_0 c}{(k_{MC} + c)} m \quad (3)$$

The terms  $r_h = \frac{r_j}{Y}$ , and  $r_k = k_2 m$  depict the VFA

consumption rate and the MB decay/death rate respectively. VFA consumption rate is associated to the MB growth rate  $r_j$  through a substrate yield coefficient  $Y$ . The methanogenic decay rate is related to  $k_2$ , the MB decay rate constant (day<sup>-1</sup>). Finally, it is possible to set up a system of ordinary differential equations to describe the accumulation rates of SDF ( $S$ ), VFA ( $c$ ) and MB ( $m$ ) by equations Eq. 4 to 6 respectively.

$$\frac{\partial S}{\partial t} = -\theta \frac{162}{60} r_g \quad (4)$$

$$\frac{\partial c}{\partial t} = [r_g - r_h] \quad (5)$$

$$\frac{\partial m}{\partial t} = [r_j - r_k] \quad (6)$$

The model was proved with different combinations of parameters and initial conditions as shown in Table 1, as reported in [20,21], which refers to measurements in different landfills in the USA. The parameters were further optimized for better adjustment of the simulation with the field data.

Table 1. Parameter values for different landfill data cases

Parameter	CAR1	CAR2	MI	TX	AZ	AC
Initial volumetric moisture content (%)	56.3	64.3	27.0	49.0	38.0	42.0
Volumetric residual moisture content (%)	11.0	11.0	7.7	15.0	12.0	16.0
Percentage of degradable solids (%)	55.0	55.0	30.2	11.7	24.0	9.0
Degradable solids density (kg m <sup>-3</sup> )	745.0	745.0	882.0	1044.0	955.0	1338.0
Inert solids phase density (kg m <sup>-3</sup> )	1735.0	1735.0	895.0	1727.0	1716.0	1660.0
Initial SDF concentration (kg m <sup>-3</sup> )	240.6	196.6	93.4	70.1	111.6	57.4
Initial VFA concentration (g <sub>[VFA]</sub> m <sup>-3</sup> <sub>[aqueous]</sub> )	300.0	300.0	0.0	0.0	8500.0	0.0
Initial MB concentration (g <sub>[VFA]</sub> m <sup>-3</sup> <sub>[aqueous]</sub> )	1000.0	1000.0	300.0	100.0	1200.0	10.0
Maximum hydrolysis rate (g <sub>[VFA]</sub> m <sup>-3</sup> <sub>[aqueous]</sub> day <sup>-1</sup> )	18000.0	24000.0	9000.0	2000.0	5200.0	2000.0
Product inhibition factor (m <sup>3</sup> g <sup>-1</sup> ) kVFA	1 × 10 <sup>-4</sup>	1 × 10 <sup>-5</sup>	8.5 × 10 <sup>-4</sup>	4.2 × 10 <sup>-4</sup>	1.2 × 10 <sup>-4</sup>	6.3 × 10 <sup>-3</sup>
Structural transformation parameter (-) n	0.06	0.06	1.00	0.70	1.00	0.70
Maximum specific growth rate for MB k(day <sup>-1</sup> )	0.047	0.047	0.128	0.150	0.070	0.70
Methanogen death rate (day <sup>-1</sup> )	0.0040	0.0040	0.0050	0.0005	0.0040	0.0005
Half saturation constant	4000	4000	1000	1500	3500	700
kMC(g m <sup>-3</sup> aq.)						
Cell to substrate yield coefficient	0.08	0.08	0.30	0.40	0.40	0.30

Source: taken from [20]

### 3 Results and Discussion

Fig 2 illustrates the biodegradation process, wherein degradable waste undergoes hydrolysis, acidogenesis/acetogenesis, and methanogenesis to transform SDF material into VFA and MB. Over time, Figs. 3 to 5 display the concentrations of SDF, VFA, and MB. A comparison between field data and model results from six experiments conducted across various waste landfills is available for analysis.

As shown in Fig. 3, a non-linear drop in SDF is presented as the initial fraction consumed by chemical processes under anaerobic conditions. The comparison between field data and model results for MI, TX, AZ and CA samples shows a very similar behavior of SDF over time, suggesting the model parameters are well calibrated. The experimental results are not available for CAR 1 and CAR2, but the simulated results are like the other samples in trend. In the case of CAR2, the results suggest additional parameter refinement could be done to improve the results, as other references suggest the decay time of SDF is shorter for this sample [16].

