



Doctoral Thesis

**MODELING THE DEGRADABLE ORGANIC CARBON IN  
MUNICIPAL SOLID WASTE LANDFILLS**

submitted in satisfaction of the requirements for the degree of  
Doctor of Science in Civil Engineering  
of the Vienna University of Technology, Faculty of Civil Engineering

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Dissertation

**MODELLIERUNG DES BIOCHEMISCHEN ABBAUS DES  
ORGANISCHEN KOHLENSTOFFS IN  
SIEDLUNGSABFALLDEPONIEN**

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*“Read! In the name of your Lord who has created the world and everything in it. He has created the man from a clot.*

*Read! And your Lord is the most generous. He has taught the man with His words. He has taught the man anything they do not know”*

*(Al Alaq 1 – 5)*

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## Abstract

Landfilling of municipal solid waste (MSW) represents an important source of long-term emissions due to the degradation of organic matter. Hence, numerous generic studies have been carried out to explore the transformation of landfilled wastes for assessing future environmental loadings. However, specific investigations into the behavior of organic carbon, taking into account the substantial variability in persistence to degradation, are rare. Thus, the objective of this study was to develop a model for the degradation of organic carbon in MSW landfills, taking into account different refractory levels of organic matter as well as landfill parameters such as temperature, pH, leachate recirculation, and climatic conditions

In order to create a suitable model, two approaches based on the batch reactor and the packed bed reactor principles were combined. The solid organic matter was assumed as a fixed-state matrix, while the gas and liquid phases were considered counter-current flows through the solid matrix. The degradation of organic matter was modeled in parallel for three differently degradable organic carbon fractions, assuming sequential three-stage biochemical reactions (acidogenesis, acetogenesis, and methanogenesis). All biochemical reaction steps and species were encoded using a C++ object oriented program under a Windows user interface.

The model was tested and improved by employing (i) data and results from an existing laboratory landfill simulation reactor, and (ii) field data from the Breitenau land-fill. Modeling and field results corresponded reasonably well: Of the readily degradable organic carbon, about 100% are degraded during the first 17 years, while of the slowly degradable only 3.5%, and none of the refractory carbon are transformed. Several simulations were performed to analyze the model sensitivity with regards to parameters influencing the degradation. It appears that within the boundaries of this study, landfill body temperature has a more profound effect on the degradation of organic matter than pH or leachate recirculation. The modeling results allow conclusions about operation and management of landfills with regard to shortening the expensive landfill after care.

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## Kurzfassung

Die Deponierung von Siedlungsabfällen stellt eine wichtige, durch den Abbau organischer Substanz bedingte Quelle von langfristigen Umweltbelastungen dar. Zahlreiche Autoren haben deshalb die Transformationen von Abfällen in Deponien zur Bestimmung zukünftiger Emissionen untersucht. Allerdings gibt es nur wenige Studien, in denen berücksichtigt wird, dass organische Kohlenstoffverbindungen unterschiedliche Persistenzen aufweisen. Das Ziel dieser Arbeit ist die Entwicklung eines Modells zum Abbau organischen Kohlenstoffs in Siedlungsabfalldeponien unter Berücksichtigung unterschiedlicher Persistenz sowie von Deponieparametern wie Temperatur, pH Wert, Sickerwasserrezirkulierung und klimatischen Bedingungen.

Der Modelansatz besteht in der Kombination eines diskontinuierlichen Reaktors mit einem Festbettreaktor. Die organische Substanz wird als feste Matrix behandelt, Gas- und Flüssigphase fließen im Gegenstrom durch den porösen Festkörper. Der Abbau der organischen Substanz wurde parallel für drei unterschiedlich refraktäre organische Kohlenstofffraktionen unter der Annahme von dreistufigen sequentiellen biochemischen Reaktionen (Acidogenese, Acetogenese, Methanogenese) modelliert. Alle biochemischen Reaktionsschritte und resultierenden chemischen Spezifizierungen wurden mit C++ und einem Windows Userinterface programmiert.

Das Model wurde anhand von (i) fremden Daten und Resultaten eines Labordeponiesimulationsreaktors, sowie (ii) eigenen Feldmessdaten der Deponie Breitenau validiert und optimiert. Die Resultate der Modellierung stimmten mit denjenigen aus Experiment und Feld recht gut überein: In den ersten 17 Jahren wurden 100% des leicht abbaubaren Kohlenstoffs, 3.5% des schwerer abbaubaren Kohlenstoffs sowie kein persistenter Kohlenstoff abgebaut. Die Modellsensitivität bezüglich Einflussgrößen des Abbaus wurde anhand verschiedener Simulationen ermittelt. Innerhalb der geprüften Intervalle hatte die Temperatur im Deponiekörper den größeren Einfluss auf den Abbau organischer Substanz als der pH Wert oder die Sickerwasserrezirkulation. Die Modellierungsergebnisse erlauben Schlussfolgerungen für den Deponiebetrieb hinsichtlich Gestaltung und Verkürzung der kostspieligen Nachsorge.

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## Nomenclatures

$a$	proportional constant of substrate concentration to supports half-maximum specific growth rate (dimensionless)
$c_g, c_l$	specific heat capacity of gas and liquid phases ( $\text{kJ kg}^{-1}$ )
$c_i$	concentration of $i$ th species in gas and liquid phases ( $\text{kg m}^{-3}$ )
$h$	depth of landfill cell (m)
$k$	thermal conductivity ( $\text{W m}^{-1} \text{K}^{-1}$ )
$k_C$	Contois saturation constant (dimensionless)
$k_{VFA}$	VFAs influence on organic matters hydrolyzing rate ( $\text{m}^3 \text{kg}^{-1}$ )
$kh$	hydrolysis rate constant ( $\text{kg m}^{-3} \text{day}^{-1}$ )
$k_M$	Monod saturation constant (dimensionless)
$k_{O_2}$	oxygen partial pressure saturation constant (Pa)
$p_{O_2}$	partial pressure oxygen (Pa)
$q$	flux heat transfer ( $\text{kJ day}^{-1}$ )
$q_G, q_L$	mass flow rate of gas and liquid phase ( $\text{kg day}^{-1}$ )
$q^{evp}$	evaporation rate of the moisture ( $\text{kg day}^{-1}$ )
$r_g, r_l, r_s$	biological reaction rate of gas, liquid, and solid phase ( $\text{kmol day}^{-1}$ )
$r_x$	microorganism growth rate ( $\text{kg m}^{-3} \text{day}^{-1}$ )
$u_m$	microorganism growth parameters that constant
$v$	volume of landfill cell ( $\text{m}^3$ )
$v_G$	volume gas in landfill cell ( $\text{m}^{-3}$ )
$v_L$	volume liquid in landfill cell ( $\text{m}^{-3}$ )
$v_W$	volume of water contained in the substrate ( $\text{m}^3$ )
$x$	concentration of microorganism ( $\text{kmol m}^{-3}$ )
$x, y$	fraction of gas and liquid phases (dimensionless)
$x_{ini}$	initial amount of microorganism ( $\text{kmol m}^{-3}$ )
$A$	surface area of landfill cell ( $\text{m}^2$ )
$B$	microorganism growth parameters that constant (dimensionless)
$E$	activation energy ( $\text{kcal mol}^{-1}$ )
$I_{VFA}$	VFAs influence on organic matters hydrolyzing rate (dimensionless)

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$K$	kinetic model parameter constant (dimensionless)
$K_H$	Henry's constant ( $\text{Pa m}^3 \text{ kmol}^{-1}$ )
$K_{sp}$	solubility constant ( $\text{kmol m}^{-3}$ )
$K_W$	water self- ionization constant ( $\text{kmol m}^{-3}$ )
$M$	total mass in landfill cell (kg)
$R$	universal gas constant ( $\text{kcal K}^{-1} \text{ mol}^{-1}$ )
$R_1, R_2$	degradable organic recovery rate ( $\text{kmol day}^{-1}$ )
$R_D$	self decayed rate of microorganism ( $\text{kmol day}^{-1}$ )
$R_G$	growth rate of microorganism ( $\text{kmol day}^{-1}$ )
$S_i$	mass of $i$ th species degradable organic matter in landfill cell ( $\text{kg m}^{-3}$ )
$T$	absolute temperature (K)
$Y$	yield microbial biomass produced by biological reaction (dimensionless)
$\Delta z$	distance heat transfer (m)
$\Delta H$	enthalpy ( $\text{kJ kmol}^{-1}$ )
$\alpha, \beta, \gamma, \delta$	stoichiometric coefficient of $i$ th species in biological reaction (dimensionless)
$\rho$	municipal solid waste density ( $\text{kg m}^{-3}$ )
$\theta$	moisture content in the substrate (%)
$\phi$	relative digestibility of organic matters (dimensionless)
$\pi$	ratio of a circles circumference to its diameter (dimensionless)
$\mu$	specific growth rate of microorganism ( $\text{day}^{-1}$ )
$\mu_{\max}$	maximum specific growth rate of microorganism ( $\text{day}^{-1}$ )
$\sigma$	constant to fit correction factor (dimensionless)
$\Omega_{(x)}$	environment inhibition factor (dimensionless)
$\Omega_{(T, pH, \theta)}$	temperature, pH, and moisture content inhibition factor (dimensionless)

### Subscripts

$a, b, c, n$  number of Carbon, Hydrogen, Oxygen and Nitrogen in chemical formula of organic matter (dimensionless)

# Chapter 1

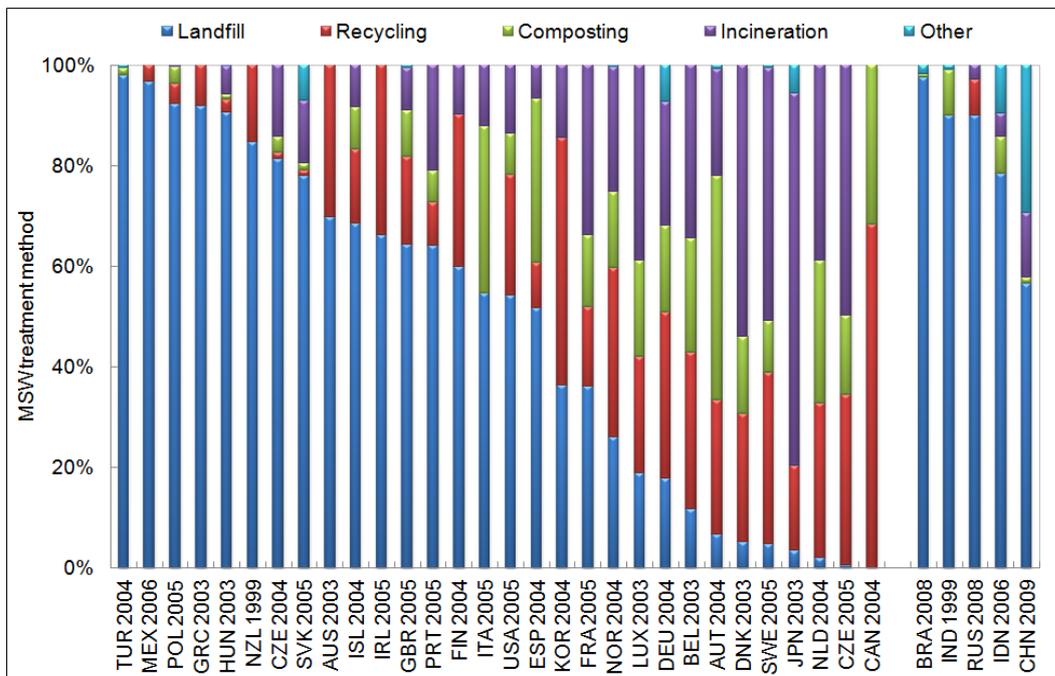
## Introduction

Change in affluence, lifestyle and consumption pattern and rapid population growth have led to a significant increase in municipal solid waste (MSW) generation. By 2006, global generation of MSW reached 2.02 billion tons per year, with an annual growth rate of approximately 7% compared to 2003, and is estimated to increase further (Wiggin, 2007). This global trend also applies to the Asia–Pacific region, where MSW generation has increased significantly due to high economic growth during the last decades. According to the International Panel on Climate Change (IPCC), MSW generation in Eastern Asian countries amounts to about 0.37 ton per capita and year, and in South Central Asia to about 0.21 ton per capita and year. In specific countries like Japan and Korea, about 0.4 ton of MSW are produced per capita and year (UNEP, 2009a).

The goals of waste management as stated in many national legislations to cope with these rising amounts of waste are: (i) to protect human health and the environment, and (ii) to conserve resources (Brunner and Rechberger, 2004). Various strategies and policies, such as the establishment of a recycling society, the “waste hierarchy”, or implementation of waste taxes have been introduced to reach these goals. The strategies are implemented by the application of technologies such as materials recycling, incineration, anaerobic digestion and landfilling. While such technologies are applicable in high GDP countries, emerging economies and developing countries have difficulties in allocating the necessary financial resources to such comparatively expensive systems. Thus, they often depend on landfilling as the main means for waste management. On a global scale, landfilling of untreated wastes remains the primary disposal method (Ding et al., 2001; Al–Yaqout and Hamoda, 2003; Kalyuzhnyi et al., 2003; Islam and Singhal, 2004; Rodríguez et al., 2004; Durmusoglu et al., 2005; Moraes and Bertazzoli, 2005; Yedla, 2005). In

addition to low costs, the simplicity of managing huge amounts of waste is another reason for landfilling in less developed regions.

Figure 1.1 shows the MSW treatment practice in selected industrialized and emerging countries. The figure indicates that landfilling is still the primary option for MSW treatment. In the European Union, about 40% of 260 million tons of MSW generated was landfilled in 2008 (Eurostat, 2013). Only a few countries, such as Germany, Denmark, Switzerland and Austria, have banned or at least restricted direct landfilling. Whereas in 1990 more than 50% of the MSW generated in Austria was landfilled, this share dropped to less than 0.5% in 2008 (BAWP, 2011). In contrast, by 2004 around 56% of 250 million tons of MSW generated in the USA had been dumped in landfills without any pretreatment. In emerging economic countries such as Brazil, India and the Russian Federation, more than 90% of the MSW generated is transported and directly disposed in landfills, while in Indonesia and China, the percentage of waste disposed in landfills is smaller. However, this is due to low MSW collection service coverage, leading to illegal MSW practices such as open burning, backyard dumping, discharging in rivers, etc.



**Figure 1.1** MSW treatment practice in industrialized (left) and emerging economic countries (right). The data compiled from OECD (2013), IBGE (2008), Maryev (2012) Sharholy et al (2008), MoE (2008) and UNSD (2013)

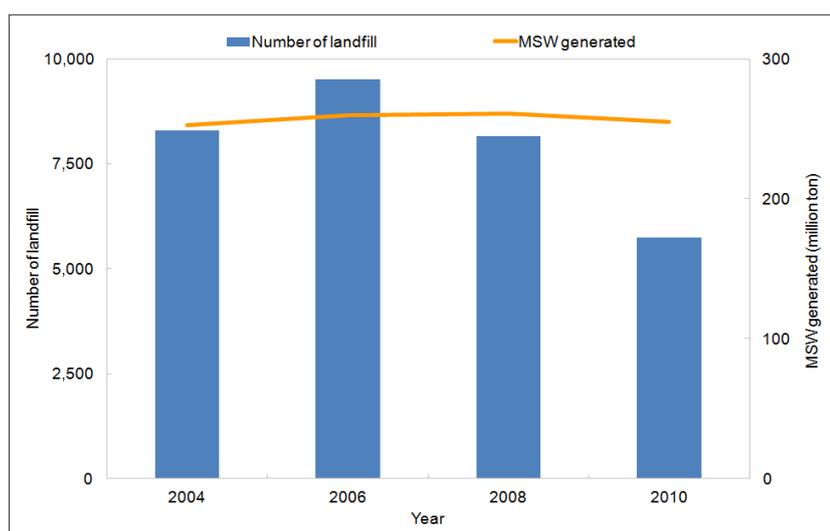
## 1.1 Background and Problem Definition

Landfilling with MSW, the globally predominant method of waste disposal is associated with long-term emissions of leachate and landfill gas. Both represent a potential hazard for the environment, in particular because of organic carbon and nitrogen. Landfill leachate contains high concentrations of dissolved organic matter, nitrogen compounds, salts and heavy metals. In order to prevent pollution of ground and surface waters and to comply with standards for discharges into receiving waters, leachate has to be properly treated. In contrast to industrial processes or other waste management processes (such as incineration), emissions from landfills have to be controlled for very long time periods (centuries) after the operation has been terminated (Belevi and Baccini, 1989). Long-term emissions from MSW landfills are determined by several factors, including the type of waste disposed of, landfill technology and operation, and the geologic and climatic conditions prevailing at the site. All of them determine the conditions within the landfill body (e.g. temperature, moisture content, pH, redox potential, etc.), which influence the rate and extent of biodegradation in MSW landfills. Favourable landfill conditions (e.g. sufficient water and nutrient supply, optimal temperature and pH, favourable gas exchange) can accelerate the degradation of organic matter by microorganisms and thus increase the release rate of emissions, resulting in shortening the aftercare period (Barlaz et al., 1990; Reinhart and Al-Yousfi, 1996; Kjeldsen et al., 2002). However, MSW contains different fractions of organic matter, from rapidly degradable to completely refractory (persistent to degradation) (Kjeldsen et al., 2002); the degradation of the latter by definition cannot be accelerated.

Landfilling with MSW and in particular its emissions pose multiple threats to human health and the environment in the short, mid and long term. In addition to the challenges mentioned above, mechanical stability is an issue of concern too. On the one hand, mechanical or static instabilities of MSW landfills are often the result of poor waste compaction, which may lead to mechanical failures causing landslides. On the other hand, degradation of organic matter can change mechanical properties of landfills too, resulting in stability problems with landfill bodies. Also, landfills

contribute significantly to greenhouse gas emissions. Landfill gas released from decomposing organic matter mainly contains methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>), both generally categorized as greenhouse gases (GHGs) and contributing to climate change. Hence, the degradation of organic carbon is an important process for landfilling, and there are plenty of reasons for analysing and controlling this process.

In order to minimize the harmful effects of landfills for human health and the environment, regulations related to the quality of the waste deposited, the degree of waste containment and the operation procedure for landfilling have increased significantly during the last decades. For instance, the Waste Frame Work Directive 2008/98/EC (EU, 2008) and the Council Directive on the Landfilling of Waste (EU, 1999) regulate standard operational procedures and technical requirements for waste management within the European Union. The latter directive also demands EU member states reduce the amount of biodegradable waste going to landfills. Moreover, according to the landfill directive, all member states are required to cover closed landfills with an impermeable cover layer to control the intrusion of precipitation into the landfill, thereby reducing leachate generation and the risk of groundwater contamination.



**Figure 1.2** Number of landfills and total MSW generated in EU 28 member states (Eurostat 2013)

As a consequence of this well-founded regulation, the number of active landfills in the EU member states decreased from 9,520 in 2006 to 5,740 in 2010. However, the

distribution was quite uneven among the states. While in most member states the number of landfills decreased by up to 93%, in some less developed states it increased by up to 43% compared to the year 2004 (Eurostat, 2013). Figure 1.2 shows the trend of the number of landfills and total amount of MSW generated in the EU between 2004 and 2010. Also, in other affluent countries a decreasing trend in the number of landfill sites can be observed. For instance, the number of MSW landfills in the USA decreased from 3,197 in 1995 to 1,754 in 2005 (U.S. EPA, 2009).

Despite the fact that the design, construction and operation of landfills has been regulated more and more in affluent countries (e.g. EU landfill directive) during the last decades, numerous questions related to the long-term behaviour of MSW landfills are still unclear. How long can a landfill cover prevent water intrusion into the waste body? The performance of cover systems depends on many factors, such as design and construction, climatic conditions, vegetation growth at the site and the composition of the landfilled waste, and is thus hardly predictable. To what extent are the biodegradation rates of organic matter in landfills reduced by the exclusion of water input? How does future intrusion of water affect waste degradation and thus landfill emissions?

Another unanswered question is how much of the organic matter remains inside the landfills, and whether the landfill emissions from the degradation of this organic matter will meet environmental standards when the low-permeability cover deteriorates in the future. Countermeasures have to be developed to ensure that the goal of waste management will be achieved. In order to design such measures, either sufficient knowledge about the degradation of organic matter in landfills over time must be available, or the status (amount, characterization) of the organic matter remaining inside the landfill must be known. The latter is complicated, costly and time-consuming, and can only be determined by collecting representative waste samples and measuring the organic matter in the laboratory. The former requires the development of a numerical model. At present, this option is likely to provide inaccurate results as most of the models available today assume similar

degradability for organic matter not differentiating between refractory and easily degradable organic carbon compounds. Also, the effects of ambient climate conditions on the degradation rates are rarely observed.

## **1.2 Objectives and Research Questions**

In the last two decades, numerous mathematical landfill models of different degrees of complexity have been developed (see Chapter 2) and applied. However, the application of most models developed has been limited either to theoretical simulations or to experiments designed by the model developer himself, thereby ensuring that all required input data of the model are measured and output data generated can be compared with experimental data. The general applicability of those models, however, suffers from this practice. In addition, the inevitable conception interdependency of mathematical model and experimental data generated by the model developer bears the risk of indistinguishable methodological errors.

In view of the facts given above, the objectives of the present thesis are:

- 1) To develop a mathematical landfill model that allows the prediction of the degradation of organic matter in MSW landfills,
- 2) To link this model to landfill emissions,
- 3) To validate the performance of the model with landfill data from laboratory experiments and full-scale landfills,
- 4) To evaluate the importance (sensitivity) of different parameters (e.g. temperature, pH, moisture content) on the degradation of organic matter in MSW landfills, and
- 5) To apply the model for the determination of the degradation of different organic carbon (easily degradable to refractory) in MSW landfills and for predicting landfill emissions.

The model to be developed aims at general applicability regarding different waste compositions, different degradability of organic matter and different climatic conditions, as well as different operational measures. Therefore the following research questions have been chosen:

- Which modelling approaches should be taken into account for predicting the organic matter degradation inside MSW landfills?
- How could these approaches be adapted in order to consider the behaviour of gas, liquid and solid phases present in MSW landfills?
- What is an appropriate definition of the different degradable organic materials, from easily degradable to completely refractory?
- How can the model simulation results be validated, and which parameter should be used to assess the model sensitivity for that parameter?
- Which kind of organic matter remains in the MSW landfill leave through over time?
- What is the long-term effect of the differently degradable organic matter on the landfill behaviour and its emissions?

### **1.3 Outline of the Thesis**

The first step of this thesis was to review and evaluate existing modelling approaches with respect to simulating the long-term emissions of landfills. Based on this evaluation, a new mathematical model was developed by adopting a combination of the Packed Bed Reactor (PBR) and Batch Reactor concepts. In a second step, the developed model was validated using data from laboratory experiments described in the literature. In addition to the model validation, sensitivity analysis was conducted in order to assess the significance of single input parameters on the degradation of organic matter and thus the emissions of MSW landfills. Lastly, the model was applied to field data in order to estimate the extent of persistent organic matter present in a field scale MSW landfill. This thesis is organized into six chapters as follows:

Chapter 2 provides the literature review of relevant previous studies. Therefore, the typical characteristics of MSW disposed in landfills, and the decomposition mechanisms of organic matter in MSW landfills including physical, chemical and biological influences, are reviewed. A state-of-the-art landfill is described to provide the background knowledge and research motivation to conduct this study, whilst the model development approach use and results that have been reported in the previous studies are described and evaluated subsequently for consideration in the model development.

Chapter 3 describes the theoretical approach and model development including material and heat balances, biological degradation pathways of decomposing organic matter, and parallel and sequential degradation of readily, slowly and refractory degradable organic MSW matter. The development of the method to accommodate the environmental condition feedback to the organic matter decomposition rate is described as well.

Chapter 4 outlines the model validation by comparing the model results to laboratory experimental data published in the literature. Also the input data for the model, mainly given by the experimental set-up, the MSW characteristics and analytical procedures, are described briefly. Then, the sensitivity analysis is carried out in order to quantify the impact of single parameters on the decomposition rate of organic matter.

Chapter 5 presents the results and discussion of the model application to a closed full-scale landfill. The simulation results are compared with available field observations. The differences of the model outcomes and field data are highlighted and evaluated. In addition, advantages and disadvantages of the current “dry tomb” strategy (Lee and Jones-Lee, 1996) with respect to the long-term landfill emissions of MSW landfills are discussed.

Chapter 6 is divided into two parts. In the first part, the conclusion of the model validation and the results of sensitivity analysis are presented and discussed. In the

second part, recommendations for future work and improvement of the models are given.

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## **Chapter 2**

### **Literature Review**

The degradation of organic matter of municipal solid waste (MSW) occurs through several stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis. This process is influenced by many factors, such as the temperature, pH and moisture content of the microorganism living environment, as well as the characteristic of organic matter content in MSW. This chapter describes the scientific concept of decomposition of degradable and refractory organic matter of MSW. Before this concept is described, the definitions of solid waste, type and source and waste management practice are discussed at the beginning to give an overview of the current conditions. This is followed by a description of the state of the art of MSW landfill and landfill emissions behaviour.

In the next section, the kinetic microorganism growth concept, which is fundamental knowledge for understanding the microorganism metabolism, is described. This aims to give an overview of the mechanism of microorganism metabolism during decomposition of organic matter under aerobic and anaerobic conditions. Finally, in the last section the model for estimating the decomposition of organic matter in MSW landfills is developed and described. The description is focused on the methodological approach and assumptions have been made to accommodate uncertain factors. This information is very important for evaluating the advantages and disadvantages of the existing model and attention needs to be paid to it during the development of the model in this study.

#### **2.1 Municipal Solid Waste**

The content of organic carbon in solid waste deposited in landfill determines the landfill gas and leachate emissions and the after-closure maintenance period. High

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organic carbon content yields significant amounts of landfill gas and organic load of leachate. Some of the organic carbon will be converted in landfill during the “bioreactor” period and emitted into the environment, where 90% of it is released as landfill gas in the form of methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>) at a ratio of approximately 60 to 40, while the rest will migrate downward as organic load of the leachate. The unconverted organic carbon during the bioreactor period remains in landfill and will be converted at a slow rate that is considered as long-term emissions.

The organic carbon content in solid waste is greatly dependent on the composition of the solid waste, which is influenced by numerous factors including region, norm and culture, income level, and the political will of the government. These factors have led to disparity in the definition and criteria of MSW as well as the waste management practice in different countries. Therefore, this section describes the definition, type and generation sources and MSW composition in developing and highly industrialized countries.

### **2.1.1 Definition of Municipal Solid Waste**

There is no universal definition of solid waste. In general, solid waste can be defined as merchandise that is useless or not wanted anymore. This matter becomes waste when discharged by the owner, but could be resources for others that are subsequently used as materials for the production of similar matter (e.g. recycling) or converted into another form such as energy (e.g. waste to energy). These human-induced resources, so-called anthropogenic resources, will increase significantly and become very important resources in the future (Brunner and Rechberger, 2004).

At legislation levels, solid waste usually refers to municipal solid waste (MSW) and is defined differently in various countries or regions depending on the strategy and goal of waste management. In Europe, MSW is defined as “waste from households, as well as other waste which, because of its nature or composition, is similar to waste from households” (EU, 1999).

The Environmental Protection Agency of the United States (US EPA) defines MSW as waste from residential, commercial, institutional and some industrial sources (Tchobanoglous and Kreith, 2002), while in developing countries like Indonesia, MSW is defined as waste from households and household-like waste deriving from commercial areas, industrial areas, special areas, social facilities, public facilities and/or other facilities (MoE, 2008). For comparison, the different definitions of MSW are compiled in the right box.

Definition of MSW
EU Directive (1999): "waste from household, as well as other waste which, because of its nature or composition, similar to waste from household"
Gol (2008): "waste from household and household-like waste derives from commercial area, industrial areas, special areas, social facilities, public facilities, and/or other facilities"
IPCC (2006): "waste collected by municipalities or other local authorities, include household waste, garden (yard and park waste, and commercial /institutional waste"
OECD (2013a): "materials that are not prime products (that is, products produced for the market) for which the generator has no further use in terms of his/her own purposes of production, transformation or consumption, and of which he/she wants to dispose"
PAHO (2010): "solid or semi-solid waste produced through the general activities of a population center. Includes waste from households, commercial businesses, services, and institutions, as well as common (non-hazardous) hospital waste, waste from industrial offices, waste collected through street sweeping, and the trimmings of plants and trees along streets and in plazas and public green spaces"
RCRA (2002): "any garbage or refuse, sludge from a wastewater treatment plant, water supply treatment plant, or an air pollution control facility and other discarded material, including solid, liquid, semi-solid, or contained gaseous material resulting from industrial, commercial, mining, and agricultural operations, and from community activities"

### 2.1.2 Municipal Solid Waste Categories

There are several categories of solid waste distinguished based on the source of origin (e.g. household, commercial, institutional, municipal services, hospitals, agriculture, manufacturing and industries, mining and quarrying, energy production, water purification, construction sites). MSW often refers to solid waste from the first four sources, while solid waste from the other sources is usually collected separately due to its hazardous properties and the huge amount generated from specific places. Table 2.1 lists the solid waste categories, sources of origin and its typical content.

MSW accounts for 25% of the 2.6 billion tons of total solid waste generated in high-income-level countries (OECD, 2013b). This amount is similar to construction and demolition (C&D) waste. In some countries such as Austria, Germany, Luxembourg and the United Kingdom, C&D waste is more than three times that of MSW. Nevertheless, the MSW generated is smaller than C&D waste; in fact, this waste is

one of the hardest waste types to manage effectively. It consists of a diverse range of materials (organic, paper and cardboard, plastic, leather, textile and rubber, wood, glass, metal, ashes, etc.) and all mixed together (see Table 2.1). The composition of MSW also varies, both seasonally and geographically, from country to country, and urban to rural areas. In contrast, C&D and other solid waste tend to be more homogenous (McDougall et al., 2001).

### **2.1.3 Composition of Municipal Solid Waste**

Although MSW contains various materials (see Table 2.1), the composition of MSW usually used in waste management streams is classified into six major components (i.e. organic, paper and cardboard, plastic, glass, metal and other). This classification can be further expanded depending on the waste management goals to be achieved and the waste treatment facilities that exist. For example, the composition of MSW in Europe is classified into 52 categories as listed in the European waste catalogue. This catalogue was later adopted together with hazardous waste into Irish legislation, under the Waste Management Act 1996 (EU, 1996).

The composition of MSW is influenced by numerous factors, such as region, norm and culture and waste management policies, but income level might be the main factor, because consumption habits and lifestyle greatly depend on income level. Figure 2.1 shows the MSW composition from different income-level countries. In general, the organic fraction of MSW in low-income countries is highest and decreases steadily as income level increases. This is typical waste in low-income countries and has a high organic fraction (Diaz et al., 1993). The high fraction of organic matters results in high waste density and moisture content. The organic fraction of MSW in low-income countries is more than twice that of high-income countries. In contrast, the paper and cardboard fraction of MSW in high-income countries is more than six times that of low-income countries. As the MSW comprises high paper and cardboard content, anaerobic treatment such as bio-gasification and landfilling is not suitable. Degradation of the cellulosic compounds

contained in paper and cardboard is slower under anaerobic conditions (Podkaminer et al., 2012).

**Table 2.1** List of solid waste classes, origin source, and typical solid waste content

Waste category	Waste origin source	Typical content of solid waste
Household waste	Single- and multi-family dwelling	Organic (e.g. foods and compostable wastes), papers and cardboards, plastics, leather, textile and rubber, woods, glass, metals, ashes, special waste (e.g. furniture, consumer electronics, batteries, tires), hazardous waste (e.g. insecticide and cleaning agent, batteries), and e-waste (e.g. computers, phones, TVs).
Commercial waste	Stores, markets, restaurants, hotels building offices, station, and airports	Organic, papers and cardboards, plastics, woods, glass, metals, special waste, hazardous waste, and e-waste
Institutional waste	Schools, hospitals (excl. medical waste), government offices.	Same as commercial waste
Municipal services waste	Streets sweeping, parks, and recreational areas	Grass, leaves and wood from trimmings tree, sand, mud, rocks, other debris from unpaved soils, and litter especially in developing countries
Medical waste	Hospitals, dental practices, blood banks, and veterinary clinics	Bandages, culture dishes and other glassware, gloves, hazardous waste (e.g. needles, lancets), cultures stocks, swabs, removed body organs, pharmaceutical waste, and radioactive waste from cancer therapies.
Agricultural waste	Agriculture land	Rice husks, cotton stalks, coconut shells, coffee waste, and hazardous waste (e.g. pesticides)
Mining and quarrying solid waste	Fuels resources and raw materials mining	Excavated soils, overburden (e.g. overlying material of mineral deposit), waste rock and tailing
Manufacturing and industrial wastes	Chemicals plants, iron and steel production, cement plant, pulp and paper, plastics and resin manufacturing	Hazardous waste (e.g. organic and inorganic chemicals), metals (e.g. iron, steel), ashes, woods, paper and cardboard, plastics and resin manufacturing
Energy production waste	Waste to energy, coal and nuclear power plants	Slag, fly ash, and radioactive waste from nuclear power plant
Water purification waste	Wastewater treatment plant	Sewage sludge, biosolids, sand, disinfectant and coagulant containers
Construction and Demolition waste (C&D)	Site construction	Concrete, wood, asphalt, gypsum, metals, bricks, glass, plastics, salvaged building components, and trees, stumps, and soils and rock

Source: Tchobanoglous and Kreith (2002)

#### 2.1.4 Degradation of MSW Organic Matters

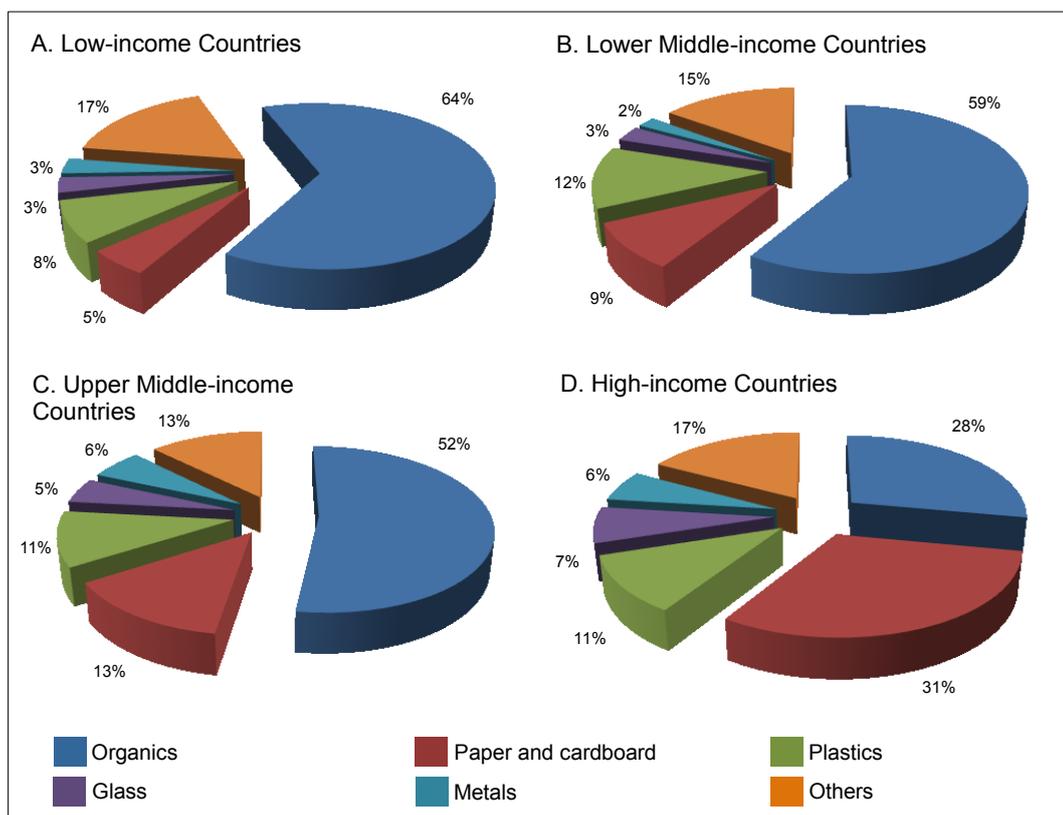
As MSW contains various materials (see Table 2.1), the content of organic matter also varies widely depending on the material and its composition. Generally, organic

matter can be distinguished into three categories based on its degradability level, namely readily, slowly and non-degradable organic matter (Henze et al., 2000). There are no specific criteria to categorize whether the organic matter is readily or slowly degradable yet, but it should be broken down naturally by microorganisms through the catabolic reactions. However, the Technical Guidance Document on Risk Assessment of the European Commission prescribes the rate constant ( $k$ ) and half-life of readily degradable organic matter as  $1.0 \text{ hour}^{-1}$  and 0.69 hours, respectively. A similar criterion is applied by the Environmental Protection Agency of the United States to describe the readily degradable organic matter in wastewater treatment using the activated sludge process (U.S. EPA, 2013). Therefore, organic matter that has a lower rate constant and high half-life is classified as slowly degradable organic matter.

Readily degradable organic matter is the fraction of organic matter that is directly available for biodegradation by heterotrophic organisms and transformed into fermentation products (Henze et al., 2000). This can be considered to be materials such as simple carbohydrates (i.e. glucose, fructose), fats and protein. The MSW components that contain a high concentration of readily degradable organic matter are food and compostable wastes. The sludge generated from wastewater treatment plants also contains large quantities of simple carbohydrates and proteins (Kapdan and Kargi, 2006; Reddy et al., 2011). During organic matter degradation, protein plays an important role as the nitrogen source for microorganism growth (Ding et al., 2008).

Slowly degradable organic matter is characterized by the high molecular weight of particulate organic matter, which must be broken down by extracellular enzymes through a process called hydrolysis, before it is available for degradation (Henze et al., 2000; Morgenroth et al., 2002). The hydrolysis usually occurs during close contact between the organisms and a surface of the organic matter. The slowly degradable organic matter in MSW waste is probably a polysaccharide compound (i.e. cellulose, hemicelluloses), which is a major component of paper and cardboard. The cellulose content in paper and cardboard ranges approximately from 75% for

low-grade to 90% for high-grade papers, while cellulose content in textiles is up to 98% of dry weight (Liu and Liptak, 2000). Most cellulose is degraded aerobically, but only 5–10 % is degraded under anaerobic conditions (Leschine, 1995).



**Figure 2.1** MSW compositions of different income countries level (Hoornweg and Bhada-Tata, 2012)

Cellulose almost never occurs alone in nature but is usually associated with other plant substances such as hemicelluloses and lignin. This association also affects cellulose degradation (Leschine, 1995). The degradation of cellulose and hemicelluloses of MSW (wood, grass and backyard wastes) is hindered by lignin. Structurally, lignin is a non-water-soluble complex polymer consisting of phenyl propane units joined together by different types of linkages. This complex structure together with high molecular weight and insoluble properties make lignin hardly degradable, particularly under anoxic conditions (Colberg and Young, 1982; Zeikus et al., 1982; Eriksson et al., 1990; Blanchette, 1995; Pérez et al., 2002). Moreover, in many studies no lignin degraded under anaerobic conditions has been observed (Hackett et al., 1977; Micales and Skog, 1997). Hence, lignocelluloses (lignin along

with cellulose and hemicelluloses) can be categorized as refractory–degradable MSW organic matter.

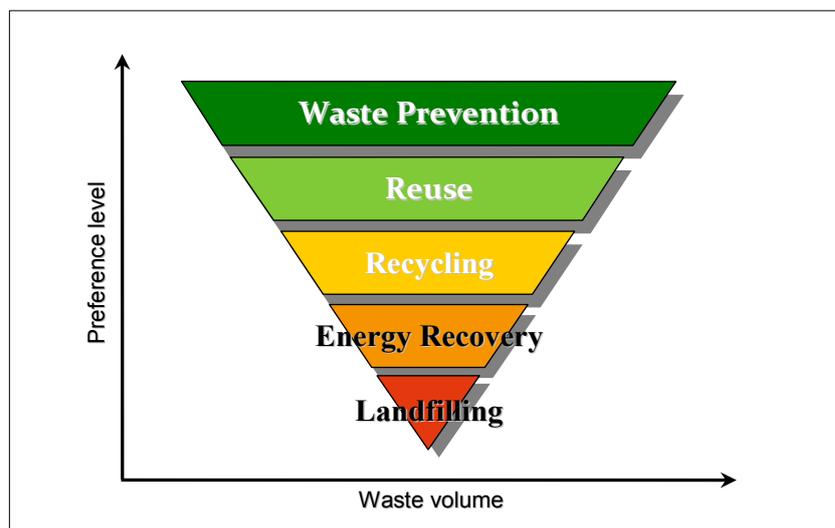
### **2.1.5 Municipal Solid Waste Treatment**

In general, there are four waste treatment methods that can be applied to deal with MSW: recycling, composting, combustion using incineration, and disposal in a landfill site. The MSW treatment methods can be used either singly or as a combination of two or more of them, depending on the existing MSW treatment facilities as well as sufficient funds being available for collection and treatment. For example, the recycling of the recyclable MSW fraction will be effective and economically viable if collection and transportation are carried out separately from other waste. Similarly, the lifetime of landfill becomes longer and landfill emissions lower when only the incineration–treated MSW is disposed in the landfill site.

In high–income countries, several waste treatment methods are carried out sequentially to achieve the waste management goals (i.e. to protect human health and the environment as well as to conserve natural resources). This approach is known as Integrated Waste Management (IWM), which is defined as the selection and application of suitable techniques, technology and management programmes. For example, the state of California in the U.S. has carried out MSW treatment in a hierarchy of source reduction, recycling and composting, waste transformation and landfilling (Tchobanoglous and Kreith, 2002).

In the EU, the MSW treatment strategy was set up by establishing the Council Directive 2008/98/EC on Waste and Repealing Certain Directives. This directive distinguishes the MSW treatment strategy into five stages. The most preferred MSW treatment practice is waste prevention, which is defined as a measure that should be taken before material becomes waste. The next preferred treatment is reuse, followed by recycling, recovery including energy recovery, and finally the least preferred method is disposal (EU, 2008). Figure 2.2 shows an illustration of the European waste management hierarchy. The key concepts, principles and objectives

to be achieved are not described in this literature review, but can be found elsewhere (Tchobanoglous and Kreith, 2002; EU, 2008).



**Figure 2.2** The European MSW treatment hierarchy

## 2.2 State of the Art Municipal Solid Waste Landfill

Landfill or final disposal is a site where municipal solid waste (MSW) is disposed of by burial into a pit in the land. This method is the oldest waste management method and still the primary method practised in many countries around the world. Approximately 2.2 billion tons of MSW were collected worldwide in 2006, and most of it was disposed of in landfill (Kwon et al., 2010). This amount increased by about 37% between 2007 and 2011 (UNEP, 2009b). The main reasons that landfill is still the primary method of MSW practised currently are the low cost and simplicity in handling the municipal solid waste, particularly in developing countries (Read et al., 1997; Warith, 2003). Nevertheless, some developed countries such as the United States, Great Britain and Finland are still highly dependent on landfill for handling their MSW; moreover, no pretreatment is carried out prior to MSW being disposed in the landfill site.

### **2.2.1 Municipal Solid Waste Landfill Criteria**

Generally, landfill sites are classified into several types according to waste criteria. In the EU, according to Council Directive 1999/31/EC, landfill sites are classified into three groups. The first is landfill for hazardous waste. This landfill was built for disposed material containing one or more hazardous trait (e.g. flammable, reactive, corrosive and/or toxic). The second is landfill for non-hazardous waste. This landfill includes landfill for MSW, industrial waste, bottom ash, etc. The last is landfill for the disposal of inert waste such as construction demolition debris (C&D) and excavated soils. However, as stated in the previous section, this study focuses only on MSW landfill including landfill criteria, landfill operation and management (O&M) and all related aspects.

In terms of disposal method, MSW landfill can also be classified into three types, namely open dump, controlled dump and sanitary landfill. The main differences among these include initial landfill selection, technology use, standard operation procedure (SOP) of daily landfill (O&M) and post-closure maintenance. According to the waste timeline, these differences were probably due to the differences in public awareness and technology available within landfill. The principal difference of each is described in the following paragraphs and summarized in Table 2.2.

#### **2.2.1.1 Open Dumping**

Open dumping is the primitive method used within MSW landfilling practice. This method has been practised since 400 BC; however, it is still used as the primary landfilling method practised around the world, particularly in low-income countries. This method is neither safe nor hygienic, so that not realistic anymore apply this method as part of MSWM even in low-income countries. The main reason open dumps are still used around the world is that they are easy and the cheapest way to manage generated MSW. In rural areas in developing countries where MSWM services are still not available, households or communities usually build open dump sites that are used for disposing their MSW.

From a technical point of view, nothing can be said about this type of site, since not all technical aspects of landfills are considered. Neither site selection nor landfilling procedures are carried out. The landfilling of MSW occurs without any planning and can take place anywhere in a vacant area, but usually within a government-owned property. Open burning is usually carried out to reduce the volume of MSW and preserve disposal space at the dump site. Since the quantity and composition of incoming MSW would not pass an inspection, the probable toxicity and hazardous waste mixed with the common MSW is very high. Therefore, the threat to human health and the environment from the operation of this site becomes very significant. For example, due to the absence of a fence to prevent animals from foraging on the dumps, the site can transmit diseases via the terrestrial food chain, as well as by pests through infestation (Rushbrook and Pugh, 1999).

#### **2.2.1.2 Controlled Landfilling**

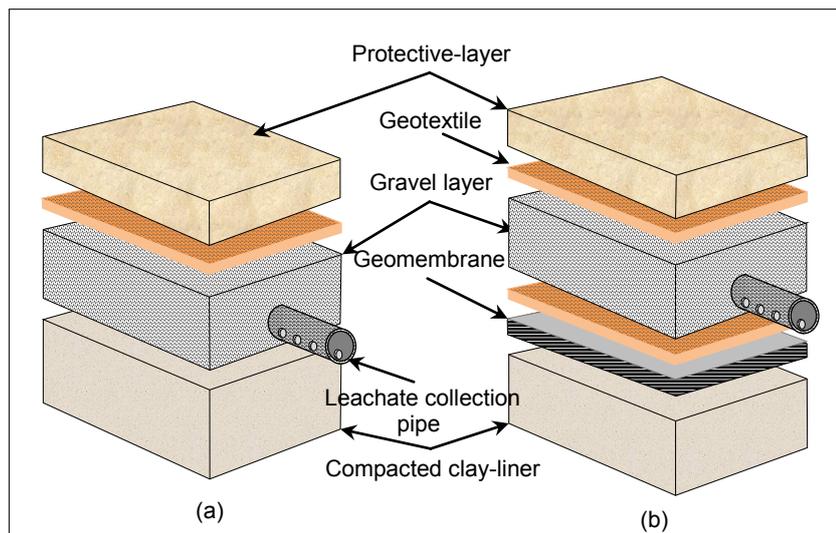
Controlled landfilling is MSW disposal on a site constructed without applying technology that can prevent landfill operation impacting on human health and the environment. However, the disposal site was built already through landfill site selection by considering the minimum standard required to protect human health and the environment. For example, the site was selected with respect to hydro-geological aspects, and distance to the residential area. The landfill capacity was also already determined by considering the average volume of waste generated.

Although the site has been through planning and site selection, a construction site for controlled landfilling is usually built under very simple constructed works to prepare the base of the landfill disposal site, leachate collection, and the necessary drainage system to control the surface water around the site. The collected leachate will flow into the sewer system either without or after thorough simple treatment. The landfill gas generated from the landfill site will be directly released into the atmosphere. Moreover, during the landfilling operation only a partial quantity of incoming MSW is controlled or there is no control at all, only basic data may be recorded, and occasionally cover applications are carried out. The scavenging

activities are unmanageable and take place the whole time from early morning until late in the evening.

### 2.2.1.3 Sanitary Landfill

Sanitary landfill is an engineered MSW disposal site that is designed, constructed and operated in a manner to protect human health and the environment. This idea was proposed by the American Society of Civil Engineers (ASCE) to replace open dumping in 1959. The idea emerged based on finding that shows the waste compaction and soils cover application could increase the safety and aesthetics aspects of MSW landfill operations. These measures were still insufficient to reduce problems associated with landfill operations that potentially threaten human health and the environment, such as leachate and landfill gas emission (Reinhart and Townsend, 1998). However, after being introduced in 1959, the sanitary landfill technology was improved significantly, particularly in planning, design, operation, closure and post-closure management. The modern sanitary landfills was equipped with baseliner and top cover systems that are able to prevent leachate and landfill gas emissions directly released into the environment.



**Figure 2.3** The schematic typical baseliner of sanitary landfill (a) single baseliner and (b) composite baseliner systems (Munawar and Fellner, 2013).

The potential of leachate to threaten human health and the environment is greatly determined by the type and effectiveness of baseliner to prevent it migrating and polluting underground. Generally, there are two baseliner types used widely in modern sanitary landfill, namely single and composite baseliner systems. The single baseliner consists of a compacted clay liner, a gravel layer, geotextile and protective layer, while the composite baseliner consists of a compacted clay liner, plastic liner (usually made of high-density polyethylene, HDPE sheet), gravel layer, geotextile and protective layer. This protective layer is traditionally composed of soil, sand and fine gravel, but many landfills now use a layer of soft refuse instead of the traditional method. Soft refuse is commonly prepared from mixed paper, organic waste and shredded tyres or rubber. Figure 2.3 presents a schematic of a typical sanitary landfill technical barrier.

Since a composite baseliner is more effective for preventing leachate migration to pollute underground water than a single baseliner, a modern MSW landfill was constructed with this baseliner system. However, many sanitary landfills in developing countries are still constructed with a single baseliner due to the unaffordable investment cost. In addition, sanitary landfills also benefit from the pre-planned installation of landfill gas control and utilization measures, extensive environmental monitoring, better organization and trained teams, detailed records of incoming MSW, and on-site leachate treatment to supplement the leachate collection system (Rushbrook and Pugh, 1999).

### **2.2.2 A Modern Sanitary Landfill Concept**

The decomposition of degradable organic matter in MSW landfills will take from decades to centuries depending on several factors, including waste characteristic, landfill operation, environmental conditions, etc. (Townsend et al., 1996; Tchobanoglous and Kreith, 2002). Common MSW landfill operations are usually carried out by piling up MSW into a landfill cell, and then the landfill is covered with soil after it has reached its full capacity. Grass and other wild plants will grow quickly over the landfill cover since rich organic content is abundantly available

inside the landfill site. Occasionally, the landfill operator staff will come to collect some samples and analyse them for aftercare management purposes. Aftercare maintenance of closed landfills typically includes monitoring landfill emission (e.g. leachate and landfill gas) and receiving systems (e.g. groundwater, surface water, soil and air) and maintenance of top covers, and leachate and landfill gas collection systems (Laner et al., 2012). This would take from several decades to centuries and require high expenditure.

**Table 2.2** The comparison key characteristic of MSW landfill

No.	Parameter	Landfill type		
		Open Dump	Controlled Landfill	Sanitary Landfill
1.	Site selection	Unplanned and often improperly sited	Selection with respect to the hydro-geology	Selection based on environment risk assessment, public and economic acceptance
2.	Landfill capacity	Unknown capacity	Under planned capacity	Under planned capacity
3.	Landfilling plan	There is no cell planned and the disposal is at anywhere	There is no cell planning, but the disposal is carried out only at designated working face	Planned cell development and disposal is carried out at the smallest designated working face
4.	Site preparation	No preparation	Grading of the bottom disposal site, necessary drainage and surface water control around of the site	Extensive preparation baseliner system
5.	Leachate collection and treatment	No leachate collection	Leachate collection without any treatment	Leachate collection and completely treatment
6.	Landfill gas management	No gas management	Partial or no gas management	Capture for energy recovery or flared
7.	Incoming waste input	No control over quantity and composition of incoming waste	Partial or no control over quantity and composition of incoming waste, but limited only for MSW	Full control over quantity and composition in coming MSW and special provision for other waste type
8.	Record keeping	No record keeping	No or basic record keeping	Completely record keeping, volume, type, source and designated site
9.	Waste compaction	No waste compaction	No or occasionally waste compaction	Daily waste compaction
10.	Daily cover application	No cover application	No or occasionally cover application	Daily cover application
11.	Security	No fencing	Partly or no fencing	Secure fencing with gate
12.	Scavenging and grazing animal	Unmanaged scavenging and grazing animal	Controlled scavenging but no grazing animal allowed	No scavenging and grazing animal allowed
13.	Closer	No final cover application	Covered with soils without or partially compacted	Fully covered and post-closure management
14.	Impact to human health and the environmental	Risky to human health and the environmental	Lesser risk to human health and the environmental compare to open dump	Minimum risk to human health and the environmental

Source: UNEP, 2009

Improvement of aftercare maintenance of MSW landfills can be achieved through implementation of modern MSW landfill methods, either bioreactor landfill or final

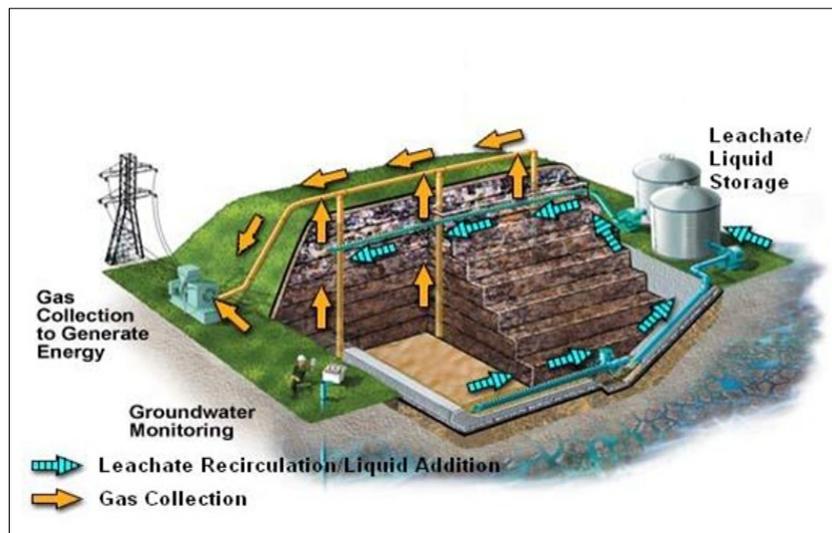
sink. Implementation of bioreactor landfill could reduce the aftercare maintenance period by accelerating the decomposition of degradable organic matter by introducing technology beyond that necessary for conventional landfill, while final sink achieves that condition through preliminary treatment of incoming waste prior to disposal in landfill sites by means of either mechanical and biological treatment (MBT) or thermal treatment. Both of these methods require greater expenditure in advance for construction and operation than the conventional landfill method, but the total cost is still comparable if not more advantageous (Berge et al., 2009). The numerous advantages that would result from bioreactor and final sink landfill operations include reduced leachate treatment costs, a high rate of landfill gas production (e.g. anaerobic bioreactor landfill), a minimal risk of landfill operation to human health and the environment, earlier beneficial reuse of landfill sites and shorter aftercare maintenance. These advantages could reduce the high costs associated with construction and operation.

#### **2.2.2.1 The Bioreactor Landfill**

A bioreactor landfill is an improved sanitary landfill constructed and introduced using additional technology beyond that necessary in conventional sanitary landfill to enhance biological processes, and to transform and to stabilize the readily and moderately decomposable organic constituents of MSW within bioreactor process implementation. A bioreactor landfill significantly increases the extent of waste decomposition, conversion rates and process effectiveness over what would otherwise occur within the landfill (Pacey et al., 1999). Stabilization means that the environmental performance measurement parameters (e.g. composition and rate of landfill gas, and concentrations of leachate) remain at steady levels, and should not increase in the event of any containment system failures beyond the lifetime of the bioreactor process (Warith, 2002).

A bioreactor landfill can be operated under either anaerobic, aerobic or hybrid conditions. For this purpose, appropriate containment and moisture/air injection systems are the most important requirement in operating the landfill under desired

conditions. Other strategies such as shredding MSW input, amendment and recalculating leachate content (i.e. pH value, nutrient content, etc.) and temperature management might be necessary to provide optimal conditions for microorganism metabolism. A bioreactor landfill can also be built from an old landfill through improvement of the containment system, and installation of moisture/air injection facilities and necessary equipment to control bioreactor functionality.



**Figure 2.4** The schematic of view a bioreactor landfill (U.S. EPA, 2012)

The advantages of bioreactor have been investigated and well documented, from laboratory– (Pohland, 1975), pilot– (Pohland, 1980; Jiang et al., 2007; Abdallah et al., 2013), and full–scale bioreactor landfills (Pacey et al., 1999; Yazdani et al., 2006; Hanchock et al., 2007). The results of these studies showed that laboratory– and pilot–scale bioreactor landfills could significantly increase the decomposition rate of readily and moderately decomposable organic constituents of MSW, and shorten leachate and landfill gas stabilization. This is probably due to MSW preparation (e.g. MSW shredding) prior to placement into the bioreactor landfill inducing a more uniform particle size of waste so that leachate recirculation and/or injected air could flow evenly to all parts of the bioreactor landfill. However, due to the heterogeneous nature of waste in a full–scale bioreactor landfill, a large fraction of recirculated leachate flowing through preferential pathways and/or injected air–filled pore space was immobilized, which made it difficult to maintain anaerobic

and/or aerobic conditions. Hence, technical challenges and further research related to the hydrodynamics of leachate recirculation and/or air injection are needed to enhance biological processes in full-scale bioreactor landfills (Reinhart et al., 2002). Figure 2.4 shows a sketch of a bioreactor landfill.

### **2.2.2.2 The Final Sink**

For some reason people make false assumptions about the practice of hoarding, so people think that by burying unwanted material in a pit or lagoon can achieve the waste management goals, protect human beings and the environment. The reality is that landfills are only temporary places, where water and air act as means of transport that will bring back to them the unwanted materials in the form of leachate and gas emissions. By increasing public awareness and the current technology available, the practice of open dumping has been improved significantly and developed into bioreactor landfill. However, this waste management practice does not guarantee that the pollutants contained in MSW will remain there forever. Although landfills are constructed with a containment system, and leachate and landfill gas collection systems, when the containment system fails or the leachate and landfill gas collection systems do not work properly, a variety of contaminants migrate and threaten human health and the environment. Moreover, many researchers have estimated that containment systems will work properly for only 10–30 years (Pivato, 2011).

The final sink is defined as a facility that ensures input is stored safely for a long-term period and that any output is released slowly enough and does not harm human health and the environment (Brunner and Tjell, 2012). The appropriate final sink for the type of material concerned is determined by the geogenic emission of the material in the storage. For example, the atmosphere is an appropriate final sink for nitrogen, the oceans for water and chlorides, and the soil for carbonates. An overloaded concentration will be released into the environment through emissions. In the context of MSW landfills, this would meet the final sink concept by transforming the waste into minerals and immobile materials prior to disposal in a

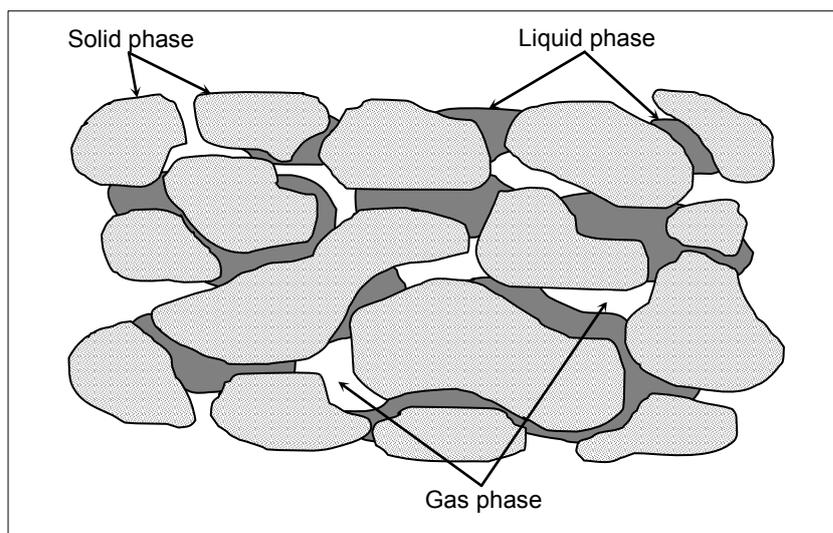
landfill site. In this way, the mineralized waste will be inert and stabilize for long time periods under changing geochemical conditions (Brunner, 2004).

### **2.2.3 Municipal Solid Waste Landfill Behaviour**

MSW landfill behaviour means all landfilling impacts of disposed waste during the operation and post-closure periods. This behaviour is determined by several factors, including disposed MSW characteristic, design and operation of landfill, environmental condition, etc. In terms of MSW characteristic, the properties of fresh waste would be very different compared to old waste that has been disposed for 30 years. In addition, the physical, biological and chemical properties of waste having pretreatment before emplacement fundamentally differs from waste without any treatment. The following subsection describes MSW landfill including an approach used to understanding its behaviour. This will cover the approach used to understand the hydro-geological behaviour of waste in landfill sites, and the influence of waste type and landfill operation on leachate and landfill emissions.