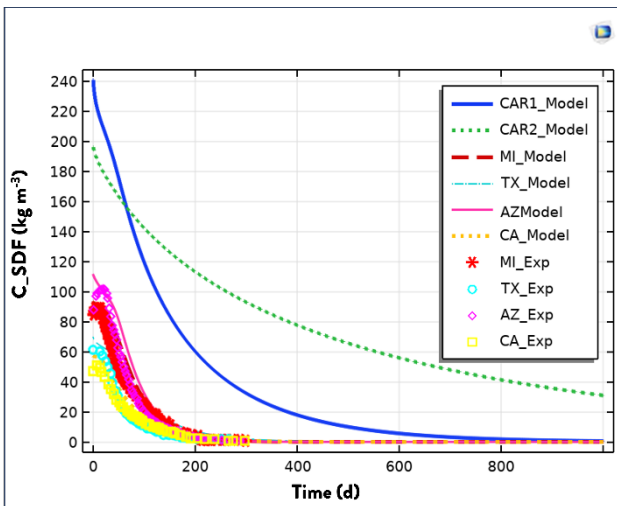


Figure 3. Concentration of Solid Degradable Fraction ( $C_{SDF}$ ) as a function of time. Source: Own

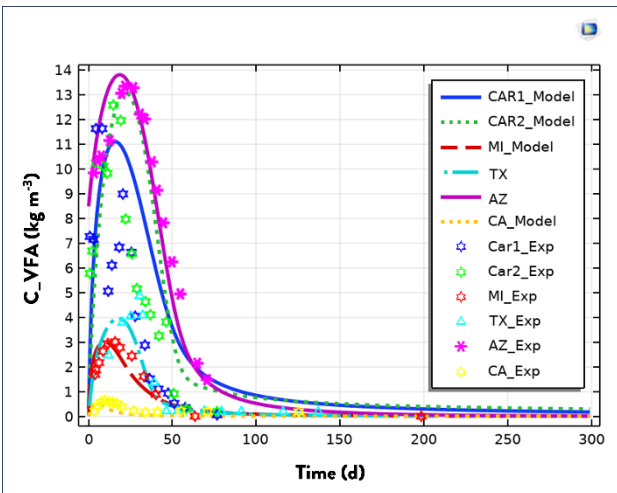


Figure 4. Concentration of Volatile Fatty Acids ( $C_{VFA}$ ) as a function of time. Source: Own

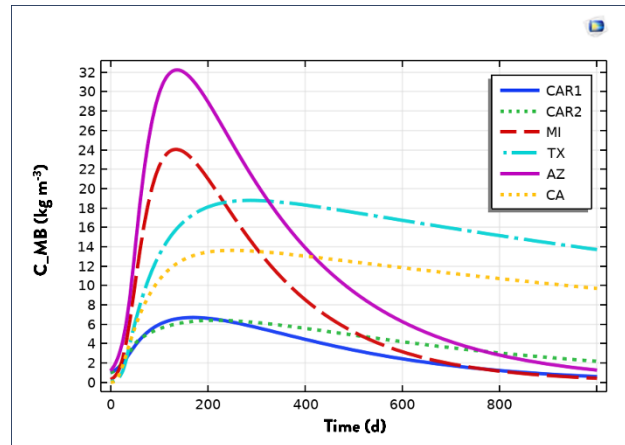


Figure 5. Concentration of Methanogenic Biomass ( $C_{MB}$ ) as a function of time. Source: Own

Fig. 3 presents only simulated results available for CAR1 and CAR2 samples. For MI, TX, AZ, and CA samples, the comparison of experimental and simulated results is available.

The VFA behavior over time is shown in Fig. 4. Fig. 4 presents all the samples (CAR1, CAR2, MI, TX, AZ, and CA), the comparison of experimental and simulated results is available. The comparison between field and simulated data shows a good agreement for all the samples. As SDF is consumed, the maximum VFA peaks after 25 to 50 days, then decays exponentially leading to MB generation. For all the samples, 150 to 200 days are required to consume all the VFA.

On the other hand, Methane production/consumption occurs slower (Fig. 5), reaching a peak after 150 days just when the VFA has been depleted, controlled by the specific decay rate ( $k_2$ ). For all the samples (CAR1, CAR2, MI, TX, AZ, and CA), only simulated results are available.

The numerical results spanning 1000 days of simulation, as depicted in Figs. 3-5, align closely with the anticipated outcomes based on the chemical processes inherent to the waste site. Moreover, the model accurately reproduces curve trends, with peak values closely resembling those reported by the authors [20,21].

### 4 Conclusion

The mathematical model proposed by McDougall in 2007 has been successfully implemented in COMSOL. Its validation was achieved through comparison with biochemical data collected from six laboratory experiments conducted on samples sourced from real MSW landfills in both the United States and the United Kingdom. In summary, the model delineates the biodegradation process within a bioreactor landfill, comprising three phases transitioning from SDF to MB via intermediate VFA stages. Graphical representations underscore the correlation between the consumption of the VFA phase and the subsequent increase in the MB phase, offering insights into the dynamics of the system.

Upon calibration of the model, we have successfully determined biodegradation parameters. These parameters exhibit strong agreement with laboratory experimental data, particularly concerning variations in biochemical parameters such as volatile

fatty acids and degradable solids within the waste samples. This alignment underscores the model's reliability in capturing the intricate dynamics of the biodegradation process. These refined parameters serve as a foundation for executing coupled Multiphysics models in subsequent analyses.

Integrating thermal dynamics, mechanical settlement, and hydraulic processes is essential for advancing the present waste backfill model. Thermal dynamics account for temperature's impact on biodegradation, while considering mechanical settlement ensures structural stability and deformation analysis. Hydraulic processes govern fluid flow, gas migration, and leachate transport. By incorporating these physics, we develop a comprehensive model that predicts temperature variations, structural integrity, and fluid dynamics within landfill systems, enhancing our management strategies.

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