#### **2.2.3.1 Landfill as a Porous Media**

In general, MSW landfill can be divided into three phases, namely solid, liquid and gas phases. The solid phase is the MSW itself, which consists of organic and inorganic compounds in a wide range of shapes and particle sizes, and also a very heterogeneous chemical composition. The solid phase is dispersed randomly with unpredictable pore spaces forming in between due to the highly non-uniform shapes and particle sizes of the solid phase. Soil is the most comparable porous Media to landfilled MSW; however, soil particle size is more homogeneous than MSW (Fellner, 2004). According to pore size and its soil behaviour characteristics, soil scientists have distinguished soil porosity into three types, usually called micropore, mesopore and macropore.



**Figure 2.5** Illustration of landfill as a porous media. Redrawing based on Fellner (2004)

The first type, micropore, is the smallest pore, which is always filled by water. This pore is too small for plant roots to absorb the water inside. Therefore this pore plays an important role in maintaining the soil's moisture and creating anaerobic conditions for microorganism metabolism. The second type is mesopore, also called storage pores due to their ability to store water, as they do not have capillary forces that encourage water into the soils surface. This pore's function is to maintain the water availability for plants for the photosynthesis process and growing up. Mesopore properties have been studied by many researchers in order to improve agricultural soils and irrigation systems. The last is macropore, a large space in the soil usually formed by cracks in the soil, plant roots or underground animals. In terms of size, soil scientists have specified that these pores have sizes of  $2\ \mu\text{m}$ , between  $2$  and  $5\ \mu\text{m}$ , and more than  $5\ \mu\text{m}$ , respectively (Rouquerol et al., 1995).

In landfill sites, the pore space are filled with liquid and/or gas generated from the decomposition of degradable organic matter (Figure 2.5). As the liquid quantity increases by water infiltration from precipitation, the liquid phase moves by gravity throughout the pore space and wets the solid phase as it moves to the bottom. At the beginning of the process when the water quantity is very low, the liquid movement occurs in a thin film form. However, on the one hand, the liquid film becomes thicker when in contact with the wet solid phase surface. This phenomenon is called

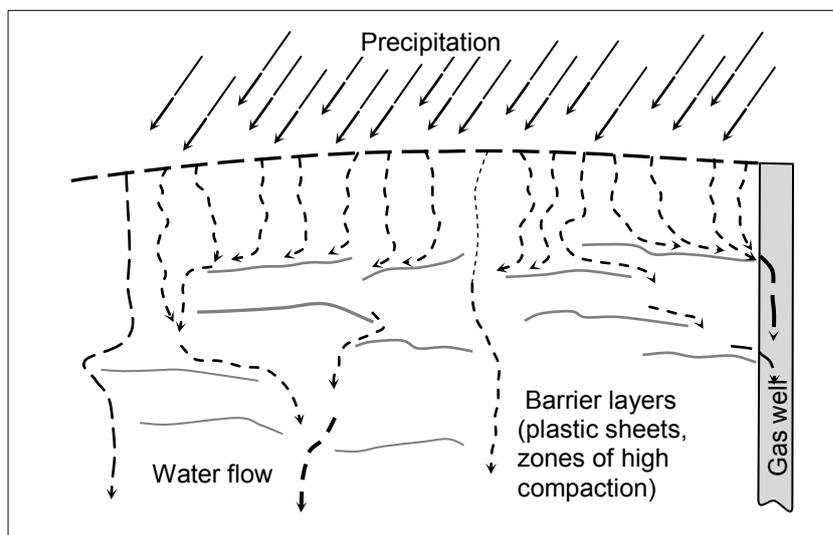
“*channelling*”. On the other hand, the liquid film becomes thinner when the liquid comes into contact with the dry solid phase surface.

### **2.2.3.2 The Water Flow Pattern in Municipal Solid Waste Landfill**

The water flow pattern in MSW landfills can be considered to be a water pattern that flows through soil layers that consists of preferential and matrix flows. Preferential flow refers to the uneven and often rapid movement of water through porous media, characterized by regions that enhance the flux of the water flow, such as wormholes, root holes and cracks, whereas matrix flow is a relatively slow and even movement of water through porous media pore spaces that obeys the convective–dispersion theory that assumes that water follows an average flow path through porous media. However, since the MSW particle size is much more heterogeneous than that of the soil, this condition causes the landfill site to have a high fraction of preferential flows. These two types of flow pattern affect solute transport in landfill sites differently. The concentration of solute in leachate would be opposite to the flow rate between preferential and matrix flows. This was confirmed by Laner et al. (2011) when they measured electric conductivity and the concentration of selected leachate substances, and the link between their concentration and the leachate generation rate. In contrast, the concentration of solute in matrix flow is higher than in preferential flow when a fertilizer or tracer is applied in field drainage experiment.

Figure 2.6 shows a schema of the water flow pattern inside MSW landfills. This illustration is adopted from the work of Mesu (1982), who was the first to point out the importance of impermeable layers for the water movement in MSW landfills. He simplified and compared the water transport inside MSW landfills with the water flow from roofs. The heterogeneous landfill structure leads to the water flows in landfills in channelling to form preferential flows towards the bottom of the landfill. However, the preferential flows formed are not only dependent on the structure of the landfill, but also determined by the water precipitation rate. New preferential

flows may develop within high precipitation rate periods due to higher water retention above impermeable surfaces (Jasper et al., 1985).



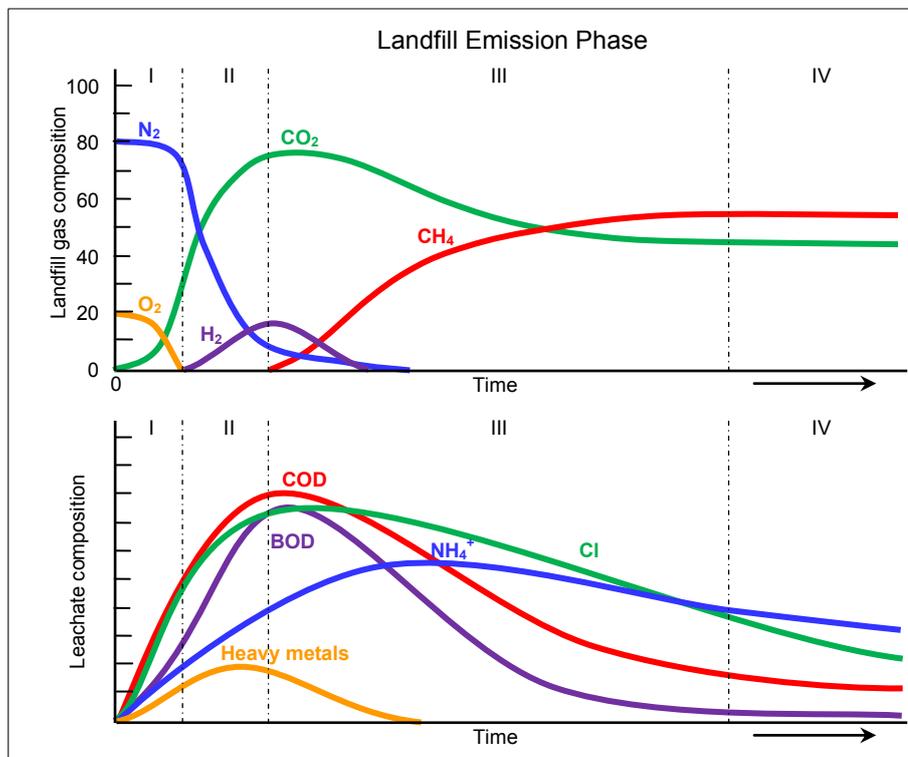
**Figure 2.6** The schematic of liquid movement in MSW landfill (Fellner, 2004)

### 2.2.3.3 Municipal Solid Waste Landfill Emissions

MSW landfills are still attracting the attention of environmentalists. The biggest concern coming from these waste management facilities is the release of leachate and landfill gas emissions into the environment. Landfill gas emissions are the result of the decomposition of degradable organic matter released into the atmosphere. Carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) are major components of landfill gas. These gases are powerful infrared absorber gases that cause the earth's temperature to increase, the so-called greenhouse effect (Popov and Power, 1999), whereas substances contained in leachate such as nitrogen compounds, heavy metals and water soluble organic matter potentially pollute surface and underground waters.

The emissions behaviour of MSW landfills can be seen from observed emissions from laboratory- (Pohland, 1975), pilot- (Pohland, 1980; Jiang et al., 2007; Abdallah et al., 2013) and full-scale bioreactor landfills (Pacey et al., 1999; Yazdani et al., 2006; Hanchock et al., 2007). Based on the results of these studies, a model to predict the substance release and emission profile for MSW landfills can be

developed. The landfill emission behaviour is controlled by a series of biological and chemical reactions from the decomposition of degradable organic matter.



**Figure 2.7** The profile of landfill gas (top, redrawing based on Farquhar and Rovers, 1973) and leachate emissions (bottom, redrawing based on Kjeldsen et al. 2002)

In general, the emission characteristic of MSW landfill emissions corresponds to the decomposition of degradable organic matter, namely the aerobic phase, anaerobic acid phase, initial methanogenic phase and stable methanogenic phase as illustrated in Figure 2.7 (Christensen and Kjeldsen, 1995). During the aerobic stage, the trapped oxygen in air spaces in deposited waste is consumed rapidly by aerobic bacteria. This process will result in CO<sub>2</sub> and heat, which causes an increase in the temperature within the landfill. The aerobic stage in landfills occurs in only a few days; the oxygen is not replenished once the new waste disposed over previous one or soils cover applied. As oxygen sources are depleted, the landfill environment switches from an aerobic to an anaerobic condition. This condition is a suitable environment for the metabolism of anaerobic bacteria. The pH in landfills is around neutral during the aerobic phase, but it gradually decreases as the anaerobic acid phase begins. This condition is caused by the accumulation of carboxylic acid,

which is produced during the anaerobic acid phase. As the pH decreases, the solubility of organic matter and metals increases. Therefore, the concentration of substances contained in the leachate is also measured during this phase (Barlaz and Ham, 1993; Reinhart and Grosh, 1998).

Once carboxylic acid is produced, substrate for methanogens is available. However, the growth rate of methanogens is still very slow during this phase, because the pH is very low, which inhibits their growth. When the pH in landfills becomes sufficient for at least limited growth, the initial methanogenic phase begins. This is indicated by measurable quantities of methane being produced. During this phase, carboxylic acid is converted to methane and carbon dioxide by methanogenic bacteria, and the methane production rate increases. The pH begins to increase as carboxylic acid is consumed and BOD, COD and other substances contained in the leachate begin to decrease as the pH landfill ecosystem increases.

In the stable methanogenic phase, the methane production rate continues to increase until it reaches its maximum value and tends to a constant. Within this phase, the methane production rate depends on the rate of hydrolysis of degradable organic matter. In the stable methanogenic phase, methane concentrations in the landfill gas are typically around 50 to 60 %. The pH continues to increase until steady-state concentration is reached because carboxylic acid is consumed immediately it is produced. These schematic landfill emission characteristics have been confirmed by various studies, both laboratory and field scale; however, the landfill emissions beyond the stable methanogenic phase are still not confirmed due to insufficient information on long-term landfill emissions that have been monitored (Kjeldsen et al., 2002).

Although the landfill gas emissions will gradually decrease as degradable organic matter reduces, in theory the concentration of methane will be stable until no more decomposition of degradable organic matter occurs. However, the decomposition process may occur continuously either under anaerobic or aerobic conditions. The oxygen intrusion into landfills due to the failure of a containment system will

oxidize the methane produced to become carbon dioxide. This will be indicated by gradually decreasing methane concentration in landfill gas, and carbon dioxide concentration is expected to increase through its production from the methane oxidation reaction. The decomposition of degradable organic matter in landfills switches from anaerobic to aerobic condition when the containment system completely fails. In this condition, the methane concentration will be insignificant, and the intruding oxygen will be consumed for oxidation of any residual methane, degradable organic matter and reduced inorganic species (sulfur, nitrogen and iron-containing species) buried in the landfill. Under aerobic conditions, additional degradable organic matter will be available, since some of the lignocelluloses substances are more degradable under aerobic conditions than under anaerobic conditions. The gas composition will be comprised largely of carbon dioxide, oxygen and nitrogen (Kjeldsen et al., 2002).

### **2.3 The Kinetic Decomposition of Degradable Organic Matter**

The decomposition of degradable organic matter could be represented by microorganism growth, which plays an important role in the decomposition process. Microorganism growth generally involves a respiration and conversion of substrate to products (catabolism) that release energy in the form of adenosine 5-triphosphate (ATP). The energy obtained from the catabolic reaction is used for both the synthesis of new cells and the maintenance of old ones (anabolism). The quantity of new cells formed could be described by kinetic theory of microorganism growth. Kinetic microorganism growth is based on two fundamental relationships, namely growth and substrate utilization rates. These relationships have been described by various mathematical models; however, the most widely used kinetic microorganism growth is the Monod kinetic model and its extended modification based on newly gained knowledge. The Monod kinetic model and its extended modification approach are described in the following subsection and summarized in Table 2.3 with other kinetic models.

### 2.3.1 Monod Kinetic Model

The Monod kinetic model was proposed by Jacques Lucien Monod (1910–1976), a French biologist, based on his series of studies focused on the effect of limiting substrate on bacterial growth. The Monod kinetic model describes the microorganism growth rate as a function of time in limited substrate condition as expressed by the series of equations below:

$$r_x = \mu \cdot X \dots\dots\dots (2.1)$$

where  $r_x$  is the microorganism growth rate ( $\text{kg m}^{-3} \text{ day}^{-1}$ ),  $\mu$  is the specific microorganism growth rate ( $\text{day}^{-1}$ ), and  $X$  the microorganism concentration ( $\text{kg m}^{-3}$ ). Monod (1949) suggested the specific microorganism growth rate as expressed by the equation below:

$$\mu = \mu_{\max} \frac{S}{K_M + S} \dots\dots\dots (2.2)$$

where  $\mu_{\max}$  is the maximum specific growth rate of bacteria ( $\text{day}^{-1}$ ),  $S$  is concentration of substrate ( $\text{kg m}^{-3}$ ) and  $K_M$  is the substrate concentration which supports half-maximum specific growth rate ( $\text{kg m}^{-3}$ ). Combining Eq. (2.1) and (2.2) we have the microorganism growth rate as expressed by equation below:

$$r_x = \mu_{\max} \frac{S}{K_M + S} X \dots\dots\dots (2.3)$$

Whereas the specific substrate consumption rate is determined by taking into account yield microorganisms as expressed by the equation below:

$$r_s = \mu_{\max} \frac{S}{Y(K_M + S)} X \dots\dots\dots (2.4)$$

where  $Y$  is yield microorganism (dimensionless), defined as the ratio of the net amount of microorganisms (e.g. amount of new microorganisms minus decay) per substrate consumed. In general, the decay coefficient of microorganisms is around 5% of the maximum specific growth rate. Nevertheless, methanogens have a

relatively low decay coefficient (almost 1% of their maximum specific growth rate) and thus can be ignored during modeling and simulations of the anaerobic process (Gavala et al., 2003).

### 2.3.2 Contois Kinetic Model

The Contois kinetic model is an extension of the Monod kinetic model. This model was proposed by Contois based on the results of his work when he applied the Monod model to *Aerobacter aerogenes* on defined mineral salt media containing ammonium as a nitrogen source and glucose or succinic acid as carbon sources. The results of this study indicated that the specific growth rate of microorganisms was not only a function of limiting nutrients, but also of the population density of the microorganisms (Contois, 1959). Contois suggested the specific growth rate of microorganisms as defined by the following equation:

$$\mu = \mu_{\max} \frac{S}{aS_0 + S} \dots\dots\dots (2.5)$$

where  $a$  is a proportional constant of substrate concentration that supports half the maximum specific growth rate (dimensionless). Furthermore, by neglecting the initial microorganism population density, since it is usually insignificant and will be washed out of the culture in time, Contois proposed the specific growth rate of microorganisms for continuous culture as defined by the following equation:

$$\mu = u_m \frac{S}{BX + S} \dots\dots\dots (2.6)$$

where  $u_m$  and  $B$  are the microorganism growth parameters that are constant. Contois furthermore defines these parameters as expressed by the equation below:

$$u_m = \frac{\mu_{\max}}{1 + a} \dots\dots\dots (2.7)$$

$$B = \frac{a}{Y(1 + a)} \dots\dots\dots (2.8)$$

### 2.3.3 Chen and Hashimoto Kinetic Model

The Chen and Hashimoto kinetic model is an extension of the Contois kinetic model for continuous culture that takes account of the refractory coefficient of the non-degradable portion of the organic substrate. The study was carried out by using aerobic treatment for synthetic substrate data and anaerobic digestion for dairy waste. These studies show the Contois kinetic model's very good fit to the kinetic data (Chen and Hashimoto, 1980). Moreover, the Contois kinetic model was a better fit to the aerobic kinetic data than the first-order kinetic model. Thus, the Contois kinetic model was extended as defined by the following equation:

$$\mu = \mu_{\max} \frac{S}{K \cdot S_0 + (1 - K) \cdot S} \dots\dots\dots (2.9)$$

where  $K$  is the kinetic model parameter constant (dimensionless) equal to multiplying  $Y$  and  $B$  as defined by Eq. (2.8),  $S_0$  is the concentration of substrate in influent to the culture system ( $\text{kg m}^{-3}$ ), and  $S$  is the concentration of substrate in effluent out of the culture ( $\text{kg m}^{-3}$ ).

## 2.4 The Mechanism of Organic Matter Degradation

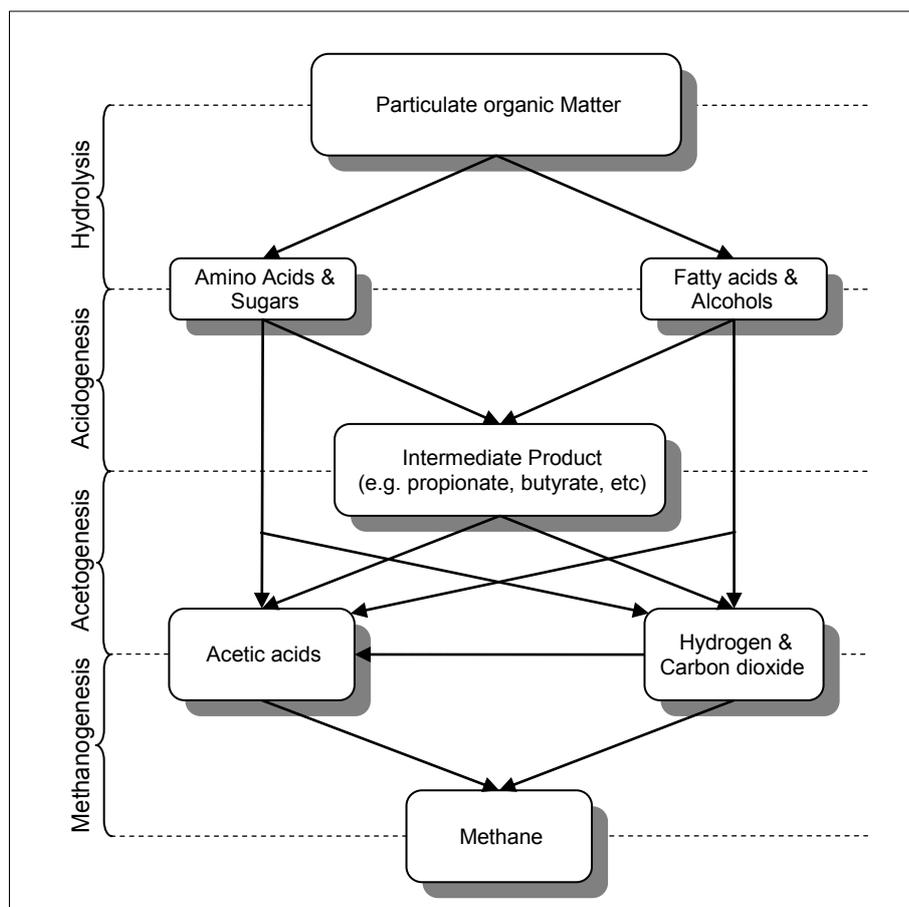
The degradation of organic matter can occur either aerobically or anaerobically. Aerobic decomposition of degradable organic matter is carried out by consortia bacteria in the presence of an oxygen environment usually known as aerobic bacteria. These bacteria consumed oxygen twice during the decomposition process, firstly as a catalyst to decomposed substrate at the beginning of the metabolism process, and secondly for respiration at the end of the metabolism process (Fritsche and Hofrichter, 2004). Conversely, anaerobic decomposition of degradable organic matter is carried out by consortia bacteria in the absence of oxygen. These bacteria usually use ionic nitrate, sulfate, iron, manganese and carbon dioxide as electron acceptors.

The decomposition of degradable organic solid matter in MSW landfills can occur in three ways, namely aerobic, anaerobic or a combination of aerobic and anaerobic simultaneously. However, aerobic decomposition probably only occurs in the top layer of landfilled waste due to the limited amount of oxygen penetrating landfill covers. This process will not occur anymore after the fresh waste over disposed waste or the landfill surface is covered with soil. Since most of the degradable organic solid matter of MSW in landfills will decompose anaerobically, the description of kinetic decomposition of degradable organic solid matter will focus on this process.

**Table 2.3** Kinetic model of decomposition organic matter

Kinetic model	Kinetic parameters	
	Specific microorganism growth	Substrate consumption rate
First-order	$\frac{k \cdot S}{S_0 + S}$	$k \cdot S$
Teissier (1936)	$\mu_{\max} \left\{ 1 - \exp^{-\left(\frac{S}{K_S}\right)} \right\}$	$\mu_{\max} \frac{X}{Y} \left\{ 1 - \exp^{-\left(\frac{S}{K_S}\right)} \right\}$
Monod (1949)	$\mu_{\max} \frac{S}{K_M + S}$	$\mu_{\max} \frac{X \cdot S}{Y \cdot (K_M + S)}$
Contois (1959)	$u_m \frac{S}{B \cdot X + S}$	$u_m \frac{X \cdot S}{Y \cdot (B \cdot X + S)}$
Moser (1959)	$\mu_{\max} \frac{S^n}{K_S + S^n}$	$\mu_{\max} \frac{X \cdot S^n}{Y \cdot (K_S + S^n)}$
Grau et al. (1975)	$\mu_{\max} \frac{S}{S_0}$	$\mu_{\max} \frac{X \cdot S}{Y \cdot S_0}$
Chen & Hashimoto (1980)	$\mu_{\max} \frac{S}{K \cdot S_0 + (1 - K) \cdot S}$	$\mu_{\max} \frac{X \cdot S}{K \cdot X + Y \cdot S}$

In general, the decomposition of degradable organic solid matter occurs through four stages. The decomposition process is initially the dissolution of degradable organic matter by extracellular enzymes that are released from microorganisms; this is known as the hydrolysis stage. At this stage, the degradable organic matter will also break down to a simple form that can pass the membrane cell of bacteria. After degradable organic matter dissolves into liquid phase, the substrates for microorganisms are available and the decomposition of degradable organic matter begins. The simple form of organic matter results from hydrolysis and is then fermented to acetic acids and other volatile fatty acids (VFAs) with carbon dioxide and hydrogen as by-products.



**Figure 2.8** General schematic biodegradation pathway of organic matter in anaerobic environment. Redrawing based on Pavlostathis and Giraldo-Gomez (1991).

A small amount of ammonia and hydrogen sulfide might be produced from fermented protein. The long- and short-chain VFAs resulting from fermentation are broken down further to simple VFAs before being utilized by methanogenic bacteria. The breakdown of long- and short-chain VFAs to simple VFAs was performed by acetogenic bacteria. Finally, simple VFAs were utilized by methanogenic bacteria where methane and carbon dioxide are generated as the product of metabolism. Anaerobic decomposition of degradable organic matter is shown schematically in Figure 2.8 and a detailed description of each process is given in the following subsection.

### 2.4.1 Hydrolysis

Hydrolysis is dissolution and depolymerization of particulate organic matter into solute that can pass the cell membrane of bacteria. Hydrolysis of solid organic matter is usually carried out by extracellular enzymes (i.e. hydrolases) and it may or may not be the limiting stage of organic matter decomposition (Gavala et al., 2003). Hydrolyzed cellulose will produce cellobiose and glucose, whereas hemicelluloses are pentoses, hexoses and uronic acid (Colberg, 1988). Amino acids were produced from hydrolyzed protein, while long-chain VFAs, and galactose and glycerol, were produced from lipids (Pavlostathis and Giraldo-Gomez, 1991).

Hydrolysis of solid organic matter is often described by the first-order kinetic model, where enzymatic activity is not directly influenced by bacterial growth (Gujer and Zehnder, 1983; Pavlostathis and Giraldo-Gomez, 1991). Eastman and Ferguson (1981) and Vavilin et al. (1996; 2008) found first-order kinetics suitable for describing the anaerobic decomposition of solid organic matter, whose hydrolysis is the first stage of the overall process. In contrast, Schober et al. (1999) found that zero-order kinetics better described the hydrolysis of organic matter during two-stage anaerobic digestion in thermophilic conditions. Furthermore, Miron et al. (2000) reported that no primary sludge component (e.g. carbohydrate, protein, lipids) followed first-order kinetics during hydrolysis, either under acidogenic or under methanogenic conditions. The authors also concluded that hydrolysis still less defined steps in anaerobic digestion of complex heterogeneous substrates such as primary sludge. However, Vavilin et al. (2008) found the Contois kinetics and two-phase kinetics fit for the hydrolysis of a wide range of particulate organic matter.

Although hydrolysis is performed by extracellular enzyme activity, there are many other factors involved. Gavala et al. (2003) mentioned that hydrolysis of organic polymers in anaerobic digestion strongly depends on several physicochemical factors including particle size, solubility of organic matter, origin of anaerobic culture, and enzyme diffusion and adsorption rates into particles of organic matter.

Moreover, temperature, pH and moisture content are the most important factors that are influenced by the hydrolysis rate. Veeken et al. (2000) reported there was no accumulation of hydrolysis products found in the anaerobic decomposition of organic solid waste that is operated at pH 6 and 7. In other words, all hydrolysis products are converted by acidogenic bacteria immediately to VFAs, CO<sub>2</sub> and H<sub>2</sub> after hydrolysis products are formed.

### **2.4.2 Acidogenesis**

Acidogenesis is fermentation of monomers and dimmers of organic polymers that have resulted from hydrolysis. The fermentation of these monomers and dimmers was performed by heterogeneous microbial population. The bacteria are species predominantly found in an anaerobic digester, while populations such as protozoa, fungi and yeast have been reported as being very small (Toerien and Hattingh, 1969). The main product of anaerobic fermentation carbohydrate is ethanol and a small amount of acetate, H<sub>2</sub> and CO<sub>2</sub> in the absence of H<sub>2</sub> utilizing bacteria. In contrast, acetate is the main product of acidogenesis carbohydrate in the presence of H<sub>2</sub> utilizing bacteria. Short-chain VFAs such as succinate, amino valerate and hydrogen gas are the main products was resulting from amino acid fermentation (Pavlostathis and Giraldo-Gomez, 1991).

Many studies have been conducted to observe the decomposition pathway and kinetics of acidogenesis carbohydrate. Most of the researchers assumed that decomposition of dissolved organic matter followed the Monod kinetic model (Gavala et al., 2003). In contrast, although anaerobic acidogenesis of the amino acid pathway and its corresponding products has been extensively studied, only few data are available.

### **2.4.3 Acetogenesis**

Acetogenesis is decomposition of VFAs carried out by bacteria, which results in acetic acids as the main product. In a continuous process, long- and short-chain VFAs produced at the acidogenic stage were converted to acetic acids and other

simple form VFAs (e.g. formic acids, methanol, methylamine, etc). Therefore, bacteria that are responsible for converting these VFAs are called acetogenic bacteria. The predominant bacteria populations were found in digested alcohol and the VFAs was the species *Acetobacterium*, *Acetobacter*, *Syntrophobacter*, *Syntrophomonas* and a small population of the species *Desulfovibrio* (Bryant, 1979; McInerney and Bryant, 1981). The growth rate of these bacteria was very slow due to the low free energy resulting from this metabolism process, whereas their doubling time was about 1.5 to 4 days (Lawrence and McCarty, 1969).

The acetogenesis hydrogenation breakdowns of long- and short-chain VFAs were performed by hydrogen-producing group bacteria (e.g. *Enterobacter*, *Citrobacter*, *Serratia* and *Syntrobacter*) to produce acetic acid as the main product and either hydrogen or carbon dioxide depending on the condition and structure of VFAs, whereas the acetogenesis dehydrogenation produced acetic acid from hydrogen or carbon dioxide carried out by hydrogen-consuming group bacteria (e.g. *Clostridium* and *Acetobacterium*). However, the acetogenesis in anaerobic digestion usually refers to acetogenesis dehydrogenation (Gavala et al., 2003).

The degradation of long- and short-chain VFAs can also be carried out by  $\beta$ -oxidation (Jeris and McCarty, 1965). But they are inhibited by hydrogen even in very low concentration. Consequently, they can only be carried out by syntrophic with microorganisms that consume hydrogen such as acetogenic dehydrogenation and methanogenic bacteria. Therefore, the complete decomposition of long- and short-chain VFAs strongly depends on the consumption rate of hydrogen by acetogenic dehydrogenation and methanogenic bacteria.

#### **2.4.4 Methanogenesis**

Methanogenesis is the final stage of decomposition of degradable organic matter. Within this stage, organic compounds resulting from the previous stages are converted by methanogenic bacteria to methane (CH<sub>4</sub>). Very limited types of organic compounds can be utilized by methanogenic bacteria for their metabolism. So far, CO<sub>2</sub>, CO, formic acids, acetic acids, methanol, methylamines and dimethyl

sulfide have been identified as substrates and energy sources for methanogenic bacteria (Gavala et al., 2003).

There are two types of methanogenic bacteria, namely acetotrophic and hydrogenotrophic methanogens. Acetotrophic methanogens are bacteria that are responsible for converting organic substrate (e.g. acetic acids and methanol) to produce  $\text{CH}_4$  (Bradley and Chapelle, 1999). Therefore, these bacteria play an important role in maintaining pH due to the accumulation of fermentation products by turning them into  $\text{CH}_4$  and  $\text{CO}_2$  (Mosey, 1983), while hydrogenotrophic methanogens are bacteria that utilize inorganic substrates (e.g.  $\text{CO}_2$  and  $\text{H}_2$ ) to produce  $\text{CH}_4$  and  $\text{H}_2\text{O}$  (Bradley and Chapelle, 1999). In general, around 65–75 % of the methane from decomposed organic matter is produced by acetotrophic methanogens (Pavlostathis and Giraldo–Gomez, 1991; Gavala et al., 2003).

Numerous studies related to methanogenesis have been conducted particularly on acetic acid and/or hydrogen reducing kinetics. Lawrence and McCarty (1969), Ghosh and Klass (1977), Smith and Mah (1966), Kaspar and Wurnmann (1978), Robinson and Tiedje (1982), Ahring and Westermann (1987a), Zinder and Mah (1979) and Kristjansson et al. (1982) investigated the kinetic methanogenesis of acetic acids derived from sewage sludge. Van den Berg (1977) and Wandrey and Aivasidis (1983) investigated the kinetics of the methanogenesis of acetic acid by using a pure chemical compound. Karakashev et al. (2006) and Hungate et al. (1970) investigated the kinetic methanogenesis of acetic acids derived from animal waste, while Archer and Powell (1985) investigated the kinetic model and specific growth rate of methanogenic mutuality co-cultures on methanogens by using ethanol as carbon and energy sources. Most authors reported the Monod kinetic model fit to their studies.

## **2.5 Environment Influence on Degradation of Organic Matter**

There are several factors affecting microorganism growth that would affect the decomposition rate of degradable organic matter. These are usually distinguished as intrinsic (e.g. moisture content, pH, redox potential) and extrinsic (e.g. temperature, partial pressure of gas component in air) factors. Most intrinsic factors are interrelated with extrinsic factors and vice versa, so it is very difficult to determine the individual effect of those factors on microorganism growth. For example, the dissolution and dissociation of calcium carbonate to calcium and carbonate ions will change the pH of the microorganism living environment, where dissolution and dissociation of calcium carbonate are highly dependent on temperature and partial pressure of carbon dioxide in the gas phase.

Temperature, pH, moisture content and redox potential are the major factors understood to affect microorganism growth. Understanding the effect of these factors on microorganism growth would help us to develop a model to determine the decomposition rate of degradable organic matter in landfill sites. Therefore, these factors have been considered in this literature review and described in the following paragraph.

### **2.5.1 Temperature**

Temperature has a dramatic effect on promoting or preventing microorganism growth. The fluidity membrane cell decreases at low temperature and would interfere with the substrate transport into the microorganism cell. In contrast, the membrane cell would denature and inactivation of heat-sensitive enzymes occurs at high temperature. The effect also varies significantly across microorganism groups; therefore, generally the microorganisms have been classified into four major groups distinguished based on their response to the temperature, namely psychrophilic, psychrotrophic, mesophilic, and thermophilic. Each group has a defined minimum, maximum and optimum temperature in which they grow as listed in Table 2.4.

In general, the microorganism growth rate increases with the temperature until the optimum temperature is reached. A further increase of the temperature beyond its optimum value will reduce the microorganism growth rate dramatically. The most widely used method to define the temperature correlation to microorganism growth is the Arrhenius equation.

$$k = A \exp\left(-\frac{E}{RT}\right) \dots\dots\dots (2.10)$$

where  $k$  is the temperature dependence growth rate constant (dimensionless),  $A$  is the pre-factor growth rate constant (dimensionless),  $E$  is the activation energy (kcal mol<sup>-1</sup>),  $R$  is the universal gas constant (kcal K<sup>-1</sup> mol<sup>-1</sup>) and  $T$  is the temperature (K).

The effect of temperature on microorganism growth has been studied and reported by many researchers, and several of these are summarized in Table 2.4. The results of these studies show that the optimum temperature was various in wide ranges depending on the substrate characteristics, type of reactor use, digestion parameters, such as hydraulic retention time (HRT), solids retention time (SRT) and organic loading rate (OLR), as well as the pH system in the reactor (Banerjee et al., 1998). However, in general, it has been reported that the optimum temperature can be distinguished into two temperature ranges, that is, between 34 and 40 °C and higher than 45 °C. These ranges of temperature can be characterized as the mesophilic and thermophilic temperature range, of respectively.

Table 2.4 The effect of temperature on microorganism growth

Authors	Substrate	Method	Mechanism stage	Temperatur (°C)		Results
				Range	Optimum	
Ahring et al. (2001)	Cattle manure	CSTR	Acidogenesis	55 – 65	55	1.8 – 2.4 kg FVA/m <sup>3</sup>
Chae et al. (2008)	Swine manure	Batch digester	Methanogenesis	55 – 65	55	0.20 m <sup>3</sup> CH <sub>4</sub> /kg VSS–day
Donoso-Bravo et al. (2009)	Starch	Batch culture	Methanogenesis	25 – 35	35	0.403 m <sup>3</sup> CH <sub>4</sub> /kg VS–day
			Methanogenesis	11.1 – 46.3	34.1	0.72 kg/kg VSS–day
			Acidogenesis	28.9 – 45.2	37	33.6 kg/kg VSS–day
			Hydrolysis	4.2 – 45.5	40.3	22.8 day <sup>-1</sup>
Joubert and Britz (1986)	Sucrose	Up flow digester	Hydrolysis	27 – 39	35	85% Sucrose hydrolyzed
Kim et al. (2010)	Wastewater	CSTR	Acidogenesis	40 – 60	50	1.71 TFVA kg/ m <sup>3</sup>
Komemoto et al. (2009)	Food waste	Batch digester	Methanogenesis	15 – 65	35	0.65 m <sup>3</sup> CH <sub>4</sub> /kg VSS–day
			Acidogenesis	15 – 65	45	73 % VSS removed
Langenhoff & Stuckey (2000)	Wastewater	ABR	Acidogenesis	10 – 35	35	95% COD removed
			Methanogenesis	10 – 35	35	3.0 m <sup>3</sup> CH <sub>4</sub> /day
Lee et al. (2008)	Food waste	Batch digester	Methanogenesis	55 – 80	55	80% VS removed
			Acidogenesis	70 – 80	70	43.1% COD removed
Lim et al. (2008)	Food waste	SCR	Acidogenesis	25 – 45	35	2.88 – 3.00 kg FVA/ m <sup>3</sup>
Meher and Ranade (1993)	Organic salt medium	Batch culture	Methanogenesis	25 – 60	35	5.38 mM CH <sub>4</sub>
Mu et al. (2006)	Glucose	Batch digester	Acidogenesis	33 – 41	39	3.92 m <sup>3</sup> H <sub>2</sub> /kg VSS–day
Penaud et al. (1997)	Wastewater	Batch digester	Acidogenesis	25 – 65	35	17 TFVA kg/m <sup>3</sup>
van den Berg et al. (1977)	Acetic acid	Batch digester	Methanogenesis	5 – 60	40 – 45	0.014 FVA kmol/ m <sup>3</sup> day
Varel et al. (1980)	Beef cattle waste	CSTR	Methanogenesis	30 – 65	45	0.24 m <sup>3</sup> CH <sub>4</sub> /kg VSS–day
Yu and Fang (2003)	Wastewater	Up flow digester	Acidogenesis	20 – 55	55	1.53 kg TVFA/m <sup>3</sup>
			Methanogenesis	20 – 55	55	40 kPa CH <sub>4</sub>
Zehnder and Wuhrmann (1977)	Organic salt medium	Batch culture	Methanogenesis	20 – 45	33 – 40	2.3 – 2.7 kg/kmol CH <sub>4</sub>
Zeikus and Wolfe (1972)	Organic salt medium	Batch culture	Methanogenesis	30 – 80	65 – 70	9.0 – 12.0 kmol CH <sub>4</sub>

### 2.5.2 pH

pH is the acidity or basicity level of an aqueous solution, usually measured as the hydrogen ion concentration in a solution. Another common term related to the pH is pKa, a term that describes the dissociation fraction of acid into its ions in a solvent, usually water. In an equilibrium state, pKa is the pH at which the concentration of dissociated and undissociated acids is equal. The pKa of strong acids is lower than that of weak acids, which means that the fraction of strong acids dissociated into their ions is higher than that of weak acids. Thus, the pH of strong acid solutions is lower than that of weak acids. For example, the pH of 0.1 M hydrogen chloride and acetic acid solutions at 25 °C is 1.08 and 2.6, respectively. The pH is a function of the hydrogen ion concentration in the solution as expressed in the equation below:

$$\text{pH} = -\log_{10}[\text{H}^+] \dots\dots\dots (2.11)$$

where  $[\text{H}^+]$  is the concentration of the hydrogen ion ( $\text{mol l}^{-1}$ ). As well as to the temperature, microorganisms are also tolerant to pH for their growing rate. Some microorganisms can survive in an acidic environment. These species usually produce acid during their metabolism such as the acetic or lactic acids producing bacteria. However, mostly they grow best at neutral or near to neutral pH.

As well as the temperature, the effect of pH on microorganism growth has also been widely reported (see Table 2.5). However, the results of these studies show that the optimum pH for methanogenesis was in a narrower pH range. The optimum pH for methanogenesis was near neutral to neutral, while the optimum pH for acidogenesis was in the range of 5.5 – 8.0 depending on type of substrate and experimental method used.

Table 2.5 The effect of pH on microorganism growth

Authors	Substrate	Method	Mechanism stage	pH		Results
				Range	Optimum	
Bengtsson et al. (2008)	Cheese whey permeate	CSTR	Acidogenesis	3.5 – 6.0	5.5	0.83 kg COD/kg VSS–day
	Paper mill wastewater	CSTR	Acidogenesis	3.5 – 6.0	5.5	0.76 kg COD/kg VSS–day
ten Brummeler et al. (1985)	Acetate-Propionate mix	UASB reactor	Methanogenesis	5.8 – 7.5	6.6 – 7.2	80 – 90% HAC removed
Fang and Liu, (2002)	Glucose	CSTR	Acidogenesis	4.0 – 7.0	5.5	2.1 kmol H <sub>2</sub> /kmol glucose
Hu et al. (2004)	Cellulose	Batch digester	Acidogenesis	4.8 – 7.3	6.8	78% cellulose removed
Hu et al. (2006)	Cattail	Batch digester	Acidogenesis	5.8 – 7.6	6.9	1.737 kg TVFA /m <sup>3</sup>
Joubert and Britz (1986)	Sucrose	Up flow digester	Hydrolysis	5.8 – 7.5	6.5	5.7% COD removed
Kisaailta et al. (1987)	Lactose	Batch digester	Acidogenesis	4.0 – 6.5	6.1	1.969 kg HAC/ m <sup>3</sup>
Lim et al. (2008)	Food waste	SCR	Acidogenesis	5.0 – 6.0	5.5	2.88 – 3.0 kgFVA/m <sup>3</sup> –day
Meher and Ranade (1993)	Organic salt medium	Batch culture	Methanogenesis	4.5 – 9.0	7	1.9 – 5.4 10 <sup>-6</sup> kmol CH <sub>4</sub>
Mu et al. (2006)	Synthetic wastewater	UASB reactor	Acidogenesis	3.4 – 6.3	5.7	99% sucrose degraded
Oktem et al. (2006)	Synthetic wastewater	CSTR	Acidogenesis	5.0 – 6.3	5.5	13% COD removed
Penaud et al. (1997)	Synthetic wastewater	Batch digester	Acidogenesis	5.0 – 9.0	8	19 kg TVFA /m <sup>3</sup>
Shin and Youn (2005)	Food waste	CSTR	Acidogenesis	5.0 – 6.0	5.5	1 m <sup>3</sup> H <sub>2</sub> / m <sup>3</sup> –day
van den Berg et al. (1977)	Acetic acid	Batch digester	Methanogenesis	4.0 – 7.6	6.5 – 7.1	0.014 FVA kmol/m <sup>3</sup> –day
Yu and Fang (2003)	Wastewater	Up flow digester	Acidogenesis	4.0 – 7.0	6.5	1.57 kg TVFA/m <sup>3</sup>
			Methanogenesis	4.0 – 7.0	7	40 kPa CH <sub>4</sub>
Yu et al. (2002)	Rice winery wastewater	Up flow digester	Acidogenesis	4.5 – 6.0	5.5	8.02 m <sup>3</sup> H <sub>2</sub> /kg VSS–day
Zehnder and Wuhmann (1977)	Organic salt medium	Batch culture	Methanogenesis	6.0 – 8.5	7	2.3 – 2.7 kg/kmol CH <sub>4</sub>
Zhang et al. (2005)	Food waste	Batch digester	Acidogenesis	5.0 – 11	7	36 kg TVFA/m <sup>3</sup>
Zoetemeyer et al. (1982)	Synthetic wastewater	CSTR	Acidogenesis	4.5 – 7.9	6	9% COD removed

### 2.5.3 Moisture Content

Moisture content is another important environmental factor that controls microorganisms' growth rate. Moisture content is defined as the ratio of the volume of water contained in the substrate to the total volume of the substrate expressed mathematically as the equation below:

$$\theta = \frac{v_W}{v_T} \dots\dots\dots (2.12)$$

where  $\theta$  is the moisture content in the substrate (v/v or %),  $v_W$  is the volume of water contained in the substrate ( $\text{m}^3$ ), and  $v_T$  is the total volume of the substrate, water and air space in the substrate ( $\text{m}^3$ ). The moisture content of pure water and completely dehydrated substrate is 1 or 100% and zero, respectively.

Microorganisms respond to moisture content differently depending on numerous factors. In general, moisture content affects microorganism growth directly together with other environmental factors such as temperature, pH, substrate availability, etc. The growth rate of aerobic microorganisms in dried environment conditions is very low and increases along with increasing moisture content to its maximum point, where a further increase in moisture content will restrict the oxygen diffusion and inhibit the microorganism growth rate. The microorganism population will shift from being predominantly aerobes to being facultative microbial anaerobes (Sommers et al., 1981).

The effect of moisture content on microorganism growth cannot be measured directly. However, it can be measured from outcomes of microorganism activities, such as oxygen consumption, transformation of nitrogen compounds or  $\text{CO}_2$  respiration rate. Iovieno and Bååth (2008) investigated the effect of soil moisture on bacterial growth by measuring the respiration rate of microorganisms from various moisture contents of grassland sandy loam soils. The results showed that the rate of respiration increased exponentially with a soil moisture content of 5% to 40% and remained constant for higher water content.

## 2.6 Modeling of Organic Matter Degradation in MSW Landfills

Numerous models to predict organic matter degradation in MSW landfills have been developed within the last decade. Most models have been developed through a sophisticated approach and equipped with various features to accommodate the complex behaviour of MSW landfills. However, only some of them are described in the following subsection, mainly those considered as major factors influencing the degradation of organic matter described above. Simple single-factor models will be described first, followed by more complex ones, which are seen as a combination of all those factors.

### 2.6.1 Model Effect of pH on Degradation of Organic Matter

White et al. (2004) developed a numerical model of landfill degradation and transport processes (LDAT) to support laboratory and field tests being carried out by the Southampton University Waste Management Research Group. This model considers that MSW contains four types of degradable organic matter (i.e. protein, fats, short- and long-chain carbohydrates), which degrade through three stages of degradation pathway. During the first stage, the particulate protein and fats were converted into their aqueous form, while acetic and butyric acids result from hydrolyzed short- and long-chain carbohydrates, respectively. The dissolved protein, fats and butyric acid were subsequently decomposed to acetic acid within the second stage (i.e. acidogenesis). Finally, the acetic acid was converted to CH<sub>4</sub> and CO<sub>2</sub> in the third stage of the degradation process (i.e. methanogenesis).

The degradation rate of organic matter throughout all stages is represented by the growth rate of microorganisms. The microorganisms' growth rate is modeled by multiplying the maximum growth rate by the pH inhibition factor as expressed by the equation below:

$$\mu = \alpha_{(pH)} \cdot \mu_{\max} \dots\dots\dots (2.13)$$

where  $\mu_{\max}$  is the biomass growth rate at neutral pH value ( $\text{day}^{-1}$ ), and  $\alpha_{(\text{pH})}$  is the pH inhibition factor (dimensionless). The pH inhibition factor is distinguished into three pH ranges as defined by the following equation:

$$\alpha_{(\text{pH})} \begin{cases} \frac{\text{pH}}{1.5} - 3, & 4.5 < \text{pH} < 6.0 \\ 1, & 6.0 < \text{pH} < 8.0 \\ 6.33 - \frac{\text{pH}}{1.5}, & 8.0 < \text{pH} < 9.5 \end{cases} \dots\dots\dots (2.14)$$

### 2.6.2 Model Effect of Moisture Content on Degradation of Organic Matter

McDougall and Pyrah (1999) developed a model for organic matter degradation for landfilled waste that takes into account moisture content in the enzymatic hydrolysis of organic matter. The degradation pathway of organic matter is believed to occur in two stages, combining the hydrolysis and acidogenesis stages into a single stage followed by methanogenesis as the final stage. The degradation of organic matter by hydrolysis is proportional to the acetic acid production rate given by the following equation:

$$\frac{d(S)}{dt} = \alpha_{(\theta)} k_h \phi I_{\text{VFA}} \dots\dots\dots (2.15)$$

where  $\alpha_{(\theta)}$  is the moisture content of the inhibition factor (dimensionless),  $k_h$  is the hydrolysis rate of organic matter ( $\text{kg m}^{-3} \text{ day}^{-1}$ ),  $\phi$  is the relative digestibility, which varies between zero and one depending on the remaining concentration of organic matter (dimensionless), and  $I_{\text{VFA}}$  is the influence of VFAs on the organic matter hydrolyzation rate (dimensionless). The volumetric moisture content, relative digestibility and VFA influence on the organic matter hydrolyzation rate are defined by the following equations:

$$\alpha_{(\theta)} = \frac{\theta - \theta_R}{\theta_S - \theta_R} \dots\dots\dots (2.16)$$

$$\phi = 1 - \left( \frac{S_0 - S}{S_0} \right)^n \dots\dots\dots (2.17)$$

$$I_{VFA} = \exp^{(-k_{VFA} \cdot c)} \dots\dots\dots (2.18)$$

where  $\theta$  is the volumetric moisture content (v/v) with  $R$  and  $S$  subscripts referring to residual and saturated moisture content, respectively. Meanwhile,  $S_0$  is the initial concentration of organic matter ( $\text{kg m}^{-3}$ ),  $S$  is the remaining concentration of organic matter at  $t$ -time ( $\text{kg m}^{-3}$ ),  $n$  is the structural transformation factor (dimensionless),  $k_{VFA}$  is the influence of VFAs on the organic matter hydrolyzation rate constant ( $\text{m}^3 \text{kg}^{-1}$ ), and  $c$  is VFA concentration ( $\text{kg m}^{-3}$ ).

### 2.6.3 Model Effect of Temperature and pH on Degradation of Organic Matter

The model of temperature and pH influences on the degradation of organic MSW matter was developed by El-Fadel et al. (1996a) to predict gas and heat generated from Mountain View controlled landfill in California, USA. Organic MSW matter was distinguished into three categories, and each category has different hydrolysis and biodegradation rates. The hydrolysis of particulate organic matter was assumed to follow the first-order kinetic model, while acidogenesis and methanogenesis were assumed to follow the Monod kinetic model. Glucose is assumed to be a product of the hydrolyzation of all the particulate matters that are degraded in the subsequent decomposition process.

$\text{CO}_2$  and VFAs (i.e. acetic, propionic and butyric acids) are produced from acidogenesis of glucose, which controls the pH and the microorganism growth rate. The effect of pH on the microorganism growth rate was assumed to follow a linear function as proposed by Clark and Speece (1970).  $\text{CH}_4$  produced from methanogenesis is considered to be water insoluble, whereas  $\text{CO}_2$  is partly dissolved and the rest is accounted for as gas transport and released into the atmosphere. The amount of  $\text{CO}_2$  dissolved is limited by Henry's constant ( $K_H$ ) as a function of temperature. The effect of temperature on first and second carbonate equilibrium constants ( $K_{a1}$  and  $K_{a2}$ ), the calcium carbonate solubility constant ( $K_{sp} \text{CaCO}_3$ ) and the water dissociation constant ( $K_W$ ) was assumed to follow third- to fourth-order polynomial function. The temperature at the top and bottom of landfills is assumed to be equal to the air and the ground temperature, respectively. Therefore, the

temperature effect on microorganism growth is determined using the Arrhenius relationship by considering the proportional constant and activation energy from experimental results.

Haarstrick et al. (2004) developed a model to simulate the degradation of easily hydrolysable organic matter in landfills, and the amount of gas and heat released. The degradation of organic matter comprises hydrolysis, acidogenesis and methanogenesis. Hydrolyzed organic matter is converted by acidogenesis to CO<sub>2</sub>, short- and long-chain VFAs followed by fermentation of long-chain VFAs and methanogenesis stages. In total, eight chemical reactions of organic matter degradation have been considered. All degradation stages are assumed to follow the Monod kinetic model.

The degradation rate of organic matter represented by the growth rate of microorganisms is influenced by the pH and temperature of the local environment. The pH and temperature effect on the microorganism growth rate is approached with linear and exponential functions, respectively, as proposed by Henze et al. (1997). The amount of CH<sub>4</sub> and CO<sub>2</sub> produced dissolves into aqueous phase and is assumed to be negligible and considerable, respectively. The amount of CO<sub>2</sub> in aqueous phase is calculated according to Henry's constants and its partial pressure.

#### **2.6.4 Model Effect of Temperature, pH and Moisture Content on Degradation of Organic Matter**

A model that takes into account the effect of moisture content on the degradation of organic matter in MSW landfills was developed by Young (1989). In his model, Young assumed that MSW contained fats, protein, carbohydrates and inert fraction, where the first three components represent easily, medium and slowly degradable organic matter. The degradation pathway of this organic matter was divided into three stages, hydrolysis, acidogenesis and methanogenesis, where hydrolysis was considered as a limiting stage of the degradation of organic matter. It is assumed that within the hydrolysis stage, the organic matter will break down to form dissolved sugars, alcohol, acetic acid and long-chain carboxylic acids (i.e. propionic and

butyric acids). These hydrolyzed products (excluding acetic acid) will break down further to form acetic acid and CO<sub>2</sub> within the acidogenesis stage and convert to form CH<sub>4</sub> afterwards. All stages of the degradation of organic matter are assumed to follow the Monod kinetic model.

The degradation rate of organic matter is assumed to be influenced by landfill environment conditions including temperature, pH and moisture content. The temperature influence on the degradation of organic matter for the acidogenesis and methanogenesis stages is assumed by following the normalized function with optimum rate at 60 and 37 °C, respectively. The optimum pH for microorganism growth rate for both stages is a pH value of 7 with minimum and maximum values for acidogenesis and methanogenesis ranging between 2 to 12 and 5 to 9, respectively, distributed evenly following the normal distribution function, whilst the moisture content influence on microorganisms is assumed to be directly proportional to the fraction of water bound relative to its maximum value. Combining these three factors and the specific substrate consumption rate (Eq. 2.4), he formulated the reduction of the  $i^{\text{th}}$  organic matter over time as expressed in the equation below:

$$\frac{d(S_{ij})}{dt} = -\alpha_{(T,pH,\theta)} \cdot r_s \cdot S_{(ij)} \dots\dots\dots (2.19)$$

where  $\alpha_{(T,pH,\theta)}$  is the combination of temperature, pH and moisture content inhibition factors on the microorganism growth rate, which is defined by the equation below:

$$\alpha_{(T,pH,\theta)} = \frac{T\theta \exp\left\{-\left(pH-7\right)^2 \ln\left(\frac{4}{3}\right)\right\}}{\theta_{\max} \left\{1 + \exp\left(\frac{T-18}{4}\right)\right\}} \dots\dots\dots (2.20)$$

where  $T$  is the landfill temperature (°C),  $\theta$  is the moisture content (%),  $\mu$  is the specific microorganism growth rate (day<sup>-1</sup>), and  $X$  is the microorganism concentration (kg m<sup>-3</sup>). By taking the specific microorganism growth rate for fats,

protein and carbohydrates, which are  $8.03^{-10}$ ,  $1.61^{-10}$  and  $26.8^{-10}$ , he calculated the half-life of these organic matters, which would be 1, 5 and 30 years, respectively.

Kim et al. (2007) developed a one-dimensional compartment model to predict organic matter degradation in MSW landfill compartments. The model designed has a feature to shift the degradation of organic matter from anaerobic to aerobic conditions and vice versa due to the changing landfill operation. The shifting of the degradation of organic matter from anaerobic conditions was designed in a manner that depends on the local oxygen partial pressure within the landfill site. The idea behind this feature is to accommodate the current landfill operation trend in accordance with the regulation in force, which requires avoidance of the landfill emissions. On the other hand, the long period of aftercare maintenance, which takes from several decades up to a century, needs to be shortened to reduce the aftercare maintenance cost. Therefore, operating the landfill as a bioreactor landfill either by recirculation the leachate into landfill during post-operation to enhance anaerobic degradation for methane harvesting or by injecting air to enhance the aerobic degradation for early landfill stabilization is widely applied in the USA and European countries.

In this model, organic matter was distinguished into three categories according to its degradability, easily, slowly and non-degradable organic matter. The degradation pathway of these organic matters is determined by the  $O_2$  partial pressure in the landfill site. First, the organic matters are degraded aerobically if the  $O_2$  partial pressure is higher than 100 Pa. There is no assumption that intermediate product results from this degradation mechanism. Second, the organic matters are degraded aerobically when  $O_2$  partial pressure is less than 100 Pa. The intermediate product resulting from anaerobic degradation (i.e. acetic acid,  $NH_3$  and  $NO_3$ ) is subsequently converted into other products either aerobically or anaerobically depending on the partial  $O_2$  pressure. Third, the methanogenesis of acetic acid, and  $CO_2$  and  $H_2$ , occurs when the  $O_2$  partial pressure is less than 10 Pa. The  $O_2$  partial pressure per unit volume landfill cell is calculated by using the equation below:

$$p_i = \left( \frac{RT}{v_G} \right) \sum_{j=1}^n r_{(ij)} - (p_T - p_{atm}) \left( \frac{p_i}{p_T} \right) \dots\dots\dots (2.21)$$

where  $p_i$  is the partial pressure of oxygen (Pa),  $R$  is the universal gas constant ( $\text{m}^3 \text{ Pa K}^{-1} \text{ kmol}^{-1}$ ),  $T$  is the temperature (K),  $v_G$  is the volume of air space in the landfill cell ( $\text{m}^{-3}$ ),  $p_T$  is the total gas pressure gas in the air space (Pa), and  $p_{atm}$  is the atmospheric pressure (Pa).

The degradation rate of organic matter is assumed to correspond to the microorganism growth rate, which is controlled by the landfill environment conditions, including temperature, pH and moisture content. The specific aerobic microorganism growth rate of easily degradable organic matter is assumed to follow the Contois kinetic model, while the rest is set to follow the Monod kinetic model. The temperature influence on the microorganism growth rate was developed using a linear function according to the Arrhenius relationship with optimum temperature for mesophilic and thermophilic microorganisms ranging between 40 and 50, and 60 and 70, respectively. The aerobic bacteria growth rate is assumed to increase as moisture content increases up to 35% and to decrease as moisture content further increases. Meanwhile, beyond 35% moisture content the growth rate of anaerobic bacteria is assumed to be constant. Kim et al. (2007) distinguished microorganism sensitivity to acidity into four groups, but the pH range among them is not very different. The minimum pH for growing very sensitive microorganisms (e.g. nitrifiers, denitrifiers and methanogenic bacteria) was set at 4.5, whereas for the least sensitive (e.g. acidogenic) the pH value was defined as 4.0.

Table 2.6 summarizes a model developed to simulate organic matter degradation in MSW landfills and variables are taken into account. It should be noted that although some models have considered the effect of temperature and moisture content on microorganism growth, these variables are set up not to be influenced by climate condition (e.g. daily mean temperature and precipitation). The model simulation is carried out under constant ambient temperature and water input.

**Table 2.6** Summary modeling degradation organic matter in MSW landfills

Model variable	Model feature Degradation pathway	Substrate	Transport model	References
pH	1) Acidogenesis 2) Acetogenesis	1.1) Protein 1.2) Fats 1.3) Carbohydrate 1.4) Cellulose 2.1) Protein 2.2) Fats 2.3) CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> COOH	Gas and leachate	White et al. (2004)
Temp., pH	3) Methanogenesis 1) Hydrolysis 2) Aerobic degradation 3) Anaerobic degradation 4) Acetogenesis 5) Methanogenesis	3.1) CH <sub>3</sub> COOH 1.1) Organic matter 2.1) Cellulose 3.1) Cellulose 4.1) CH <sub>3</sub> CH <sub>2</sub> COOH 4.2) CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> COOH 5.1) CH <sub>3</sub> COOH 5.2) CO <sub>2</sub> + H <sub>2</sub>	not considered	Haarstrick et al. (2004)
Temp., pH	1) Hydrolysis 2) Acidogenesis 3) Acetogenesis 4) Methanogenesis	1.1) Cellulose 2.1) Glucose 3.1) CH <sub>3</sub> CH <sub>2</sub> COOH 3.2) CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> COOH 4.1) CH <sub>3</sub> COOH 4.2) CO <sub>2</sub> + H <sub>2</sub>	Gas and heat	El-Fadel et al. (1996a)
Temp., pH, moisture	1) Aerobic degradation 2) Acidogenesis 3) Methanogenesis	1.1) Easily degradable 1.2) Slowly degradable 1.3) CH <sub>3</sub> COOH 1.4) NH <sub>3</sub> 2.1) Easily degradable 2.2) Slowly degradable 3.1) CH <sub>3</sub> COOH 3.2) CO <sub>2</sub> + H <sub>2</sub>	Gas, heat and leachate	Kim et al. (2007)
Temp., pH, moisture	4) Denitrification 1) Hydrolysis 2) Acidogenesis 3) Acetogenesis 4) Methanogenesis	4.1) NO <sub>3</sub> + CH <sub>3</sub> COOH 1.1) Carbohydrate 1.2) Protein 1.3) Fats 2.1) Glucose 2.2) Alcohols 3.1) Carboxylic acids 4.1) CH <sub>3</sub> COOH 4.2) CO <sub>2</sub> + H <sub>2</sub>	Gas and leachate	Young (1989)

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## **Chapter 3**

### **Model Development**

Numerous laboratory experiments followed by field testing have been conducted to implement, evaluate and further develop the bioreactor landfill concept in MSW landfills. However, the rapid development in computer technology has encouraged researchers to create computer-based models for an improved understanding and modeling of the degradation of solid organic matter in landfills prior to the field application. The earlier landfill models considered only moisture flow and leaching of soluble organic matter (Straub and Lynch, (1982a, b), moisture flow for unsaturated conditions (Korfiatis and Demetracopoulos, (1984) and solute generation and transport from landfills (Demetracopoulos et al., 1986).

More complex models were developed afterwards through consideration of the effect of pH on the biodegradation of organic matter by White et al. (2004), the effect of moisture content on the biodegradation of organic matter by McDougall and Pyrah (1999), the effect of temperature incorporated with pH on the biodegradation of organic matter by El-Fadel et al. (1996a) and Haarstrick et al. (2004), and the combined effect of temperature, pH and moisture content by Young (1989) and Kim et al. (2007), as was described in the previous section. Although the last two models considered the most relevant factors affecting the biodegradation of organic matter, they do not take into account the environmental influences of these factors. Therefore, the atmospheric temperature and precipitation rate, which greatly influenced these factors, were set up at a fixed value for the entire simulation time. This approach obviously differs from real conditions where the atmospheric temperature and rate of precipitation fluctuate greatly depending on region and seasonal climate conditions. Moreover, the model has also not been experimentally verified to measure the model calculation accuracy.

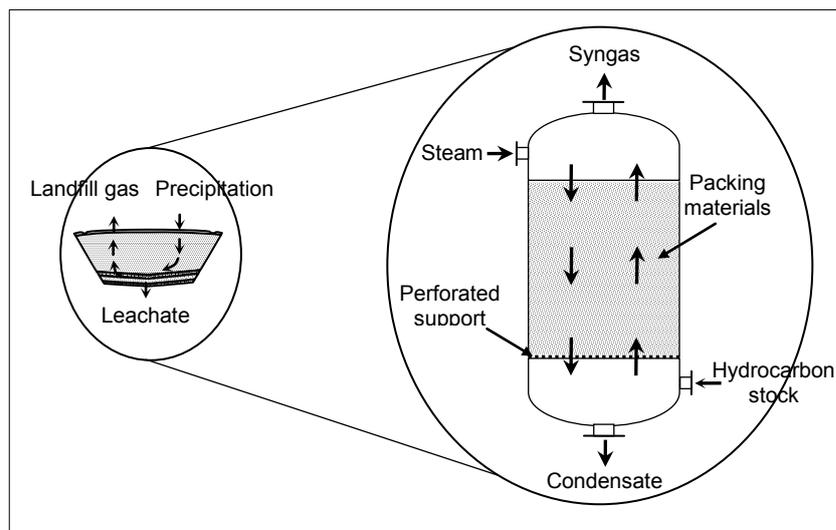
The present study aims to develop the computer-based model to simulate biodegradation organic matter in landfill sites by considering the effect of temperature, pH and moisture content on the biodegradation of organic matter in landfill cells, taking into account the fluctuation of atmospheric temperature and precipitation rate according to region and seasonal climate condition. For this purpose, the Packed Bed Reactor (PBR) coupled with batch reactor concepts widely used in industrial processes is adopted within the model development. The method approach, detailed mathematical model formulation and assumptions used in this study are described in the following sections. The model was also verified by a laboratory experiment and assesses the sensitivity of biological parameters that control biodegradation organic matter, contaminant concentration in leachate and landfill emissions.

### **3.1 Model Analogy and Governing Balance Equations**

In industrial processing, PBRs are very important equipment for the synthesis of chemicals or intermediate products. In this reactor, the reaction takes place during intimate contact between the reactants within the transport process. The contact between the two phases to separate a solute from a mixed component (e.g. absorption, extraction, leaching, etc.) or to reactants to produce new product (e.g. catalytic reaction) is applied in many processes. These processes involve mass transfer and/or mass transfer followed by chemical reaction. In most cases, the contact between the two phases is intimately tied to the presence of the solid phase, so-called packing materials or packed bed.

The hydro-cracking of heavy petroleum feedstock using a zeolite-based catalyst is an example of application contact between two phases in the PBRs (Penick, 1985). In this process, the heavy petroleum feedstock feeds into the reactor through a mean inlet for the liquid on top of the reactor and flows downward due to gravity through catalyst bed interstices to the outlet to withdraw the hydro-cracking product at the bottom reactor. On the opposite side, the hydrogen ( $H_2$ ) under pressure feeds into

the reactor through a gas inlet at the bottom of the reactor. The  $H_2$  and heavy petroleum feedstock flow counter, and current and intimate contact occurs along the catalyst bed. The rich  $H_2$  leaves from the reactor through a mean outlet at the top of the reactor and flows to the absorber column to remove the contaminant before re-feeding into the reactor.



**Figure 3.1** Schematic diagram the theoretical approach of landfill cells considered as PBR

Figure 3.1 shows a comparison of the gas and liquid flow patterns throughout the solid phase in PBR and a landfill site. In general, there is a similarity between them, where the liquid phase flows downwards from the top to the bottom sides, while due to its properties and incorporated mechanical device the gas phase produced by the biodegradation of organic matter flows counter currently to the liquid phase. During the transport process, the gas reacts with liquid or other gases due to intimate contact in the presence of a solid phase. Moreover, some miscible gases will dissolved in the liquid phase. This process is a common phenomenon that occurs in industrial processes involving a packed bed column.

Although the flow patterns of liquids and gases in landfill sites and PBR are similar, there are also substantial differences between both processes. For example, in PBR the solid phase acts only as a catalyst. This means that no interaction between solid, gas and liquid phases has occurred, while in the landfill site a solid phase also acts as a reactant, which degrades during the biodegradation process. Therefore, an

additional approach is required to describe the material balance of the solid phase in the landfill cell. For this purpose, PBR coupled with batch reactor concepts could be suitable for describing the material balance of landfill sites. A typical feature of the batch reactor operation is that the reactant is fed into the reactor prior to the process taking place and no in and out flows after the process takes place can represent degradable organic matter in landfill sites.

### **3.1.1 Governing Mass Balance Equations**

As previously mentioned, the PBR coupled with batch reactor concepts is adopted to model the biodegradation of organic matter in an MSW landfill. A unit cell of landfill is analogous to a stage of the PBR. The degradable organic matter is surrounded by low permeable material (i.e. daily soil cover). Therefore, material balances for landfill sites were formulated based on this low permeable material as calculation boundary. The solid phase is considered to be in a fixed state, while the liquid and gas phases flow counter currently throughout the solid phase. The liquid phase is represented through water precipitation and other liquid components flowing downward from the upper side throughout organic matter and discharges at the bottom side. Within the liquid phase transport, it is assumed that there is no solid organic matter transported in the liquid phase.

The gas phase represents biogenic gases produced from biological reaction and assumed to flow only in an upward direction throughout the solid phase due to the pressure difference between the landfill and the atmosphere. Within the gas transport, some miscible gas (e.g. carbon dioxide) will dissolve in the liquid phase. The concentration of gases dissolved in the liquid phase is assumed to be in equilibrium within the gas phase and limited by Henry's constant.

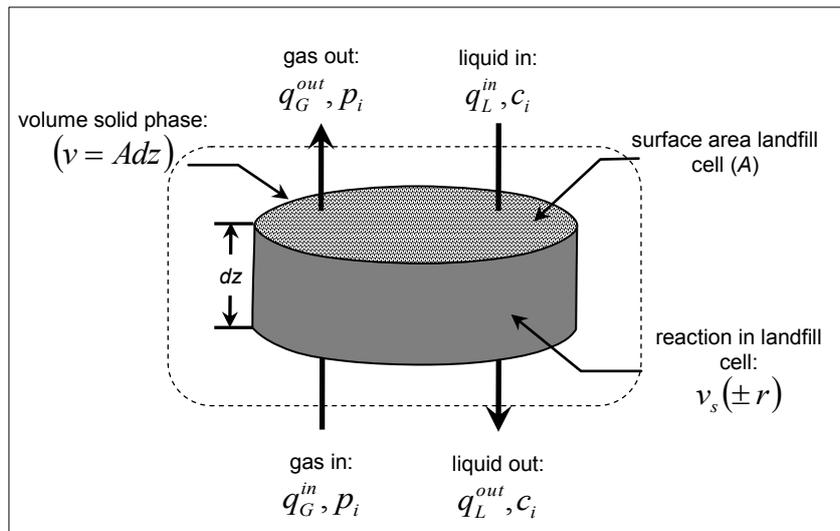


Figure 3.2 System boundaries material balance of a unit landfill cell

According to these assumptions and mass conservation principle, the general mass balances of one unit landfill cell can be drawn based on the system boundary as illustrated in Figure 3.2 and shown by the following equation:

$$\frac{\partial M}{\partial t} = \sum_{j=1}^n (r) + q^{in}c - q^{out}c \dots\dots\dots (3.1)$$

where  $M$  stands for the mass of degradable organic matter ( $\text{kg day}^{-1}$ ),  $r$  is the production/consumption rate of degradable organic matter at the  $j$ th reaction stage ( $\text{kg day}^{-1}$ ),  $q^{in}$  and  $q^{out}$  are total volumetric liquid and gas flow rates to enter and leave the landfill cell ( $\text{m}^3 \text{ day}^{-1}$ ), and  $c$  is the concentration of organic matter in liquid and gas flow rates to enter and leave the landfill cell ( $\text{kg m}^{-3}$ ).

As solid organic matter is in a fixed state, it is assumed that no solid organic matter in liquid enters and leaves the landfill cells. Therefore, Eq. (3.1) can be rewritten to describe the mass balances of solid organic matter as follows:

$$\frac{\partial S_i}{\partial t} = \sum_{j=1}^n (r_i) \dots\dots\dots (3.2)$$

where  $S_i$  stands for the mass  $i$ th constituent of solid organic matter ( $\text{kg day}^{-1}$ ), and  $r_i$  is the production/consumption rate of the  $i$ th constituent of solid organic matter at the  $j$ th biological/chemical reaction stage ( $\text{kg day}^{-1}$ ).

Although the liquid phase was considered to flow only in a downward direction, parts of the moisture and volatile aqueous species may evaporate and flow upward. By taking into account the amount of moisture that evaporated, the mass balance for the moisture can be written as:

$$\frac{\partial L_i}{\partial t} = \sum (r_i) + q_L^{\text{in}} c_i - q_L^{\text{out}} c_i - q^{\text{evp}} \dots \dots \dots (3.3)$$

where  $L_i$  is the mass of the  $i$ th constituent in the liquid phase ( $\text{kg day}^{-1}$ ),  $q_L^{\text{in}}$  and  $q_L^{\text{out}}$  are volumetric precipitation and leachate discharge of landfill cells ( $\text{m}^3 \text{ day}^{-1}$ ),  $c_i$  is the concentration of the  $i$ th constituent in precipitation and discharge of landfill cells ( $\text{kg m}^{-3}$ ), and  $q^{\text{evp}}$  is the evaporation rate of the moisture ( $\text{kg day}^{-1}$ ). The volumetric leachate discharge of landfill cells depends on the difference between the total liquid phase (e.g. the sum moisture and aqueous species) and the field capacity as expressed by the following equation:

$$q_L^{\text{out}} = (v_L - \theta_F v) \dots \dots \dots (3.4)$$

The evaporation rate is driven by the difference between the saturated and moisture vapour pressures as expressed by equation (3.5).

$$q^{\text{evp}} = (p_{H_2O}^s - p_{H_2O}) \dots \dots \dots (3.5)$$

where  $p_{H_2O}^s$  and  $p_{H_2O}$  are saturated and moisture vapour pressures (Pa). The saturated vapour pressure is defined as a temperature function:

$$p_{H_2O}^s = \exp\left(20.386 - \frac{5132}{T}\right) \dots \dots \dots (3.6)$$

where  $T$  is the temperature of the landfill ecosystem (K). As concentration species of aqueous organic matter (e.g.  $\text{CH}_3\text{COOH}$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{CO}_3$ ,  $\text{HCO}_3^-$ ,  $\text{CO}_3^{2-}$ ,

$H^+$  and  $OH^-$  in precipitation are considered to be zero and these species will not evaporate, the mass balance for aqueous organic matter is defined by equation (3.7).

$$\frac{\partial L_i}{\partial t} = \sum (r_i) - q_L^{out} c_i \quad \dots\dots\dots (3.7)$$

where  $q_L^{in}$  is the volumetric leachate discharge of the landfill cell ( $m^3 \text{ day}^{-1}$ ), and  $c_i$  is the concentration of the  $i$ th aqueous organic matter in the discharge of the landfill cell ( $kg \text{ m}^{-3}$ ).

The biogenic gas produced from the degradation of solid and aqueous organic matter is assumed to flow only in an upward direction. Thus the mass balance of gaseous organic matter can be written as follows:

$$\frac{\partial G_i}{\partial t} = \sum (r_i) + q_G^{in} p_i - q_G^{out} p_i \quad \dots\dots\dots (3.8)$$

where  $q_G^{in}$  and  $q_G^{out}$  are aeration volumetric flow and landfill gas release from the landfill cell ( $m^3 \text{ day}^{-1}$ ), and  $p_i$  is the partial pressure of the  $i$ th biogenic gas in the injected (e.g. through landfill aeration) and landfill released gas of the landfill cell ( $kg \text{ m}^{-3}$ ). In cases where the landfill is operated without aeration, the second term of Eq. (3.7) can be neglected. The flow rate of landfill gas released from the landfill cell is determined by using an ideal gas equation (3.9).

$$q_G^{out} = v(p_T - p_{atm}) \frac{V_G}{RT} \quad \dots\dots\dots (3.9)$$

where  $v$  is the conversion factor from mol to cubic meter ( $m^3 \text{ mol}^{-1}$ ),  $p_T$  and  $p_{atm}$  are landfill gas pressures in the landfill cell and the atmospheric pressure (Pa),  $V_G$  is the air space in the landfill cell ( $m^3$ ), and  $R$  is the universal gas constant ( $m^3 \text{ Pa K}^{-1} \text{ mol}^{-1}$ ).

The production/consumption rate  $i$ th constituent of degradable solid organic matter, aqueous and gas phases under either aerobic or anaerobic conditions is defined as the result of specific growth rate divided by the biomass yield formed per mass of

substrate utilized, and multiplied by the mass of biomass and the environmental inhibition factor. The production/consumption rate  $i$ th constituent of degradable solid, aqueous and gas organic matter is expressed by the following equation:

$$r_i = -\frac{1}{\psi_i} \Omega \mu_i x_i \dots\dots\dots (3.10)$$

where  $\Omega$  is the environmental inhibition factor as a function of temperature, pH and moisture content (dimensionless),  $\mu_i$  is the specific growth rate of the  $i$ th species of biomass ( $\text{day}^{-1}$ ),  $\psi_i$  is the yield of the  $i$ th species of biomass formed per mass of substrate utilized ( $\text{kg/kg}$ ), and  $x_i$  is the concentration of the  $i$ th species of biomass ( $\text{kg m}^{-3}$ ).

The specific growth rate of the  $i$ th species of biomass was assumed to follow either the Monod or Contois kinetic models depending on the substrate utilized and the landfill ecosystem condition. The specific growth rate of the biomass applied for the biodegradation of solid, aqueous and gaseous organics for each degradation stage is calculated using the series equation listed below:

The Contois kinetic model for aerobic degradation of organic matter is shown in equation 3.11 below:

$$\mu_i = \mu_{max} \frac{\frac{S_i}{x_i}}{k_C + \frac{S_i}{x_i}} \frac{p_{O_2}}{k_{O_2} + p_{O_2}} \dots\dots\dots (3.11)$$

The Monod kinetic models for aerobic and anaerobic degradation of organic matter are shown in equations 3.12 and 3.13 below:

$$\mu_i = \mu_{max} \frac{S_i}{k_M + S_i} \frac{p_{O_2}}{k_{O_2} + p_{O_2}} \dots\dots\dots (3.12)$$

$$\mu_i = \mu_{max} \frac{S_i}{k_M + S_i} \dots\dots\dots (3.13)$$

where  $\mu_{max}$  is the maximum specific growth rate of the  $i$ th species of biomass ( $\text{day}^{-1}$ ),  $k_C$  is the Monod saturation constant (dimensionless), and  $k_M$  is the Monod saturation constant, which is defined as the minimum substrate available for half the maximum specific growth rate ( $\text{kg m}^{-3}$ ).

The specific growth rate of biomass was assumed to follow the Monod kinetic model, except for simple carbohydrates. According to Znad et al. (2004), the Contois kinetic model fit better than the Monod kinetic model for aerobic degradation of simple carbohydrate compounds such as glucose, hence, this kinetic model is applied for the biodegradation of dissolved simple carbohydrates.

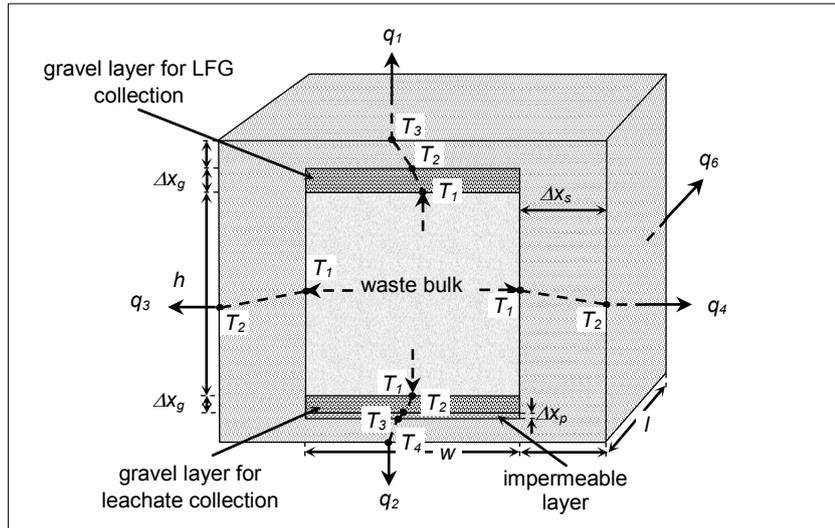
### 3.1.2 Governing Heat Balance Equations

A considerable heat of reaction (enthalpy) is generated from parallel and sequential biological reaction from the biodegradation of organic matter in landfill cells. The heat generated within the landfill cell is transferred to the environment in all directions. The amount of heat transferred depends on the heat generated and the ambient temperature. However, due to the significant temperature difference most of it will flow upwards and be lost to the environment at the landfill cover atmosphere boundary (Miller and Clesceri, 2003). The heat balance within the landfill cell can be written as follows:

$$\frac{\partial Q}{\partial t} = \sum_{j=1}^n r_i(-\Delta H) + \dot{m}^{in} c_p \Delta T - \dot{m}^{out} c_p \Delta T - \sum q_c \dots\dots\dots (3.14)$$

where  $\Delta H_i$  is the heat of reaction of the  $i$ th species of solid, aqueous and gaseous organic matter ( $\text{kJ kg}^{-1}$ ),  $\dot{m}^{in}$  and  $\dot{m}^{out}$  are mass flow rates of aqueous and gaseous organic matter that enters and leaves the landfill cell ( $\text{kg day}^{-1}$ ),  $c_p$  is the specific heat capacity of aqueous or gaseous organic matter that enters and leaves the landfill cell ( $\text{kJ kg}^{-1} \text{K}^{-1}$ ),  $\Delta T$  is the temperature difference between the landfill ecosystem

and ambient environment (K), and  $q_c$  is the heat transfer by conduction through the landfill cover, bottom liner and side walls to the environment ( $\text{kJ m}^{-2} \text{day}^{-1}$ ).



**Figure 3.3** The schematic diagram heat transfer of landfills cell to surrounding area

The biodegradation of solid, aqueous and gaseous organic matter takes place at any point in the landfill cell, thus temperature within the landfill cell was assumed to be uniform. Therefore, the heat transfer by conduction can be considered from the cell boundary to the environment. Figure 3.3 shows a schematic of heat transfer by conduction from the landfill cell to the environment. In order to minimize the landfill emissions to the top, bottom and side walls, the landfill site is usually constructed with different construction methods and materials. Hence, the heat transferred by conduction depends upon the construction material and the number of layers. According to Fourier’s law, the heat transferred from the landfill cell to the environment is distinguished into several approaches as expressed by the following equations:

For heat transfer across a single layer:

$$q_c = kA \frac{\partial T}{\partial x} \dots\dots\dots (3.15)$$

For heat transfer across double or multiple layers:

$$q_c = k_1 A \frac{\partial T_1}{\partial x} + k_2 A \frac{\partial T_2}{\partial x} + \dots + k_n A \frac{\partial T_n}{\partial x} = \sum_{i=1}^n k_i A \frac{\partial T}{\partial x} \dots\dots\dots (3.16)$$

where  $k$  is the thermal conductivity of the material traversed by heat ( $\text{kJ K}^{-1} \text{m}^{-1} \text{day}^{-1}$ ),  $A$  is the surface area of the top, bottom and side walls traversed by the heat flow ( $\text{m}^2$ ), and  $x$  is the thickness of the top, bottom and side walls traversed by the heat flow (m).

## 3.2 The Environmental Inhibition Factors

There are many factors influencing the biodegradation of organic matter in landfill cells, and all are interrelated. However, temperature, pH and water content are the main factors influencing the biodegradation of organic matter. Therefore, these three factors have been considered in this study. The approach used is described in the following paragraphs.

### 3.2.1 Temperature Inhibition Factor

The temperature of the landfill ecosystem is influenced by the biodegradation rate of organic matter through temperature affecting the biomass growth rate. Although various types of bacteria are found in extreme environmental conditions, almost all bacteria types are very sensitive to temperature changes. In general, the bacteria growth rate is rather slow when the temperature is either below or above the favourable temperature range. The bacteria cells will deteriorate when the temperature is increased further. As a consequence, no biodegradation of organic matter occurs.

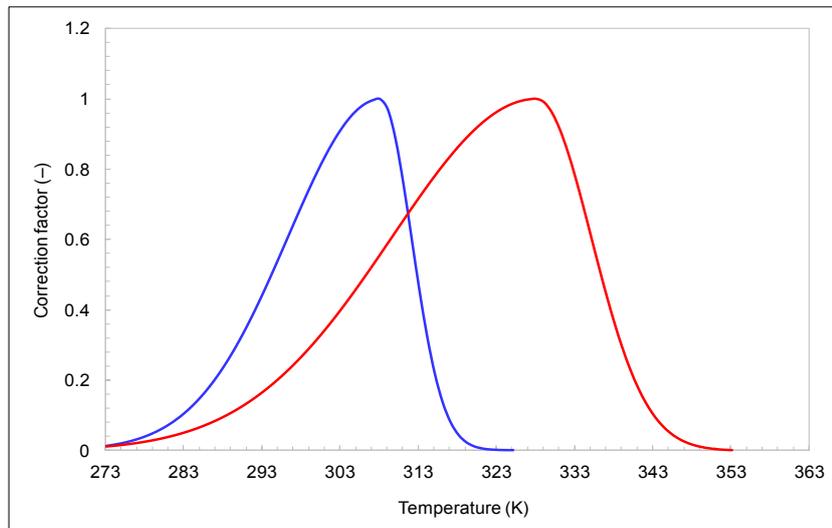
The literature survey described in the previous section shows that the bacteria growth rate occurs within a temperature range from 5 to 80 °C. However, most methanogenic bacteria are mesophilic, within a temperature range between 10 and 45 °C, and the optimum for activity is around 37 °C (Pavlostathis and Giraldo-Gomez, 1991). Hence, this temperature was selected as the optimum temperature for

methanogenic growth rates, while the optimum temperature for acidogenic bacteria growth rates was fixed at 55 °C (Yu et al., 2002; Shin et al., 2004). The temperature correction factor applied in this model is given by the following equation:

$$\Omega_{(T)} = c_T \frac{1}{\sigma\sqrt{2\pi}} e^{-0.5\left(\frac{T-T_{opt}}{\sigma}\right)^2}; \quad T \leq T_{opt} \dots\dots\dots (3.17)$$

$$\Omega_{(T)} = c_T \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(T-T_{opt})^2}{2\sigma^2}}; \quad T \geq T_{opt}$$

where  $c_T$  and  $\sigma$  are constants fitting parameters (dimensionless), and  $T$  and  $T_{opt}$  are the actual temperatures in the landfill ecosystem on the one hand and the optimum temperature for bacteria growth on the other (K). Plotting this equation into  $x$ - $y$  Cartesian will form a curve correction factor as a function of temperature (K) as shown in Figure 3.4.



**Figure 3.4** Plot temperature correction factor function, methanogenesis (blue line) and acidogenesis (red line).

### 3.2.2 pH Inhibition Factor

The second most important factor that influences the bacteria growth rate is the pH. In general, a neutral or near to neutral pH is the most favourable condition for bacteria growth. The change of the pH out of its tolerance limits will interfere with the metabolic system of the bacteria. This includes the ability to utilize carbon and

energy sources that will reduce the efficiency of substrate degradation and production of metabolism. Moreover, pH variation can affect cell morphology and the structure of the bacteria.

Numerous studies have been done related to the influence of the pH on the bacteria growth rate. Most of them conclude that the metabolic and growth rates of methanogenic and acid fermentation bacteria are different. Although acidogenesis was reported to be active in a wide range of pH, it varies with substrate and digestion technique. The optimum biodegradation was found at a pH of 6.5 (Joubert and Britz, 1986; Kisaalita et al., 1987; Yu et al., 2003), whereas the optimum methanogenesis was found at a pH of 7.0 (Zeikus and Wolfe, 1972; Farquhar and Rovers, 1973; Zehnder and Wuhrmann, 1977; ten Brummeler et al., 1985; Meher and Ranade, 1993; Chu et al., 2008; Park et al., 2010).

According to these findings, the optimum pH values for acidogenesis and methanogenesis are 6.5 and 7.0, whilst for aerobic biodegradation the optimum pH bacteria growth rate was set at 7.5. However, as methanogens, nitrifiers and denitrifiers are very sensitive to the pH value (Tchobanoglous et al., 1991), the range of pH for this bacteria group was set narrower than the range used for aerobic and acidogenic bacteria. Therefore, the pH inhibition factor is expressed by the following equation:

$$\Omega_{(pH)} = c_{pH} \frac{1}{\sigma\sqrt{2\pi}} e^{-0.5\left(\frac{pH-pH_{opt}}{\sigma}\right)^2} \dots\dots\dots (3.18)$$

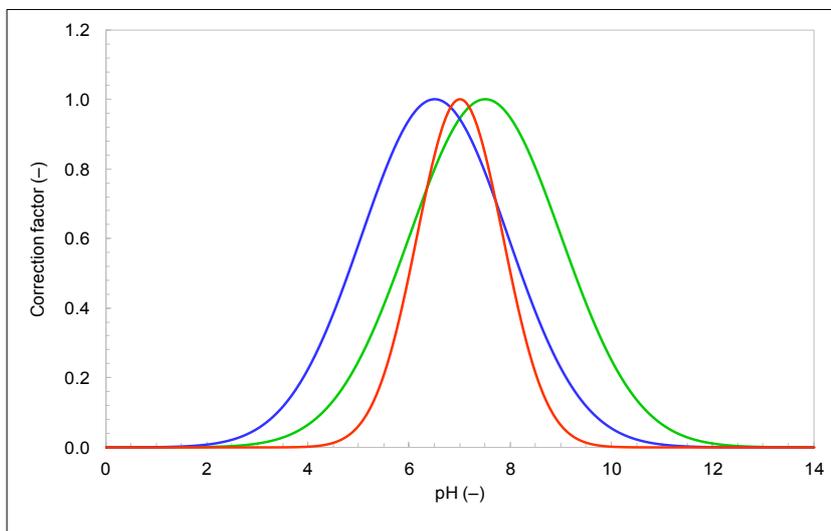
where  $c_{pH}$  and  $\sigma$  are constant fitting parameters (dimensionless), and  $pH$  and  $pH_{opt}$  are the pH in landfill cells and the optimum pH for biomass growth (unit less). Plotting this function into  $x$ - $y$  Cartesian will form a curve correction factor as a function of the pH as presented in Figure 3.5.

The pH value of the landfill ecosystem is calculated iteratively according to the charge balance or electroneutrality of the aqueous phase. The electroneutrality of the

aqueous phase is defined as the difference between anion and cation of dissociated substances in aqueous phase, and is expressed by the following equation:

$$[\text{Ac}^-] + [\text{HCO}_3^-] + 2[\text{CO}_3^{2-}] + [\text{OH}^-] - [\text{NH}_4^+] - 2[\text{Ca}^{2+}] - [\text{H}^+] = 0 \dots\dots\dots (3.19)$$

where  $[\text{Ac}^-]$ ,  $[\text{HCO}_3^-]$ ,  $[\text{CO}_3^{2-}]$ ,  $[\text{OH}^-]$ ,  $[\text{NH}_4^+]$  and  $[\text{Ca}^{2+}]$  are cogeneration aqueous acids (e.g. acetic, propionic and butyric acids), bicarbonate, carbonate, hydrogen oxide, ammonium and calcium ions, respectively.



**Figure 3.5** Plot pH correction factor function, aerobic biodegradation (green line), acidogenesis (blue line), and methanogenesis (red line).

$\text{Ca}^{2+}$  ions are assumed to derive from dissociated dissolved  $\text{CaCO}_3$ . The concentration of those ions in aqueous phase is determined by their concentration and equilibrium constant, which may also be temperature dependent; however, this was not considered in this model. The ion concentration relationships with the equilibrium constant are presented in the following equations:

$$[\text{Ac}^-] = \frac{K_{\text{Aq}}}{[\text{H}^+]} [\text{HAc}] \dots\dots\dots (3.20a)$$

$$[\text{HCO}_3^-] = \frac{K_{\text{H}_2\text{CO}_3}}{[\text{H}^+]} H_{\text{CO}_2} p_{\text{CO}_2} \dots\dots\dots (3.20b)$$

$$[\text{CO}_3^{2-}] = \frac{K_{\text{HCO}_3} K_{\text{H}_2\text{CO}_3}}{[\text{H}^+]^2} \dots\dots\dots (3.20c)$$

$$[\text{OH}^-] = \frac{K_w}{[\text{H}^+]} \dots\dots\dots (3.20d)$$

$$[\text{NH}_4^+] = \frac{K_{\text{NH}_3}}{[\text{H}^+]} H_{\text{NH}_3} p_{\text{NH}_3} \dots\dots\dots (3.20e)$$

$$[\text{Ca}^{2+}] = \frac{K_{\text{sp}}}{[\text{CO}_3^{2-}]} \dots\dots\dots (3.20f)$$

where  $K_{\text{Aq}}$ ,  $K_{\text{H}_2\text{CO}_3}$ ,  $K_{\text{HCO}_3^-}$  and  $K_{\text{NH}_3}$  are equilibrium constants of aqueous acids, bicarbonate, carbonate and ammonium ( $\text{kmol m}^{-3}$ ), respectively,  $K_w$  is the water self-ionization constant ( $\text{kmol m}^{-3}$ ),  $K_{\text{sp}}$  is the solubility constant of calcium carbonate ( $\text{kmol m}^{-3}$ ), and  $H_{\text{CO}_2}$  and  $H_{\text{NH}_3}$  are Henry's constants for carbon dioxide and ammonia ( $\text{Pa m}^3 \text{ kmol}^{-1}$ ). The equilibrium constants of gas and liquid phases and the solubility constant of calcium carbonate are given in Table 3.1.

**Table 3.1** Equilibrium constants among gas and aqueous, and solid and aqueous phases

Equilibrium constant	Unit	Value
$K_w = [\text{H}^+][\text{OH}^-]$	$\text{kmol m}^{-3}$	$1.00 \times 10^{-14}$
$K_{\text{Ace}} = \frac{[\text{H}^+][\text{Ace}^-]}{[\text{HAce}]}$	$\text{kmol m}^{-3}$	$1.74 \times 10^{-5}$
$K_{\text{Pro}} = \frac{[\text{H}^+][\text{Pro}^-]}{[\text{HPro}]}$	$\text{kmol m}^{-3}$	$1.34 \times 10^{-5}$
$K_{\text{But}} = \frac{[\text{H}^+][\text{But}^-]}{[\text{HBut}]}$	$\text{kmol m}^{-3}$	$1.52 \times 10^{-5}$
$K_{\text{H}_2\text{CO}_3} = \frac{[\text{H}^+][\text{HCO}_3^-]}{H_{\text{CO}_2} p_{\text{CO}_2}}$	$\text{kmol m}^{-3}$	$4.47 \times 10^{-7}$
$K_{\text{HCO}_3^-} = \frac{K_{\text{H}_2\text{CO}_3}}{[\text{H}^+]} \frac{[\text{HCO}_3^-]}{[\text{CO}_3^{2-}]}$	$\text{kmol m}^{-3}$	$5.01 \times 10^{-11}$
$K_{\text{NH}_3} = \frac{[\text{H}^+][\text{NH}_4^+]}{H_{\text{NH}_3} p_{\text{NH}_3}}$	$\text{kmol m}^{-3}$	$6.31 \times 10^{-10}$
$K_{\text{H}(\text{CO}_2)} = \frac{p_{\text{CO}_2}}{[\text{H}_2\text{CO}_3]}$	$\text{Pa kmol}^{-1} \text{ m}^{-3}$	$3.38 \times 10^6$
$K_{\text{H}(\text{NH}_3)} = \frac{p_{\text{NH}_3}}{[\text{NH}_3]}$	$\text{Pa kmol}^{-1} \text{ m}^{-3}$	$5.78 \times 10^3$
$K_{\text{sp}} = [\text{Ca}^{2+}][\text{CO}_3^{2-}]$	$\text{kmol m}^{-3}$	$4.70 \times 10^{-9}$

Substitute Eq. (3.20a) to (3.20f) into Eq. (3.19) and thus rearranging it will lead to the following equation:

$$[\text{H}^+] = \frac{K_{\text{Aq}}}{[\text{H}^+]} [\text{HAc}] + \frac{K_{\text{H}_2\text{CO}_3}}{[\text{H}^+]} H_{\text{CO}_2} p_{\text{CO}_2} + \frac{K_{\text{HCO}_3^-} K_{\text{H}_2\text{CO}_3}}{[\text{H}^+]^2} H_{\text{CO}_2} p_{\text{CO}_2} + \frac{K_w}{[\text{H}^+]} \dots\dots\dots (3.21)$$

$$- \frac{K_{\text{NH}_3}}{[\text{H}^+]} H_{\text{NH}_3} p_{\text{NH}_3} - \frac{K_{\text{sp}}}{[\text{CO}_3^{2-}]}$$

By solving this equation iteratively we find the concentration of  $[\text{H}^+]$  in the aqueous phase. Then, we can calculate the pH carbonate system by using  $\text{H}^+$  calculated above as follows:

---


$$\text{pH} = -\log[\text{H}^+] \dots\dots\dots (3.22)$$

### 3.2.3 Moisture Content Inhibition Factor

All biomass needs moisture for its metabolism and as an intercessor for extracellular enzymes during hydrolyzation of particulate organic matter. However, limited studies have been carried out to discover the effect of moisture content on bacteria growth rate. This is because most studies related to the biodegradation of solid organic matter have been focused on anaerobic biodegradation, which is carried out under saturated conditions.

A study carried out by Iovieno and Bååth (2008) on the effect of soil moisture on bacteria growth shows that the rate of bacterial respiration increases exponentially with an increase in soil moisture content from 5% to 40%, but remains constant with further increase of the moisture content. Since this finding does not conflict with accepted behaviour, it was adopted in this study. Nonetheless, the aerobic bacteria growth rate was assumed to decrease by increasing moisture content beyond 40%. This approach was based on the hypothesis that further increase of the moisture content will inhibit oxygen infiltration and shift the landfill ecosystem to anaerobic conditions. The moisture inhabitation correction factor was denoted by  $\Omega(\theta)$  as expressed in the following equations:

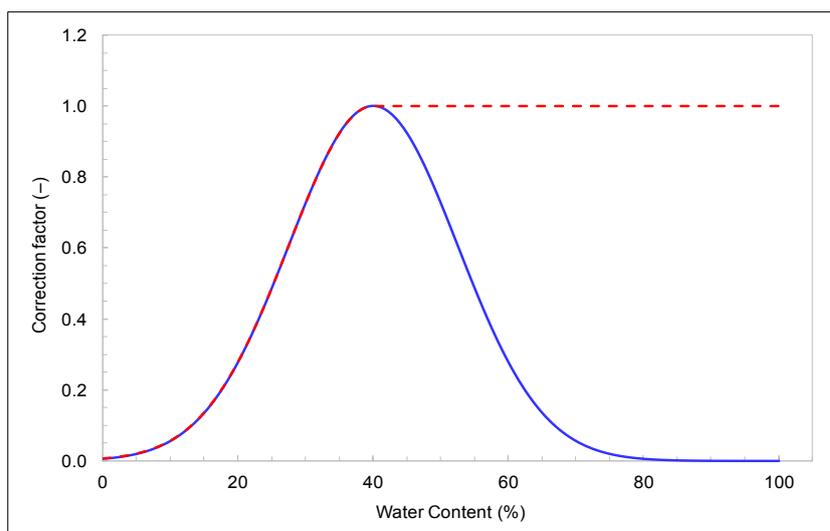
for aerobic biodegradation:

$$\Omega_{(\theta)} = c_{\theta} \frac{1}{\sigma\sqrt{2\pi}} e^{-0.5\left(\frac{\theta-\theta_{opt}}{\sigma}\right)^2} \dots\dots\dots (3.23)$$

and for anaerobic biodegradation:

$$\begin{aligned} \Omega_{(\theta)} &= c_{\theta} \frac{1}{\sigma\sqrt{2\pi}} e^{-0.5\left(\frac{\theta-\theta_{opt}}{\sigma}\right)^2}; & \theta \leq \theta_{40} & \dots\dots\dots (3.24) \\ \Omega_{(\theta)} &= 1; & \theta \geq \theta_{40} & \end{aligned}$$

where  $c_\theta$  and  $\sigma$  are constant fitting parameters of the correction factor (dimensionless), and  $\theta$  and  $\theta_{opt}$  are the moisture content landfill ecosystem and the optimum moisture content for the bacteria growth rate (%). Figure 3.6 presents the moisture inhibition correction factor as a function of the moisture content as used in this model.



**Figure 3.6** Plot moisture content correction factor function, aerobic biodegradation (blue line), and anaerobic biodegradation (red line).

### 3.3 Determining Fraction of Degradable Organic Matter

The landfill cell was considered to consist of three phases, namely gas, liquid and solid phase. The solid phase was composed of degradable organic matter, inorganic solid matter and biomass. The degradable solid organic matter was distinguished into three categories according to its degradability level, namely readily, slowly and hardly degradable organic matters.

The fraction of readily, slowly and hardly degradable organic MSW matter is determined according to its composition in each MSW constituent. Readily degradable organic matter is represented by simple carbohydrates, protein and fats, while slowly and hardly degradable organic matter is represented by cellulose and lignin. The composition of each fraction was calculated by multiplying its fraction

by the composition of MSW constituents and converted to mass weight as expressed by the equation below:

$$s_i = v_s \rho_s \sum w_i x_j \dots\dots\dots (3.25)$$

where  $s_i$  stands for the mass of the  $i$ th solid organic matter (e.g. readily, slowly and hardly degradable organic matters) ( $\text{kg m}^{-3}$ ),  $\rho$  is the density of the municipal solid waste ( $\text{kg m}^{-3}$ ),  $v_s$  is the landfill cell volume ( $\text{m}^3$ ),  $w$  is the fraction of the  $i$ th waste type (%), and  $x$  is the composition of the  $j$ th degradable solid organic matter (%). The fraction of degradable organic matter in MSW constituents is presented in Table 3.2.

**Table 3.2** Organic matter fraction in MSW constituent

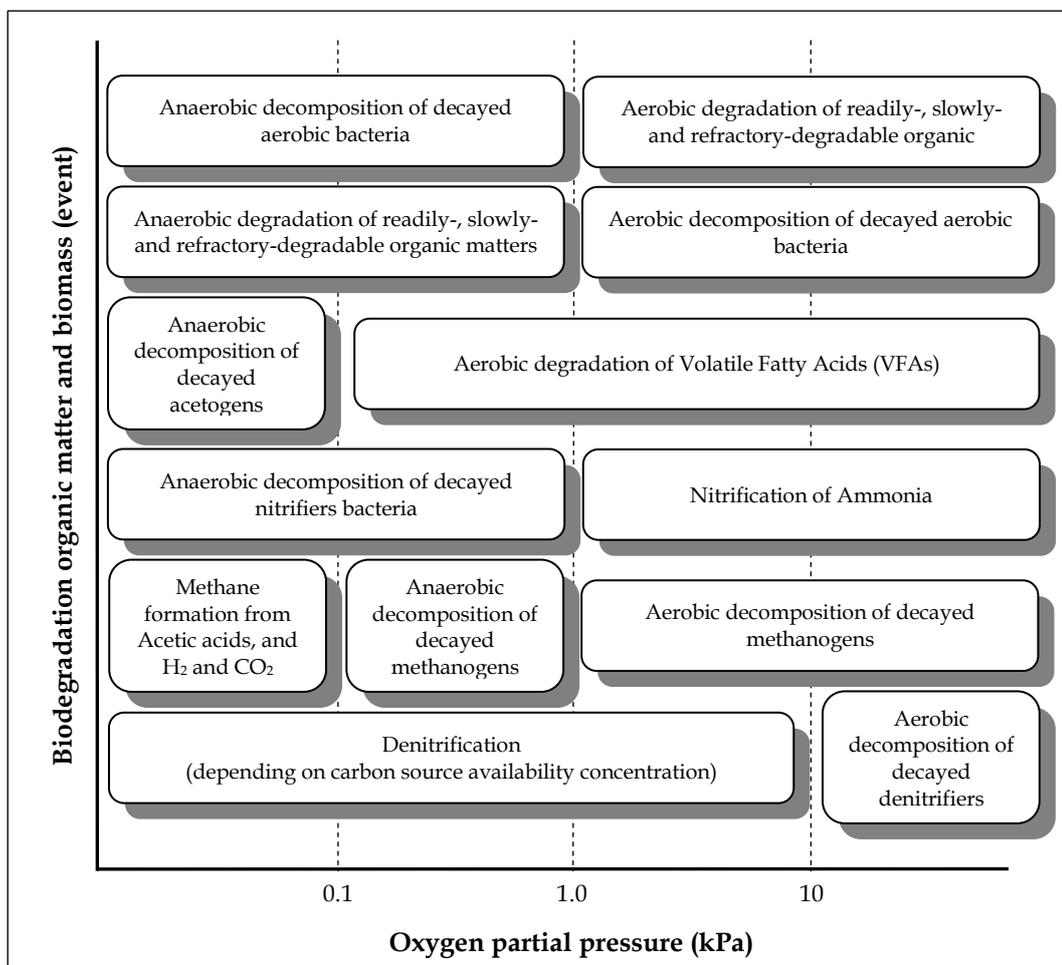
MSW component	Degradable fraction (%)					
	Sugar <sup>a)</sup>	Protein <sup>a)</sup>	Fats <sup>a)</sup>	Cellulose <sup>b)</sup>	Lignin <sup>c)</sup>	Others <sup>d)</sup>
Biogenic waste	39.1	11.0	4.8	29.3	6.0	9.9
Paper and cardboard	0.2	0.2	1.2	43.1	18.2	37.1
Plastic	–	–	–	–	–	100
Textile and rubber	0.1	3.9	1.0	48.0	2.9	44.1
Wood	1.1	1.3	7.7	59.0	30.0	0.9
Glass	–	–	–	–	–	100
Metal	–	–	–	–	–	100
Residual	–	–	–	–	–	100

a: readily-degradable; b: slowly-degradable; c: refractory-degradable; and d: non-degradable  
Source: Neumayer (1999)

### 3.4 Model of Biodegradation of Organic Matter

The biodegradation of solid, aqueous and gaseous organic matter as well as decayed biomass are modeled either by aerobic or anaerobic equations depending upon the partial pressure of oxygen in the landfill ecosystem. In total, 22 biochemical reactions have been considered, as shown in Figure 3.7. This figure shows that when the partial pressure of oxygen in the landfill ecosystem exceeds 1.0 kPa, the biodegradation of solid organic matter and the decay of biomass will occur aerobically. Acetic acid will be oxidized to form  $\text{CO}_2$  and nitrification of ammonia-nitrogen will occur. On the other hand, when the partial pressure of oxygen is less than 1.0 kPa, the biodegradation of solid organic matter and the decay of biomass

will occur under anaerobic conditions, whereas methanogenesis processes are assumed to occur only if the partial pressure of oxygen inside the landfill cell is less than 0.1 kPa.



**Figure 3.7** The schematic diagram of biodegradation of organic matter and decayed biomass by partial oxygen pressure inside landfill

### 3.4.1 Aerobic Biodegradation

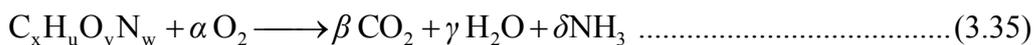
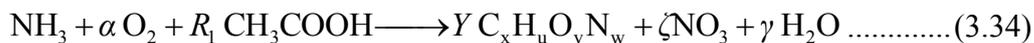
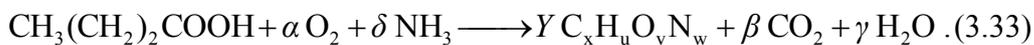
Aerobic biodegradation is the decomposition of solid, aqueous and gaseous organic matter carried out by biomass in the presence of oxygen. Under aerobic conditions, the biodegradation of solid organic matter in the landfill cell was assumed to occur only in one stage. Readily, slowly and hardly degradable organic matter is broken down by extracellular enzymes produced from aerobic bacteria to their monomer. The hydrolytic products are immediately consumed by aerobic bacteria to form new

cells and CO<sub>2</sub>. This metabolic process is assumed to follow the biological reaction below:



where  $C_n H_a O_b N_c$ ,  $C_n H_a O_b$  and  $C_6 H_{12} O_6$  are the chemical formulae of protein, fats and simple carbohydrates, which represents readily degradable organic matters.  $(C_6 H_{10} O_6)_3$  and  $C_{10} H_{12} O_3$  are cellulose and lignin, which represents slowly and hardly degradable organic matters, whilst  $C_5 H_7 O_2 N$  is the empirical formula for biomass determined based on dry matter (McCarty, 1972).

Although acetic acid, propionic acid, butyric acids and ammonia in fresh waste are assumed to be negligible, aerobic degradation of these substances is also considered and taken into account within the simulation. This is to accommodate when the landfill is operated aerobically. The biodegradation of acetic acid, ammonia and decayed biomass are assumed to follow the biological reaction below:

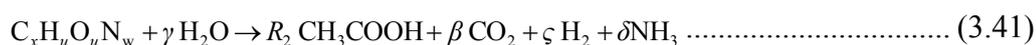
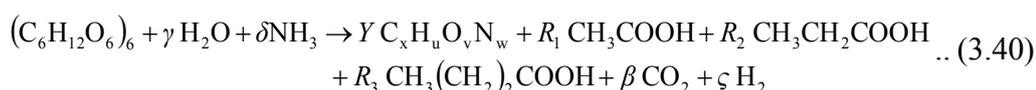
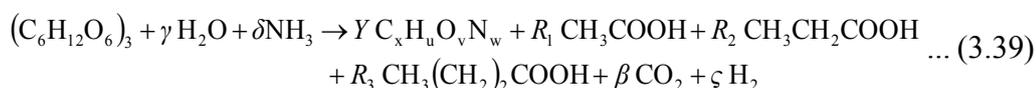
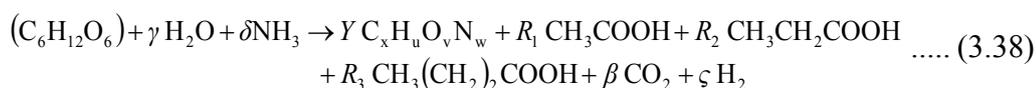
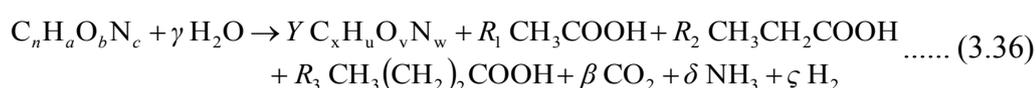


$\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  and  $\zeta$  are biochemical stoichiometric coefficients that represent the amount of mole of each constituent produced from/consumed by the biodegradation of solid, aqueous and gaseous organic matter, while “Y” is the stoichiometric coefficient of biochemical reaction that represents the amount of mole of biomass species

produced from the biodegradation of solid, aqueous and gaseous organic matter. All stoichiometric coefficients were not specified and will be calculated by the model depending on substrate and biological reaction coefficient. This was aimed at convenience and allowing the model to be used for various organic materials with different chemical formulae. The formulation of a stoichiometric coefficient model will be described in the next section and summarized in Table 3.3.

### 3.4.2 Anaerobic Biodegradation

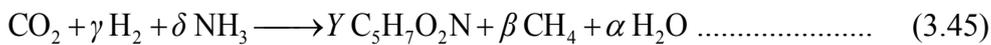
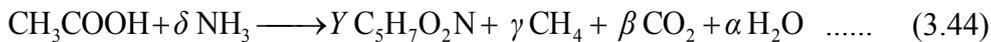
Anaerobic biodegradation is the decomposition of solid, aqueous and gaseous organic matter carried out by biomass in the absence of oxygen. Under anaerobic conditions, the biodegradation of solid, aqueous and gaseous organic matter was distinguished into three stages. First, readily, slowly and hardly degradable solid organic matter was broken down by extracellular enzymes produced from anaerobic bacteria to their monomer. Hydrolytic products are assumed to be immediately consumed by anaerobic bacteria to produce VFAs (e.g. acetic, propionic and butyric acids),  $\text{CO}_2$  and new cells. This metabolic process is assumed to follow the biological reaction below:



In the second stage, long-chain VFAs (e.g. propionic and butyric acids) are subsequently broken down by acetogenic bacteria to produce acetic acid and  $\text{CO}_2$ . This metabolic process is assumed to follow the biological reaction below:



Finally, the acetic acid produced from acidogenesis and acetogenesis is converted into  $\text{CH}_4$  and  $\text{CO}_2$ . Two types of methanogens have been considered, namely acetotrophic and hydrogenotrophic methanogens, which correspond to producing  $\text{CH}_4$  from acetic acid and from hydrogen. The biological reaction of  $\text{CH}_4$  formation is assumed to follow the chemical reaction equations below:



In addition to  $\text{CH}_4$  formation, the denitrification of nitrate has also been considered in this model. The denitrification of nitrate is assumed to follow the chemical reaction equations below:



Similarly to aerobic biodegradation, the stoichiometric coefficient of the chemical reaction for anaerobic biodegradation is also not specified and will be solved by the model.

### 3.4.3 Model of Stoichiometric Coefficient of Chemical Reaction

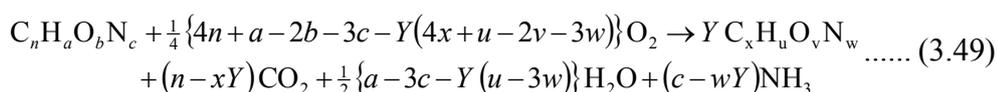
The stoichiometric coefficients of all chemical reactions used in this model were not specified and will be solved by the model itself. This was aimed to allow the model to be used for various organic materials with different chemical formulae. The stoichiometric coefficients were distinguished into two categories, dependent and independent coefficients. The dependent stoichiometric coefficients will be calculated by the model according to the chemical reaction and the given figure for the independent coefficient is based on an elemental balance in the left and right side substances of the chemical reaction. For example, the elemental balance of carbon, hydrogen, nitrogen and oxygen of Eq. (3.26) can be described as below:

$$\begin{aligned}
 \text{C} & : n = xY + \beta \\
 \text{H} & : a = uY + 2\gamma + 3\delta \\
 \text{O} & : b + 2\alpha = vY + 2\beta + \gamma \\
 \text{N} & : c = wY + \delta
 \end{aligned} \dots\dots\dots (3.47)$$

Arranging and substituting the relationship among the parameters, we can express the unknown coefficient (e.g.  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$ ) as a known parameter as expressed by the equation below:

$$\begin{aligned}
 2\alpha & = vY + 2\beta + \gamma - b \\
 \beta & = n - xY \\
 2\gamma & = a - uY - 3\delta \\
 \delta & = c - wY
 \end{aligned} \dots\dots\dots (3.48)$$

Solving the above elemental balance equations by substituting unspecified coefficients with specified coefficients will result in an equation stating the unspecified coefficient and its relationship to the specified coefficient. By substituting these equations to replace unspecified coefficients in Eq. (3.26), we can rewrite this chemical reaction with complex stoichiometric coefficients as expressed below:



All stoichiometric coefficients of chemical reaction used in this model are solved in the same manner explained above and presented in Table 3.3.

**Table 3.3** The stoichiometric coefficient biological reaction for each organic matter

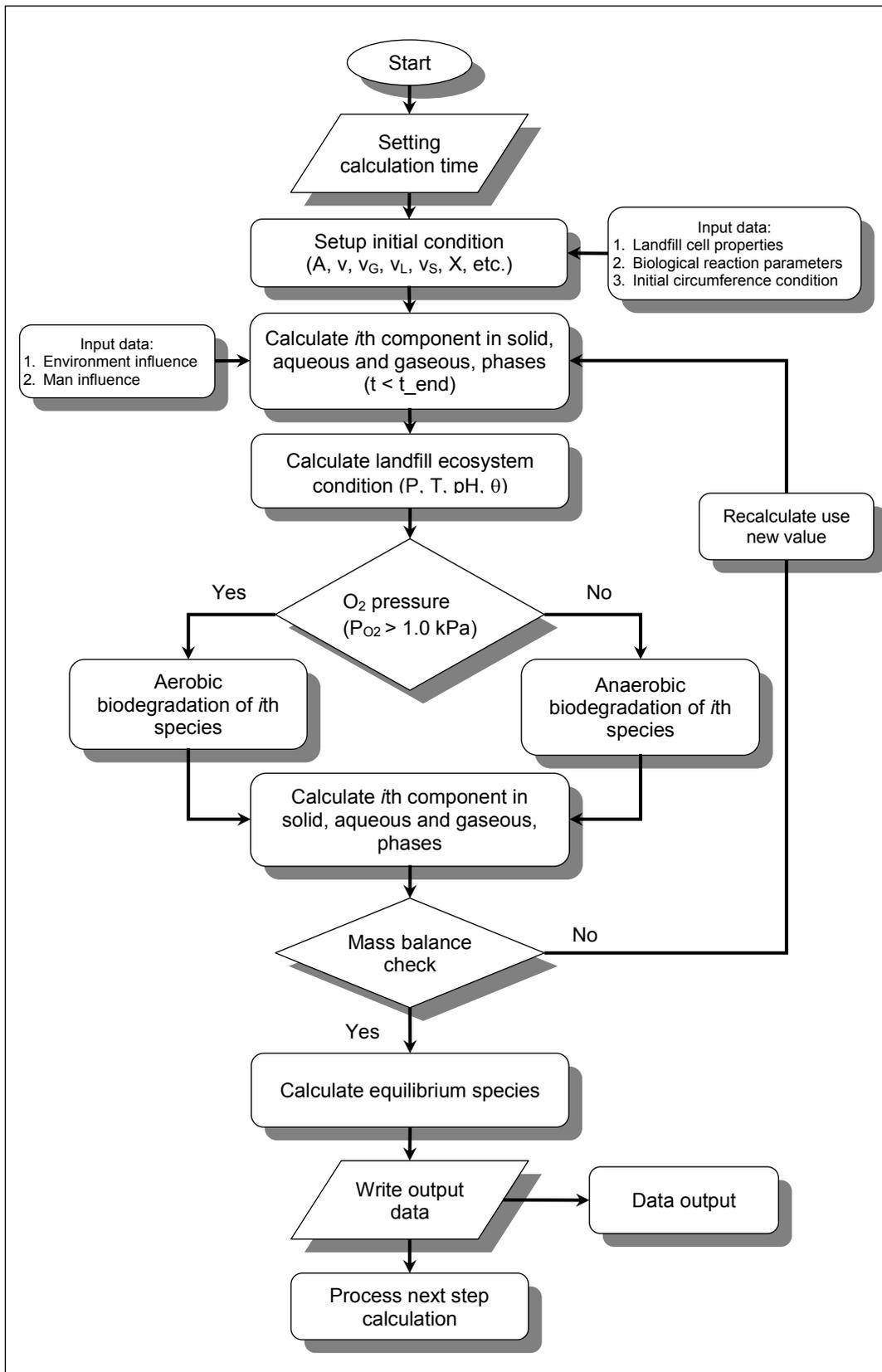
Equation no.	Organic matter (C <sub>n</sub> H <sub>a</sub> O <sub>b</sub> N <sub>i</sub> )	(C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> ) <sub>n</sub>	(C <sub>4</sub> H <sub>10</sub> O <sub>5</sub> ) <sub>n=3</sub>	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> N	CH <sub>3</sub> COOH	CH <sub>2</sub> CH <sub>2</sub> C (OOH)	CH <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> (COOH)	CO <sub>2</sub>	H <sub>2</sub>	O <sub>2</sub>	NH <sub>3</sub>	CH <sub>4</sub>	NO <sub>3</sub>	N <sub>2</sub>
3.26	-1			Y			a-xY			-1/4(4a+b-2c-3w) 3n-Y(4x+u-2v-3w)	-wY			
3.27	-1			Y			a-xY			-1/4(4a+b-2c-3w) Y(4x+u-2v-3w)	-wY			
3.28	-1			Y			6n-xY			-1/4(4a+b-2c-3w) Y(4x+u-2v-3w)	-wY			
3.29		-1		Y			6n-xY			-1/8(8-Y(4x+u-2v-3w)) 2v-3w	-wY			
3.30				Y			a-xY			-1/4(14-Y(4x+u-2v-3w)) 2v-3w	-wY			
3.31				Y	-1		2-xY			-1/4(20-Y(4x+u-2v-3w)) 2v-3w	-wY			
3.32				Y		-1	3-xY			-1/4(9-Y(u-2v+6w)) 2v+6w	-wY			
3.33				Y			4-xY			-1/4(4x+u-2v-3w)	-wY			
3.34				Y			x				-1			1-wY
3.35				-1			0.99R1				w			
3.36	-1			Y	R1	0.93R1	a-xY-8.61R1			1/4(4a+b-2c-3n-40.13R1-Y(4x+u-2v-w)) 1/4(4a+b-2c-40.13R1-Y(4x+u-2v-w))	n-wY			
3.37	-1			Y	R1		a-xY-2R1			1/4(4a+b-2c-40.13R1-Y(4x+u-2v-w)) 1/4(24-8R1-Y(4x+u-2v-3w))	-wY			
3.38		-1		Y	R1		6-xY-2R1			1/4(24n-8R1-Y(4x+u-2v-3w)) 1/2(24n-8R1-Y(4x+u-2v+3w))	wY			
3.39				Y	R1		6n-xY-2R1			1/2(4a+b-2c-8R1-Y(4x+u-2v-3w)) 1/2(4x+u-2v-3w)	-wY			
3.40				Y	R1		a-xY-2R1			1/4(4a+b-2c-8R1-Y(4x+u-2v-3w)) 1/4(4x+u-2v-3w-8R1)	-wY			
3.41				-1	R1		x-2R1				w			
3.42				Y	R1	-1	3-xY-2R1			1/4(14-8R1-Y(4x+u-2v-3w)) 2v-3w	-wY			
3.43				Y	R1	-1	4-xY-2R1			1/4(18-8R1-Y(4x+u-2v-3w)) 2v-3w	-wY			
3.44				Y	-1		1/4(16-Y(8x-2u-4v+6w))				-wY			1/4(16-Y(8x+2u-8v-6w))
3.45				Y			-1			-1/8(8-Y(4x-u+2v+3w))	-wY			1-xY
3.46				Y	-1/4(3+Y(2x+1/4u+Y))									1/4(1-wY)

### 3.5 Numerical Solution

The mass and energy balance equations governed in the previous section are encoded into a modular numerical model programmed using the C++ object-oriented language program. The numerical model consists of 60 subroutines that represent the  $i$ th species and the  $j$ th events that consider the degradation of solid, aqueous and gas organic matters. These subroutines were divided into several modules and a series of input data sets. All subroutines are linked with each other under the control of a module that acts as the main program. The source code and input data used are attached as Appendices A and B.

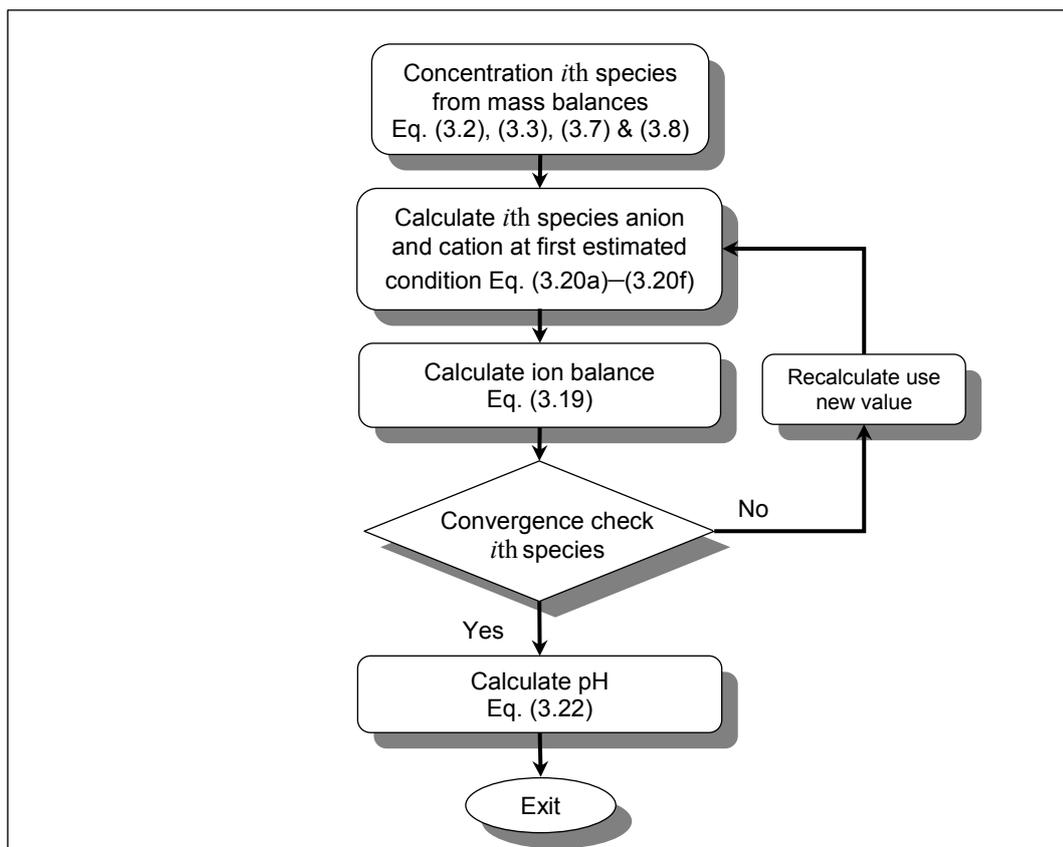
The biodegradation of solid, aqueous and gaseous organic matter is calculated over time increment in a constant-volume landfill cell system. At the beginning of the calculation, a set of given parameters (e.g. temperature, pH, moisture content, etc.) is assumed as a first estimate of landfill cell ecosystem condition. The solid, aqueous and gas organic matter change due to biodegradation, and are then computed by taking into account temperature, pH and moisture content inhabitations. Figure 3.8 shows a flow chart diagram of the numerical solution.

In the initial calculation, the total pressure and partial pressure of oxygen within the landfill ecosystem were calculated first to determine the solid, aqueous and gas organic matter biodegradation for both aerobic and anaerobic conditions. For both biodegradation methods, solid, aqueous and gas organic matter degradation is estimated using Eq. (3.2), (3.7) and (3.8). However, the kinetic model of specific microorganism growth rate depends upon the type of substrate and biodegradation method assumed. The specific microorganism growth rate for aerobic biodegradation of readily degradable organic matter is calculated using the Contois kinetic model Eq. (3.10), while the Monod kinetic model Eq. (3.12) is used for all substrates degraded under anaerobic biodegradation conditions.



**Figure 3.8** Flowchart numerical solution biodegradation *i*th organic matters

The concentrations of the  $i$ th species are represented by differential–algebraic equations, solved at every calculation with the Euler method. This method was chosen due to its simplicity in solving the differential equations with an interval increment time step. Although the calculation accuracy of this method is relatively low compared to other methods using the same step size, this can be minimized by fixing the increment time step as small as possible. The concentration of the equilibrium of the  $i$ th species is calculated independently using Eq. (3.21) by bisection method with iterative technique. Figure 3.9 shows the flow chart diagram of the equilibrium of  $i$ th species concentration. If the “error” (difference between total anions and cations) is higher than the predetermined threshold value, the iteration is continued until the error is lower than the predetermined threshold value. Once a convergent solution is obtained, this concentration is used to calculate the concentration of the  $i$ th parameters in the next increment time step.



**Figure 3.9** Flowchart equilibrium  $i$ th species concentration

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## **Chapter 4**

### **Model Validation and Sensitivity Analysis**

The landfill model is an abstraction of the real landfill with a complex behaviour and is influenced by many factors. Some inevitable assumptions must be made within the landfill model development to represent the real landfill ecosystem. In general, this is necessary as there is not enough information to develop the model as close as possible to the real condition. On the other hand, assumptions are required to achieve the modelling objectives, eliminating unnecessary details and allowing the model to focus on the specific condition of the real landfill ecosystem, which is an important aspect from the model development point of view. Some degree of inaccuracy may be necessary to make the model solution more efficient. However, the reasonable degree of error should be taken into account to minimize the uncertainty and maintain the quality of the model as a consequence of the assumptions that have been made.

There are two methods for judging how well the model represents the real landfill system. The first is by comparing the model calculation to the laboratory experimental results, and the second is by comparing the model calculation to the measurement results at the real landfill. Since the laboratory experimental work is usually carried out under fully controlled conditions, this method does not allow us to claim that the model satisfyingly represents the real landfill ecosystem behaviour. The reason is that as many of the factors that influence the landfill behaviour are not considered within the model development, only some parameters of landfill behaviour are taken into account within the model development. However, in the absence of adequate well-documented data from the landfills, the data from laboratory experimental work are used for model validation. The model validation is carried out and discussed in this chapter to measure the quality of the model developed by comparing several parameters (i.e. pH, VFAs, CO<sub>2</sub> and CH<sub>4</sub>) from the model calculation to the laboratory experimental results.

The model validation is followed by a sensitivity analysis to assess the model sensitivity to the most relevant parameters that affect the biodegradation of organic matter in the landfill site. These parameters include temperature, pH and the leachate recycling ratio to represent the effect of moisture content on the biodegradation of organic matter. These parameters are chosen as they are considered to be adjustable under bioreactor landfill operation mode. By selecting these parameters it is expected that this model can be used as a tool for bioreactor landfill operation design.

## **4.1 Model Validation**

Model validation aims to assess whether the model calculation results are reasonable enough to represent the real landfill behaviour. For this purpose, the model validation is carried out by comparing the model calculation to the laboratory experiment results. The validity of the model is analysed by measuring the deviation of each parameter considered against the laboratory experiment results. If the deviation is far from the laboratory experiment results, the deviation is discussed with regard to the theoretical analysis to judge this deviation.

The laboratory experiment carried out by Valencia et al. (2009) is chosen to validate the model. As references for the model validation, the concentration of the landfill gas released (i.e. CO<sub>2</sub> and CH<sub>4</sub>), pH and volatile fatty acid (VFAs) concentration in leachate are used. A brief description of the laboratory experiment set-up and the model validation results are given in the following section.

### **4.1.1 Description of the Landfill Simulation Reactor**

The laboratory experiment work was carried out by Valencia et al. (2009) by using a landfill simulation reactor (LSR). The LSR was made of an HDPE pipe with a diameter of 70 cm and a total height of 200 cm. The LSR was sealed at both ends with HDPE lids and rubber rings to keep it airtight. The LSR was equipped with a

dry gas meter to measure the gas volume released from it, and a leachate recirculation pump allowed the leachate discharged to be pumped back into the LSR. The LSR temperature was kept constant at  $30 \pm 4$  °C by covering the LSR with a wool fiber blanket and equipping it with an electric heating element, aluminum foil and finally wrapping it with plastic to protect it from getting wet with water.

The LSR was filled with 500 kg of MSW, which was collected from a transfer station in Wijster, the Netherlands. Prior to emplacement into the LSR, the MSW was characterized and shredded to a maximum size of 4 cm. The composition of the MSW is presented in Table 4.1. The MSW was extracted and its composition distinguished according to the degradability level as proposed by Neumayer (1999). The moisture content of the MSW was about 0.2 kg of water per kg of dry solid waste. Then, the shredded MSW was placed into the LSR in layers of approximately 0.3 m and compacted using a sledgehammer to an apparent density of  $1,040 \text{ kg m}^{-3}$  before the next layer was inserted. Finally, the MSW in the LSR was saturated with  $0.2 \text{ m}^{-3}$  of mature leachate in order to stimulate the biodegradation of the organic matter.

**Table 4.1** MSW Composition use in landfill simulator reactor and its degradable fraction

MSW component	Composition (%) <sup>a</sup>	Organic matter (w/w) <sup>b</sup>					
		Protein	Fats	Sugar	Cellulose	Lignin	Other
Biogenic waste	33.2	3.65	1.59	12.98	9.73	1.99	3.25
Paper and cardboard	15.2	0.03	0.18	0.03	6.55	2.77	5.64
Plastic	3.7	–	–	–	–	–	3.7
Textile and rubber	2.3	0.01	–	–	0.10	0.01	0.08
Wood	2.5	0.03	0.19	0.03	1.48	0.75	0.02
Glass	13.6	–	–	–	–	–	13.60
Metal	0.6	–	–	–	–	–	0.60
Residual	28.9	–	–	–	–	–	28.90
Total	100.0	3.72	1.97	13.04	17.85	5.51	55.79

Source: <sup>a</sup> Valencia et al. (2009); <sup>b</sup> calculated according to Neumayer (1999)

The leachate produced during the LSR operation was recycled into the LSR to maintain the moisture content without any treatment (i.e. pH neutralization, ammonium removal, etc.). Part of the leachate was collected and substituted by tap water for laboratory analytical purposes on a weekly basis. The analysis parameters of leachate are general parameters such as pH, electric conductivity, BOD, COD,  $\text{NH}_4^+$ , TKN and total VFAs (acetic, propionic and butyric acids). In addition to the

leachate characterization, the volume and composition of gas generated were also determined throughout the LSR operation.

**Table 4.2** Composition of leachate use to saturated landfill simulator reactor

Leachate parameter	Unit	Concentration
pH	–	7.7
Electric conductivity	mS/cm	14.3
BOD	mg/l	650
COD	mg/l	4,240
NH <sub>4</sub> <sup>+</sup>	mg/l	610
Nitrate	mg/l	100
Chloride	mg/l	5,480
Sulfate	mg/l	210
Bicarbonate	mg/l	7,200

Source: Valencia et al. (2009)

#### 4.1.2 Model Validation Set-up

The chemical formulae for protein and fats used in this model were adapted as proposed by Young (1989), while the chemical formulae for sugar and cellulose were formulated according to typical polysaccharide chemical formulae with one and three repeating units, respectively, whereas for the average molecule weight of lignin it was decided to use the chemical formula of hardly degradable organic matter. The chemical formula of organic MSW matter used in this model is presented in Table 4.3.

**Table 4.3** Chemical formula organic matters

Degradability level	Organic matter	Chemical formula
Readily	Protein	C <sub>46</sub> H <sub>77</sub> O <sub>17</sub> N <sub>12</sub>
	Fats	C <sub>55</sub> H <sub>104</sub> O <sub>6</sub>
	Sugar	(C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> ) <sub>n</sub> ; n = 1
Slowly	Cellulose	(C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> ) <sub>n</sub> ; n = 3
Refractory	Lignin	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>

The biodegradation of organic matter is carried out by microorganisms in parallel with the subsequent biochemical reaction process. Nineteen types of microorganism population are assumed to be present in the landfill ecosystem. The activity of each type of microorganism is characterized by four or five biokinetic constants for anaerobic microorganisms. They include the maximum specific growth rate constant, the half saturation constant, the decay rate constant and the yield

coefficient. In addition to these four biokinetic constants, the partial pressure of oxygen constant is considered to affect the activity of aerobic microorganisms.

**Table 4.4** The biokinetic const. for aerobic and anaerobic degradation organic matter

Degradation stages	Biokinetic const. Parameter	Symbol	Unit	Reported values	Applied value		
<b>Organic matter</b>							
<b>Aerobic degradation</b>							
Protein	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.00		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Fats	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.00		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Carbohydrate	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.00		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Cellulose	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.10		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Lignite	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.50		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Acetic acid	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.0		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Propionic acid	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.0		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Butyric acid	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.0		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.02x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
Ammonia (nitrification)	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	1.0		
	Yield coefficient	Y	–	–	0.10		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.05		
	O <sub>2</sub> saturation const.	$k_{O_2}$	Pa	–	0.05x1.013E <sup>-5</sup>		
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$		
<b>Acidogenesis</b>							
Protein	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.001		
	Yield coefficient	Y	–	0.205 <sup>(1)</sup>	0.20		
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	11.3 <sup>(1)</sup>	25	
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.01 <sup>(1)</sup>	0.05 $\mu_{\max}$	
	Fats	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.105–0.55 <sup>(2)</sup>	0.002
Yield coefficient		Y	–	–	0.038–0.11 <sup>(1,2)</sup>	0.20	
Half saturation const.		$k_S$	kg m <sup>-3</sup>	–	–	0.105–3.18 <sup>(b)</sup>	25
Decay rate		$k_D$	day <sup>-1</sup>	–	–	0.01 <sup>(1,2)</sup>	0.05 $\mu_{\max}$
Carbohydrate		Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.0125–7.2 <sup>(3-7)</sup>	0.002
	Yield coefficient	Y	–	–	0.1–0.35 <sup>(1-7)</sup>	0.05	
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	–	0.0225–0.427 <sup>(3-7)</sup>	25
	Decay rate	$k_D$	day <sup>-1</sup>	–	–	0.01–6.1 <sup>(1,5,7)</sup>	0.05 $\mu_{\max}$

**Table 4.4** The biokinetic const. for aerobic and anaerobic degradation organic matter (*continued*)

Degradation stages	Biokinetic const.				
Organic matter	Parameter	Symbol	Unit	Reported values	Applied value
Cellulose	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	
	Yield coefficient	Y	–	–	
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	0.008 <sup>(8)</sup>	
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$
Lignite	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	
	Yield coefficient	Y	–	–	
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$
Acetogenesis					
Propionic acids	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	0.042–1.2 <sup>(9-11)</sup>	0.10
	Yield coefficient	Y	–	0.025–0.051 <sup>(1,10,11)</sup>	0.05
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	0.017–1.145 <sup>(9-11)</sup>	10.0
	Decay rate	$k_D$	day <sup>-1</sup>	0.01 <sup>(1)</sup>	0.05 $\mu_{\max}$
Butyric acids	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	0.354–0.77 <sup>(9,12)</sup>	0.10
	Yield coefficient	Y	–	0.047–0.058 <sup>(1,9)</sup>	0.05
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	0.012–0.013 <sup>(9,12)</sup>	10.0
	Decay rate	$k_D$	day <sup>-1</sup>	0.01 <sup>(1)</sup>	0.05 $\mu_{\max}$
Methanogenesis					
Acetotrophic	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	0.054–1.4 <sup>(7,12-14,16,18-20)</sup>	0.009
	Yield coefficient	Y	–	0.01–0.05 <sup>(1,7,9,13-19)</sup>	0.005
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	0.011–0.93 <sup>(7-9,12-20)</sup>	30.0
	Decay rate	$k_D$	day <sup>-1</sup>	0.004–0.037 <sup>(1,7,9,14,15,18)</sup>	0.05 $\mu_{\max}$
Hydrogenotrophic	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	0.05–4.07 <sup>(7,21,23,26,27)</sup>	0.750
	Yield coefficient	Y	–	0.017–0.13 <sup>(1,7,12,23,26,27)</sup>	0.005
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	4.8x10 <sup>-8</sup> –6.0x10 <sup>-4</sup> <sup>(7,12,22-27)</sup>	15.0
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$
Denitrification					
Nitrate	Specific growth rate	$\mu_{\max}$	day <sup>-1</sup>	–	0.10
	Yield coefficient	Y	–	–	0.05
	Half saturation const.	$k_S$	kg m <sup>-3</sup>	–	0.30
	Decay rate	$k_D$	day <sup>-1</sup>	–	0.05 $\mu_{\max}$

<sup>1</sup>McCarty, (1972); <sup>2</sup>Novak & Carlson, (1970); <sup>3</sup>Ghosh et al. (1977); <sup>4</sup>Zoetemeyer et al. (1982); <sup>5</sup>Ghosh et al. (1974); <sup>6</sup>Chen et al. (2001); <sup>7</sup>Pavlostathis & Giraldo-Gomez, (1991); <sup>8</sup>Noike et al. (1985); <sup>9</sup>Lawrence & McCarty, (1969); <sup>10</sup>Heyes & Hall, (1983); <sup>11</sup>Zinder et al. (1979); <sup>12</sup>Ahring & Westermann, (1987b); <sup>13</sup>Cappenberg, (1975); <sup>14</sup>Kugelman & Chin, (1971); <sup>15</sup>Parkin & Speece, (1983); <sup>16</sup>Smith & Mah, (1978); <sup>17</sup>van den Berg, (1977); <sup>18</sup>Wandrey & Aivasidis, (1983); <sup>19</sup>Zehnder et al. (1980); <sup>20</sup>Zinder & Mah, (1979); <sup>21</sup>Archer & Powell, (1985); <sup>22</sup>Giraldo-Gomez et al. (1992); <sup>23</sup>Gujer & Zehnder, (1983); <sup>24</sup>Hungate et al. (1970); <sup>25</sup>Kristjansson et al. (1982); <sup>26</sup>Pavlostathis et al. (1990); <sup>27</sup>Robinson & Tiedje, (1982).

All the biokinetic constants are reported to be directly affected by landfill ecosystem conditions such as temperature, pH and moisture content. For example, the yield coefficient is not affected by temperature changes, but the maximum specific growth rate constant and the decay rate constant have been reported to increase with increasing temperatures. In contrast, the half saturation constant decreased with increasing temperatures (El-Fadel et al., 1996a). However, for simplifying purposes these parameters were assumed to be constant throughout the simulation time. The biokinetic constants used for all biodegradation of organic matter stages are determined by trial and error until the simulation results fit with the LSR experimental results. The biokinetic constants of best fit are listed in Table 4.4 together with the literature value. Moreover, since the temperature of the LSR was

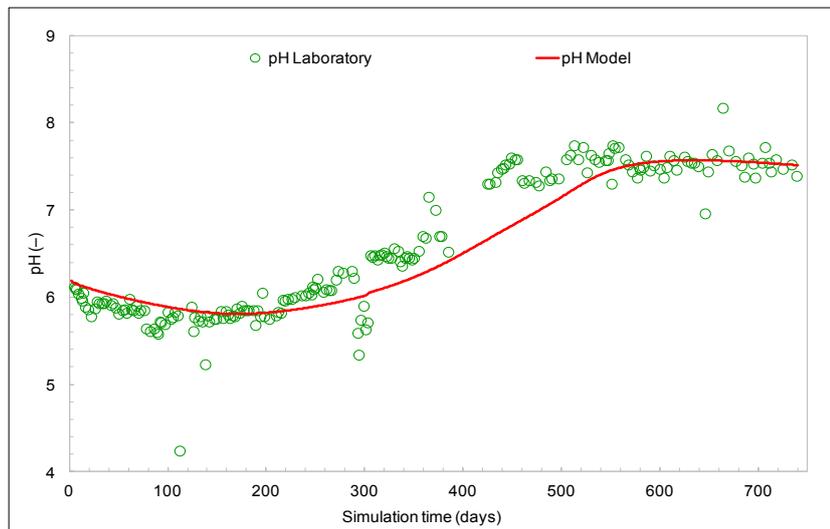
kept constant, the biodegradation of organic matter was also simulated at a constant temperature by deactivating the temperature feedback function to the microorganism growth rate. Nevertheless, the temperature changes throughout the simulation time can still be observed.

#### **4.1.3 Results and Discussion**

Although this model is able to simulate all the parameters that were analysed within the laboratory experimental work, only four of these parameters were considered to validate the model calculation results. These parameters include the pH value of discharged leachate, VFA concentration in discharged leachate, and the cumulative CO<sub>2</sub> and CH<sub>4</sub> released. The reason for this is only that these four parameters are the most reliable as measured during the whole of the laboratory experiment. Moreover, due to the complex process that occurred within the biodegradation of organic matter in the LSR, which cannot be modeled precisely, the pH value of discharged leachate was chosen as the main parameter for model validation. This means that the closer the pH value of the model calculation to the LSR experiment results is the best fits model validation event. The pH value measurement is fairly easy and usually carried out *in situ*, so that very small uncertainties may occur and affect the measurement accuracy. Unlike the pH value, measuring the concentration and volume of the gas released may be affected by leaking from the gas chamber, or VFA concentration may be under the detection limit of the instrument used, or decomposed within the sample preparation, etc.

The time profile of the pH value of leachate discharged from the LSR experiment and the model calculation result are presented in Figure 4.1. This figure shows that the model calculation result is almost identical to the pH in the LSR experiment, particularly at the beginning and end of the simulation time. The pH value of leachate decreased gradually from 6.2 to 5.8 during the first 200 days and its pH value remained constant at approximately 7.5 from day 430 until the end of the simulation time, whereas in between this period the pH value of the model calculation result is slightly higher than the LSR experiment result. However, the

differences between them are still within tolerance. Statistically, the square-means error (SME) of the model calculation compared to the LSR experimental results was approximately 0.09, indicating that the model calculation result fits the LSR experimental results.

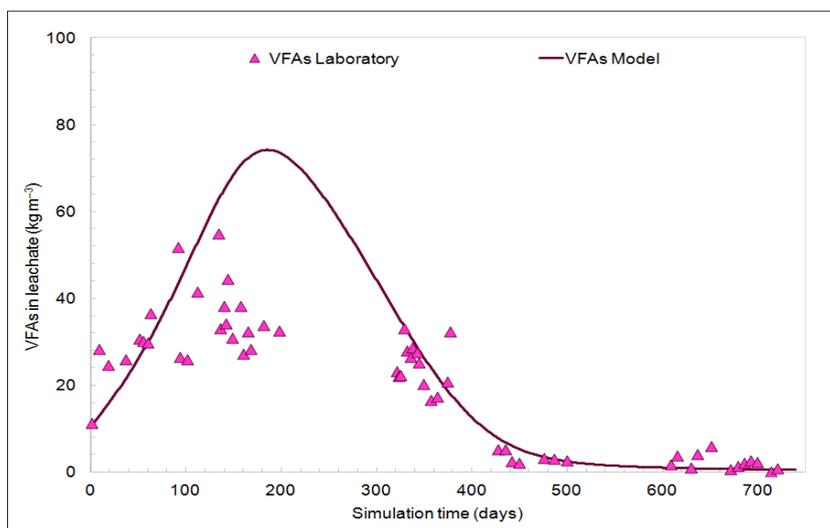


**Figure 4.1** Simulated and LSR experiment measured pH value of leachate discharged

The comparison of the VFA concentration of the model calculation and the LSR experiment results is shown in Figure 4.2. In contrast to the pH value, the concentration of VFAs increased in the first 200 days of the simulation time due to accumulated hydrolyzed and fermented products of organic matter degradation. Veeken et al. (2000) reported that the hydrolysis and fermentation of organic matter to VFAs was pH dependent, but the hydrogen ion of VFA dissociation is not the single contributor to the pH. Therefore, the pH of landfill ecosystems is not related directly to VFA concentration.

In comparison to the pH data, the number of VFA data of LSR experimental results was comparatively low and dispersed in a wide range. There were no data recorded from day 200 to day 320 of the LSR experiment time. This fact will provide low validity of the model calculation compared to the LSR experiment results. However, in general the model calculation results show a high consistency and are closely related to the other parameters. This is indicated by the concentration of VFAs, which decreases with the increasing pH of the LSR ecosystem and biogas (see

Figures 4.3 and 4.4). This confirms the reduction of VFA concentration in leachate, which is converted into biogas.

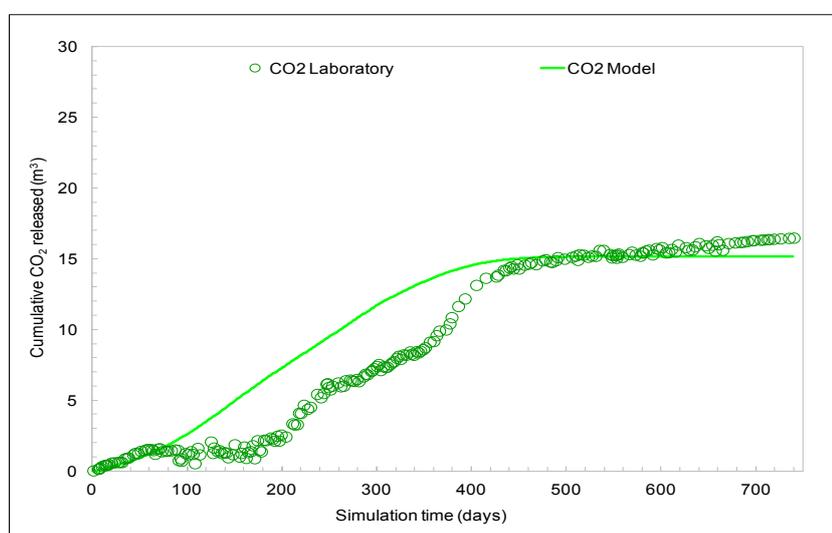


**Figure 4.2** Simulated and LSR experiment measured of VFAs concentration in leachate discharged

Organic MSW matter (i.e. sugar, protein, fats, cellulose and lignin) is hydrolyzed by extracellular enzymes into its corresponding products (i.e. soluble sugar, amino acids and alcohol), which are subsequently fermented to VFAs (i.e. acetic, propionic and butyric acids) and CO<sub>2</sub>. The VFAs (except for acetic acid) are converted by acetogens to acetic acids, H<sub>2</sub> and CO<sub>2</sub>. Lastly, the acetic acids, and H<sub>2</sub> and CO<sub>2</sub>, are converted to CH<sub>4</sub> by acetotrophic and hydrogenotrophic methanogens, respectively. The experimental results showed no accumulation of such hydrolyzed products, therefore an assumption of hydrolysis of organic matters and acidogenesis of hydrolyzed products to produce VFAs occurs simultaneously and should be an appropriate approach for modeling the degradation of organic matter.

Figure 4.3 shows the cumulative CO<sub>2</sub> released from the LSR experiment and the corresponding model simulation results. The cumulative CO<sub>2</sub> of the model calculation fits to the LSR experiment results at the beginning and the end of the simulation times, but was one order of magnitude higher in between these periods. This figure shows that the cumulative CO<sub>2</sub> of the LSR experiment from day 50 to day 200 tends to be constant even though on several particular days it was lower than the previous day, while the model calculation gradually increases with

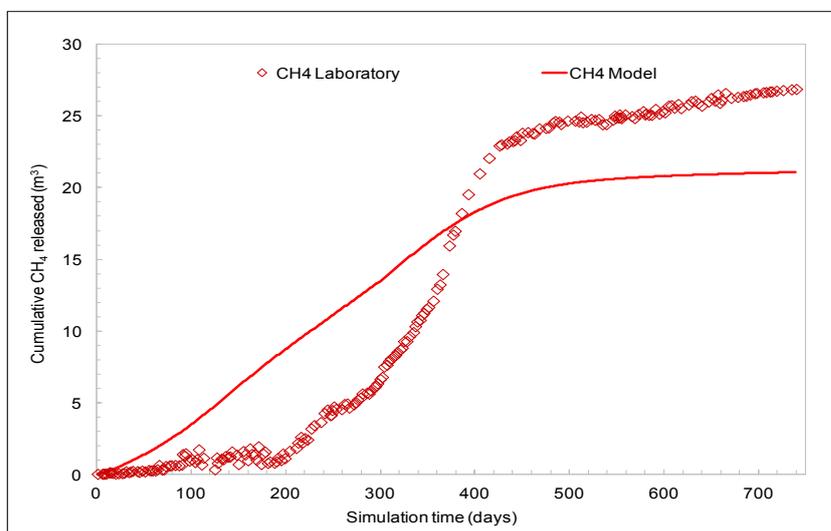
simulation time. From an algebraic perspective, the accumulation of CO<sub>2</sub> released must increase or at least be equal to the previous day when there is no CO<sub>2</sub> released on a particular day. In addition, although the cumulative CO<sub>2</sub> released from the LSR experiment from day 50 to day 400 was one order of magnitude lower than the model calculation results, at the end of the simulation time the cumulative CO<sub>2</sub> release became almost equal to the model simulation results. This might be caused by inaccuracies during the gas measurement or within data preparation. The SME of the model calculation compared to the LSR experiment results was about 34.



**Figure 4.3** Simulated and LSR experiment measured cumulative of CO<sub>2</sub> released

The time profile of released CH<sub>4</sub> of the model calculations and the LSR experiment results are presented in Figure 4.4. In contrast to CO<sub>2</sub>, the released CH<sub>4</sub> of the model calculations does not fit to the LSR experiment results during the entire simulation time. The CH<sub>4</sub> of the model calculation was released from the very beginning and increased gradually with the simulation time up to day 450 before it increased slowly until the end of the simulation time, while the CH<sub>4</sub> of the LSR experiment was released from day 200 and increased dramatically until day 500. Although the acetotrophic and hydrogenotrophic methanogens growth rate is strictly sensitive to the pH value, the pH value of the LSR ecosystem, which is indicated by the pH value of leachate, did not much differ during the first 200 days of the LSR experiment time. The long lag phase and the dramatically increased CH<sub>4</sub> release

after day 200 might also be caused by inaccuracies during gas measurement or within data preparation.



**Figure 4.4** Simulated and LSR experiment measured cumulative of CH<sub>4</sub> release

The volume percentage and yield of the CH<sub>4</sub> model calculation results also substantially differ from the LSR experimental results. CH<sub>4</sub> volume percentage and the yield of the model calculation were approximately 58% and 0.36 m<sup>3</sup> per kg VS. These figures are one magnitude lower than the LSR experiment results, which were approximately 70% and 0.46 m<sup>3</sup> per kg VS. Although the model calculation is much lower than the LSR experiment result, the figures seem to be more realistic. The typical CH<sub>4</sub> volume percentage in LFG released from organic MSW matter degradation reported by a lot of literature was approximately 40–60 % (Šan and Onay, 2001; Barlaz et al., 2002; Sponza and Ağdağ, 2004; He et al., 2005) and the yield of CH<sub>4</sub> was approximately 0.069–0.25 m<sup>3</sup> per kg VS (Šan and Onay, 2001; Sponza and Ağdağ, 2004).

The initial and final simulated organic matters in the LSR are shown in Table 4.5. The total weight of degraded organic matter was about 40 kg. This amount is only half the total weight of degraded organic matter reported from laboratory experiments (Valencia et al., 2009). The readily degradable is completely mineralized, while the slowly degradable and refractory–degradable organic matters were assumed not to be degraded at all. This is accomplished because the

cumulative amount of CO<sub>2</sub> released from readily degradable is already equal to the experiment results. As previously mentioned, the cumulative CO<sub>2</sub> and CH<sub>4</sub> might be below the real values, but we do not want to speculate how big the differences are between the actual and reported values. Therefore, the simulation was stopped after the model calculation fit to the LSR experiment results.

**Table 4.5** Simulated the fate organic matter in LSR

Organic matter	Initial (kg)	Final (kg)	Degraded (%)
Readily-degradable	39.49	0.06	99.8
Slowly-degradable	71.81	71.81	–
Refractory-degradable	25.13	25.13	–
Total	136.43	97.00	28.9

## 4.2 Sensitivity Analysis

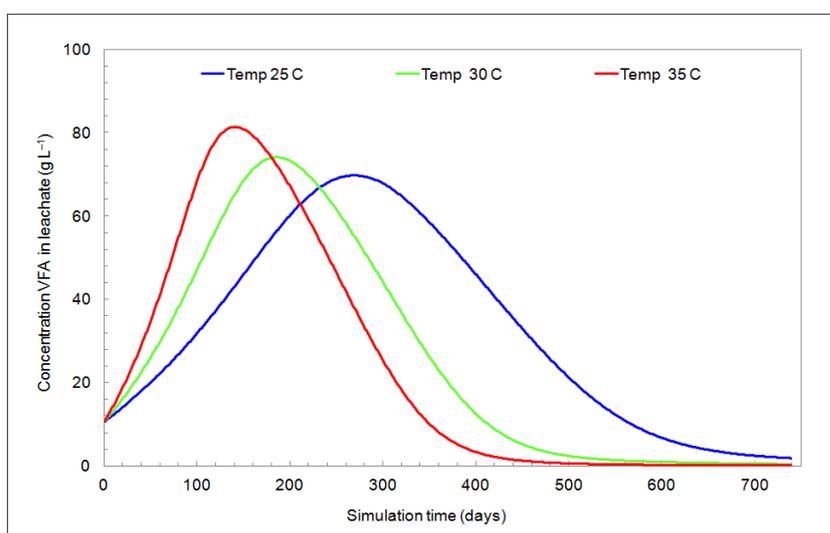
Several simulations were performed to measure the model sensitivity to the parameters that affect the biodegradation of organic matter in the landfill site. An excellent bibliography of model sensitivity analysis can be found in El-Fadel et al. (1997). The sensitivity analysis involves various biokinetic constants of the microorganism growth rate that will affect the biodegradation of organic matter. This approach will, of course, provide high accuracy in the impact of biokinetic constants on the biodegradation of organic matter under a given set of assumptions. However, this approach might be applicable at the model simulation level only, because the biokinetic constants (i.e. the maximum specific growth rate constant, the half saturation constant, the decay rate constant and the yield coefficient) are dependent on parameters that are not adjustable on the LSR experiment level.

Therefore, this sensitivity analysis focused on independent parameters that directly affect the biodegradation of organic matter in landfill sites and can also be adjusted. This means that the parameters can be controlled by means of introducing a technology to accelerate the biodegradation of organic matter such as under bioreactor landfill conditions. For example, the temperature in the LSR experiment was kept constant at a certain degree by covering the LSR with insulators and

equipping it with an electric heating element; the pH value within the LSR ecosystem was maintained close to the desired value by adding acid or base into the LSR; and the moisture content of waste in the LSR was enhanced through leachate recirculation or pumping fresh water into the LSR.

#### 4.2.1 Effect of Temperature on Organic Matter Degradation

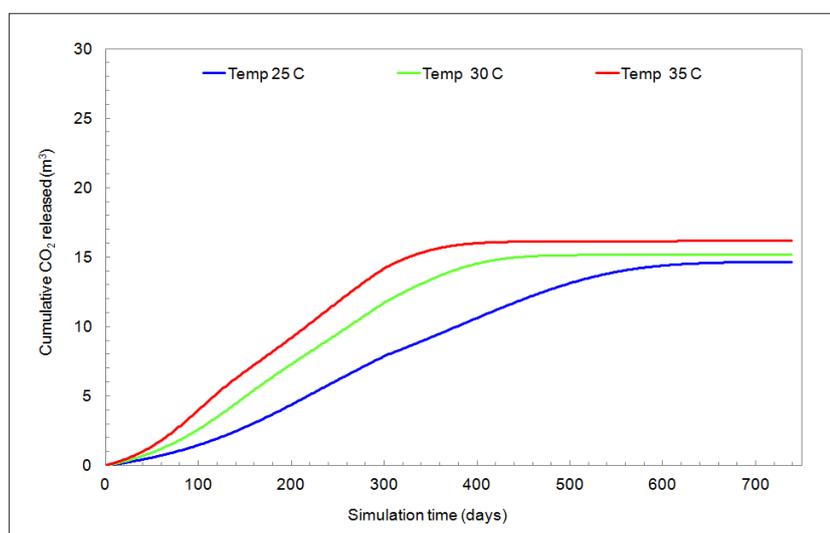
The temperature within the landfill site is controlled from both sides, in and outside of the landfill ecosystem. From the inside, heat was generated during the biodegradation of organic matter within the landfill site, while from outside the ambient temperature change was driven by heat transfer from the landfill to the environment or vice versa. This model was developed to accommodate this issue by introducing the heat transport and use of the daily mean temperature as input for model simulation. However, this heat transport function was deactivated to measure the model sensitivity on dependent parameters that have been considered and the ambient temperature input data were set up at constant levels of 25, 30 and 35 °C.



**Figure 4.5** Sensitivity analysis effect of temperature on VFA concentration in leachate discharged

Figure 4.5 shows the VFA concentration profile within the LSR experiment under various temperatures. The figure shows that the VFA concentration in the discharged leachate increased with the temperature change from 30 to 35 °C. The peak of VFA accumulation occurred 50 days earlier from day 190 for the LSR

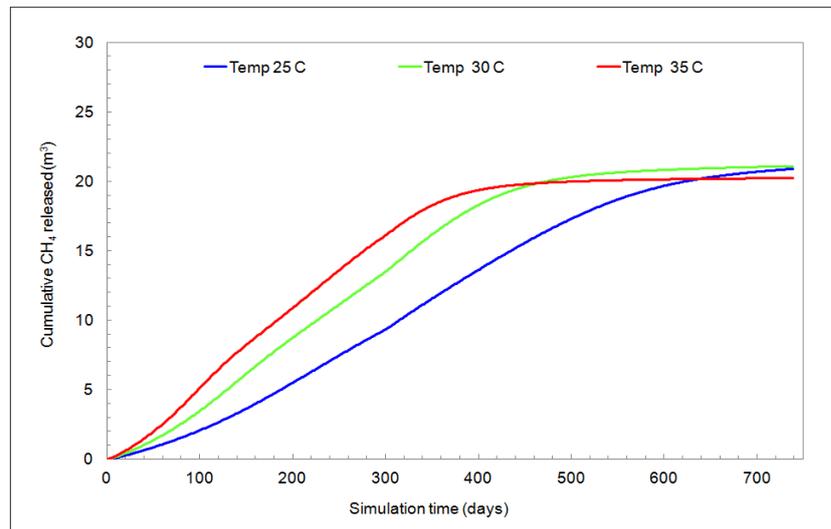
operating at 30 °C to day 140 for the LSR operating at 35 °C. The temperature change of 5 degrees from 30 to 25 °C was also affected significantly by the slowdown of the VFA production rate. The peak VFA accumulation occurred 80 days later from day 190 for the LSR operating at 30 °C to day 270 for the LSR operating at 25 °C. These results indicate that the acidogenesis and methanogenesis of organic matter are strongly dependent on the temperature.



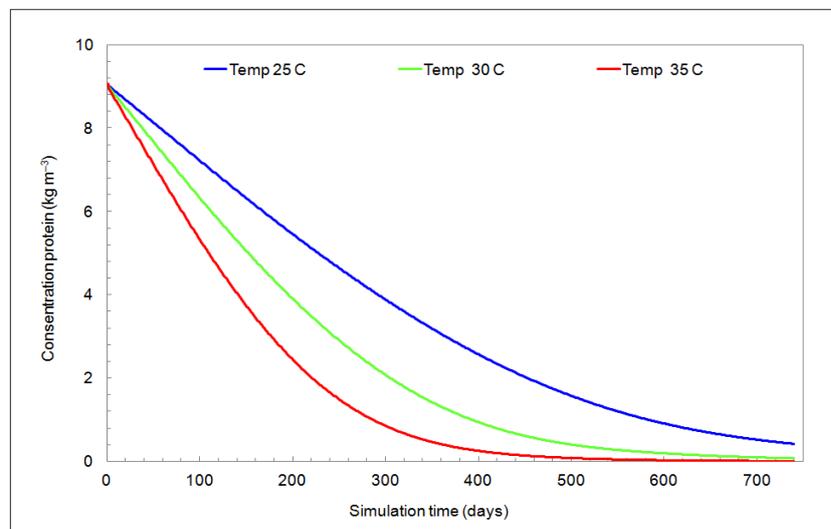
**Figure 4.6** Sensitivity analysis effect of temperature on cumulative CO<sub>2</sub> generated

Figure 4.6 illustrates the effect of temperature on the cumulative CO<sub>2</sub> release within the simulation time. This figure shows that as the biodegradation rate increased with temperature, the maximum cumulative CO<sub>2</sub> released from the LSR operating at 35 °C was achieved earlier than that of the LSR operating at 30 °C. However, the figure also shows that the cumulative CO<sub>2</sub> released from the LSR operating at 35 °C was higher than that of the LSR operating at 30 °C. This result is contrary to what was intuitively expected, where the temperature increase would enhance the stabilization time and increase the CH<sub>4</sub> volume percentage so that the landfill operation under bioreactor landfill conditions becomes feasible. This increase can be explained by the fact that acetic acid is converted to CH<sub>4</sub> and CO<sub>2</sub> by acetotrophic methanogens in a 1:1 molar ratio. On the other hand, CO<sub>2</sub> is also produced from the biodegradation of solid organic matters, whereas hydrogenotrophic methanogens can only convert a small part of the CO<sub>2</sub> produced and the rest escapes as CO<sub>2</sub> emissions. In general,

hydrogenotrophic methanogens contribute only a quarter to a third of the total  $\text{CH}_4$  production (Pavlostathis and Giraldo-Gomez, 1991; Gavala et al., 2003).



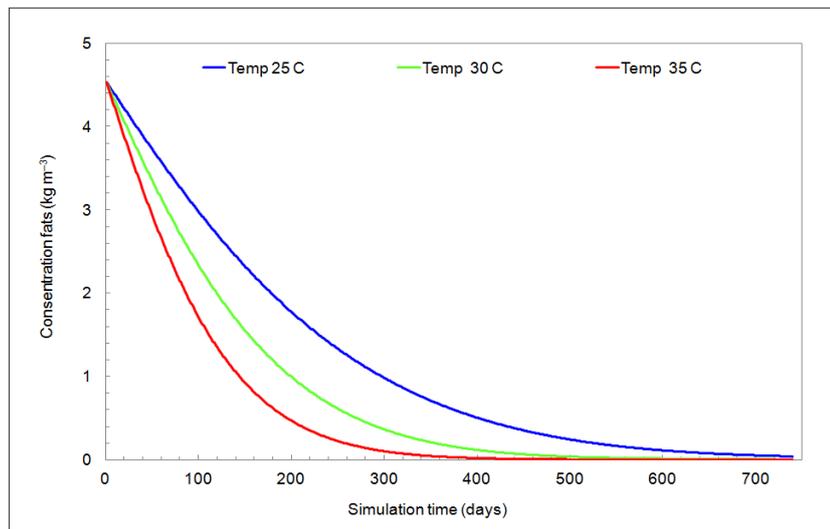
**Figure 4.7** Sensitivity analysis effect of temperature on cumulative  $\text{CH}_4$  generated



**Figure 4.8** Sensitivity analysis effect of temperature on protein degradation

As  $\text{CO}_2$  production increases more with temperature than  $\text{CO}_2$  consumption by hydrogenotrophic methanogens, the cumulative  $\text{CH}_4$  released from the LSR operating at 35 °C was slightly lower than from the LSR operating at 30 °C. The reduction of cumulative  $\text{CH}_4$  released from the LSR operating at 35 °C was approximately 4.1% below that of the LSR operating at 30 °C. This reduction is higher than when the LSR operates at 25 °C, which will reduce the cumulative  $\text{CH}_4$  released by less than 1.0% (see Figure 4.7).

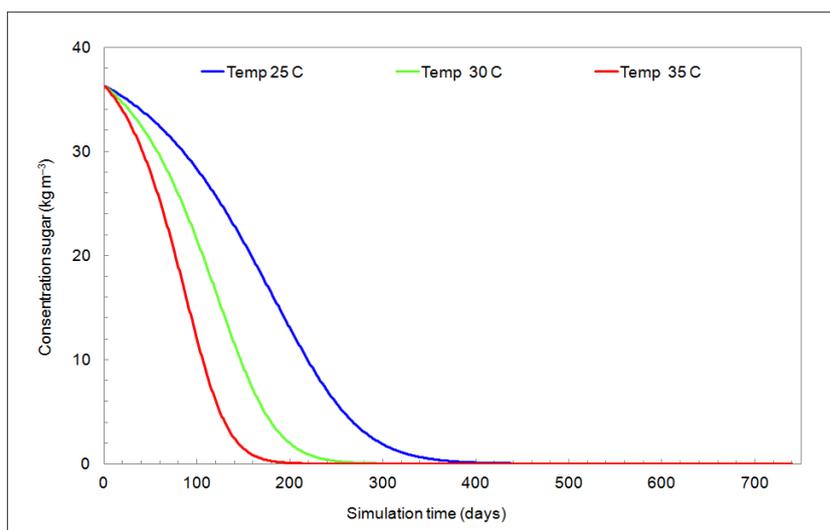
Although the model distinguished the degradable organic matter into five groups according to their degradability level (i.e. sugar, protein, fats, cellulose and lignin), the VFA and CO<sub>2</sub> production of the model calculation is equal to the LSR experiment without the contribution of cellulose and lignin degradation. Therefore, cellulose and lignin were assumed to be not degraded yet within the entire LSR experiment time. This assumption seems quite realistic since only 28.1% of 284.5 kg of total dry weight MSW placed into the LSR was degraded until the end of the experiment (Valencia et al., 2009). The weight of residue in the LSR after the experiment was higher than the total weight of cellulose, lignin and inorganic matters.



**Figure 4.9** Sensitivity analysis effect of temperature on fats degradation

Figures 4.8, 4.9 and 4.10 illustrate the model sensitivity of temperature changes in sugar, protein and fat degradation rates, respectively. The model sensitivity is measured using the dry weight per cubic meter of sugar, protein and fats left in the LSR during the simulation time. These figures show the similarity for all organic matter types, meaning that the degradation rate increases with the temperature. However, the model provides no similar response by the same order of magnitude as the temperature changes between being higher and lower than the initial condition. This difference can be explained by the temperature effect on the microorganism growth rate, which was assumed to follow a cumulative distribution function (CDF).

The microorganism growth rate at low temperature increased slowly until a certain temperature, and then increased exponentially at higher temperatures (see Temperature inhibition factor in Chapter 3).



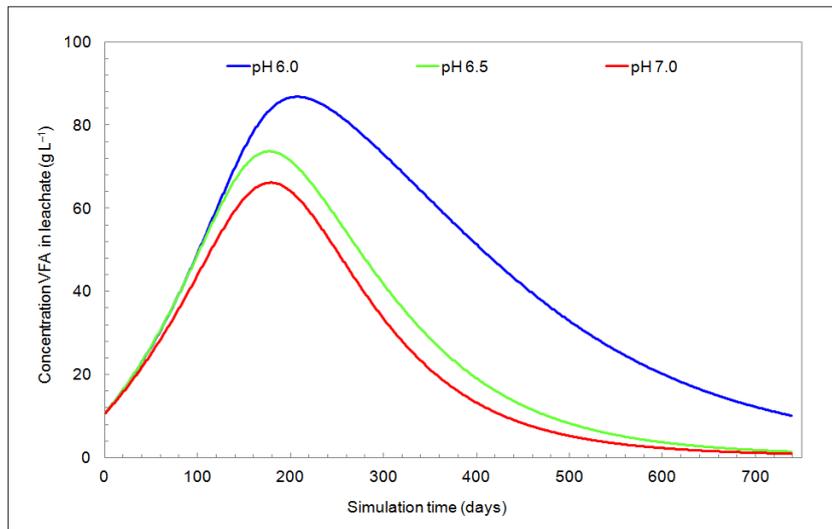
**Figure 4.10** Sensitivity analysis effect of temperature on sugar degradation

#### 4.2.2 Effect of pH on Organic Matter Degradation

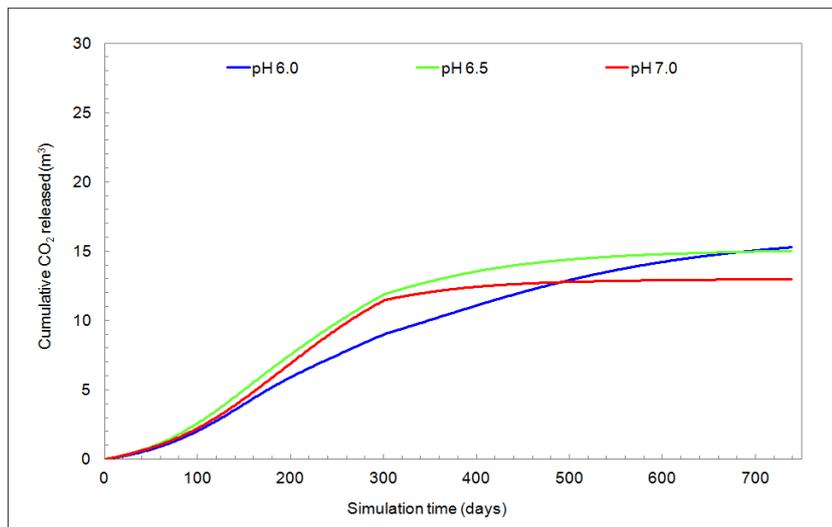
The pH values in landfill sites are dependent on several factors, including the concentration of VFAs, ammonium accumulated, calcium carbonate dissolution rate, and CO<sub>2</sub> partial pressure. All of these parameters are in equilibrium and reflected in the pH value of leachate. On the laboratory experiment scale, the pH of the LSR may remain at the desired value through leachate amendment and injecting acid or base solutions into the LSR. This method may be impossible to implement for field-scale landfill operation due to the huge amount of acid or base that would be required to maintain the pH value for large landfill sites. However, this sensitivity analysis is still useful for providing an overview of the effect of pH value on the biodegradation of organic matters in landfill sites.

Figure 4.11 shows the profile of VFA concentration in leachate generated from the LSR operating under pH values kept constant at 6.0, 6.5 and 7.0. As expected, the VFA concentration in leachate decreases with the pH value increasing to 7.0, which is the optimum value for methanogenic growth. At this pH value, the VFAs

produced from acidogenesis of organic matter were consumed immediately after being produced. However, as the growth rate of acidogens was ten times faster than methanogens, only parts of the VFAs have been converted into  $\text{CH}_4$  and  $\text{CO}_2$ . Most of them were accumulated and recycled within the LSR experiment until the organic matter depleted and VFAs were not produced anymore.



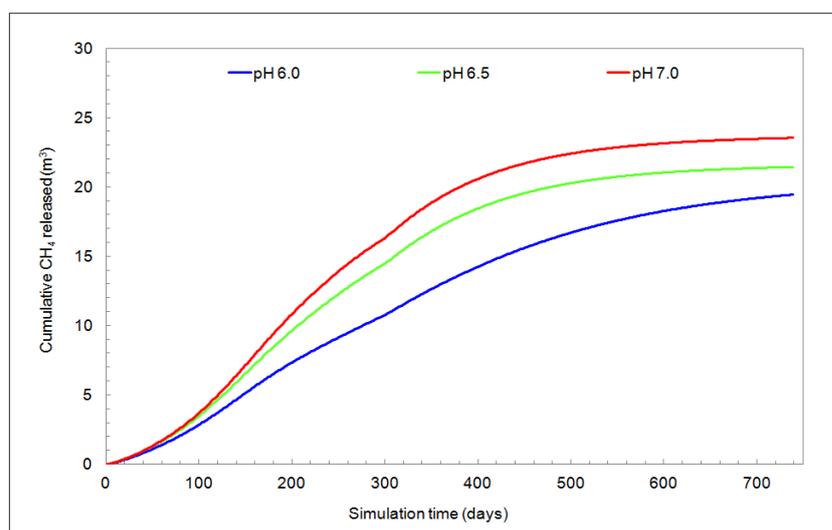
**Figure 4.11** Sensitivity analysis effect of pH on VFA concentration in leachate discharged



**Figure 4.12** Sensitivity analysis effect of pH on cumulative  $\text{CO}_2$  generated

When the pH value was adjusted to 6.0 the concentration of VFAs in leachate increased by two to three orders of magnitude higher than the reduction of the VFA concentration when the pH value was adjusted to 7.0. These increases can be explained by the fact that under a low pH value the methanogens growth rate

substantially decreased, while on the other hand the VFA production and acidogens growth rate were not affected significantly by these pH value changes.

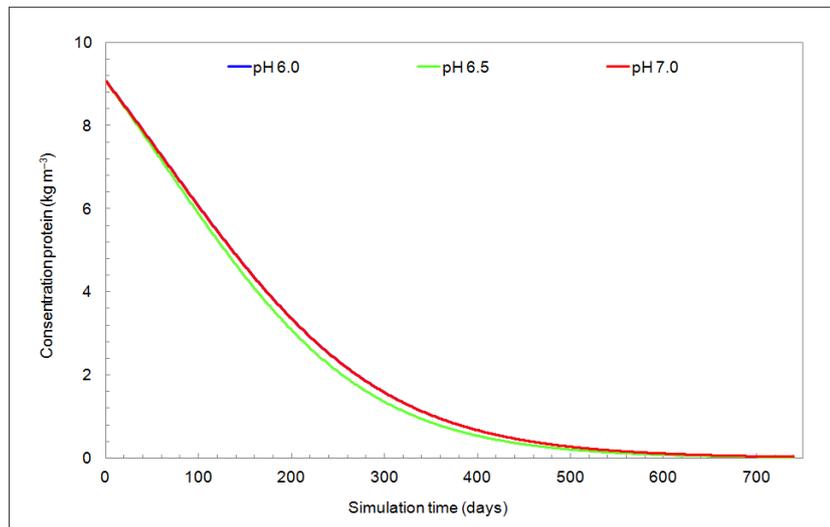


**Figure 4.13** Sensitivity analysis effect of pH on cumulative CH<sub>4</sub> generated

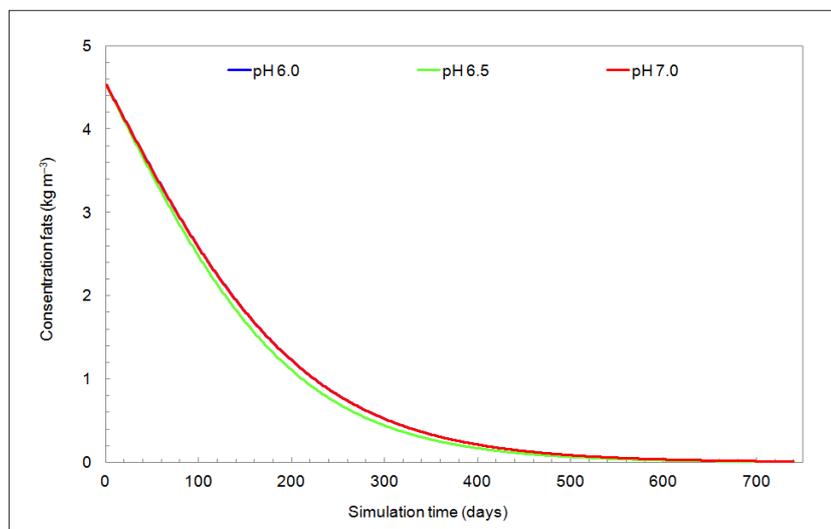
The pH value had no significant effect on the cumulative CO<sub>2</sub> released. The model simulation shows that a change of pH from 6.5 to its initial value of 7.0 results in an almost identical CO<sub>2</sub> accumulation from the beginning of the simulation time until day 300. After day 300, the cumulative CO<sub>2</sub> of the LSR operating at a pH of 7.0 was slightly lower than the LSR operating at a pH of 6.5 until the end of the simulation time. In contrast to the pH of 7.0, the cumulative CO<sub>2</sub> of the LSR operating at pH 6.0 increased steadily from the beginning until the end of the simulation time.

The explanation for judging these different results is that the hydrogenotrophic methanogens growth rate very fast from the beginning of the simulation since a pH value 7.0 is the preferred pH for methanogens. After day 300, the solid organic matter was completely degraded and the acetotrophic methanogenesis became the limiting step and the only source of CO<sub>2</sub>. This CO<sub>2</sub> is consumed immediately as it is produced by hydrogenotrophic methanogens and stays at a relatively low level. Therefore the accumulation of CO<sub>2</sub> increases at very small rates. This is confirmed by the steady increase of the cumulative CH<sub>4</sub> as shown in Figure 4.13. On the other hand, for the LSR operating at a pH of 6.0 the growth rate of hydrogenotrophic methanogens is slower than the LSR operating at a pH of 7.0. Therefore the CO<sub>2</sub>

produced is high enough to support the hydrogenotrophic methanogens growth at a steady rate.



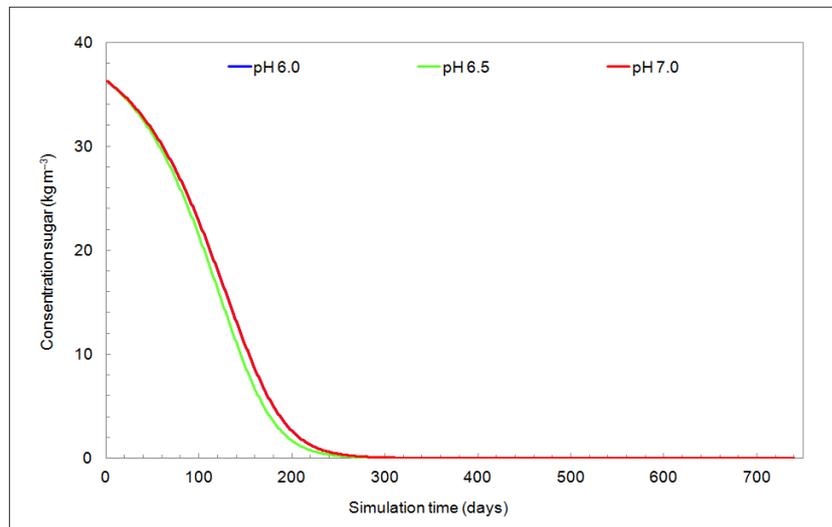
**Figure 4.14** Sensitivity analysis effect of pH on protein degradation



**Figure 4.15** Sensitivity analysis effect of pH on fats degradation

Figures 4.14, 4.15 and 4.16 illustrate the effect of pH value on sugar, protein and fat degradation rates. These figures indicate that the pH value change from 6.0 to 7.0 has an insignificant effect on the degradation of organic matter. This insignificant effect can be explained by the fact that a pH value of 6.5 is the optimum condition for the hydrolysis and acidogenesis step of the biodegradation of organic matter and an increase or decrease of the pH value from 6.5 to 7.0 or from 6.5 to 6.0 has a little and similar effect on the growth rate of acidogens (see pH inhibition factor in

Chapter 3). This means that these pH changes resulted in an identical biodegradation rate.



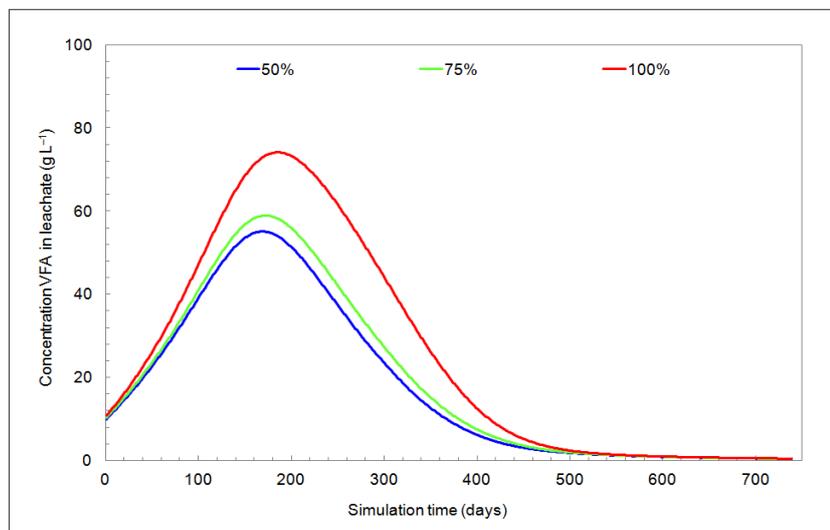
**Figure 4.16** Sensitivity analysis effect of pH on sugar degradation

#### 4.2.3 Effect of Leachate Recirculation Rate on Organic Matter Degradation

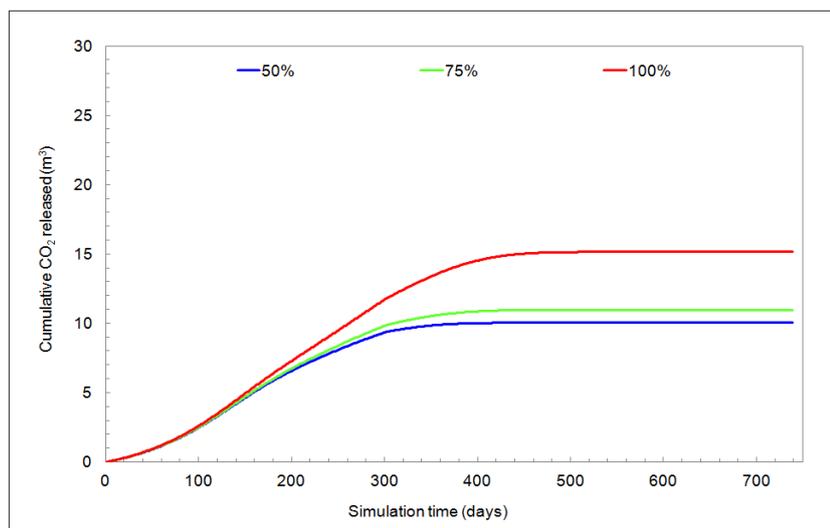
Moisture content plays an important role in biodegradation in landfill sites. The moisture content also directly affects the volume and composition of leachate produced from MSW landfills. Laner et al. (2011) reported that high infiltration rates during the landfill cover reinstallation significantly increased the concentration of chloride and ammonia–nitrogen by two to three orders of magnitude higher than under previous conditions. Furthermore, with the current trend of MSW landfill operations that is moving from the conventional concept to a bioreactor approach, information on the effects of moisture content on the biodegradation of organic matter in landfill sites is urgently required. Therefore, several simulations for the sensitivity analysis of moisture content affecting biodegradation are highlighted for this issue.

The LSR experiment was carried out under total leachate recirculation without the pH being amended (i.e. pH neutralization, ammonium removal, etc.). Therefore the sensitivity analysis effect of moisture content was also set up without adjustment of the leachate concentration. The simulation results indicate that the leachate

recirculation affected only the concentration of VFAs in discharged leachate, and the cumulative  $\text{CO}_2$  and  $\text{CH}_4$ . Figure 4.17 shows that the VFA concentration in the leachate decreased with changes of the leachate recycling rate. The model simulation results also indicated that the decreasing VFA concentration in discharged leachate from a leachate recirculation ratio of 100 to 75 % was four orders of magnitude higher than from 75 to 50 %.



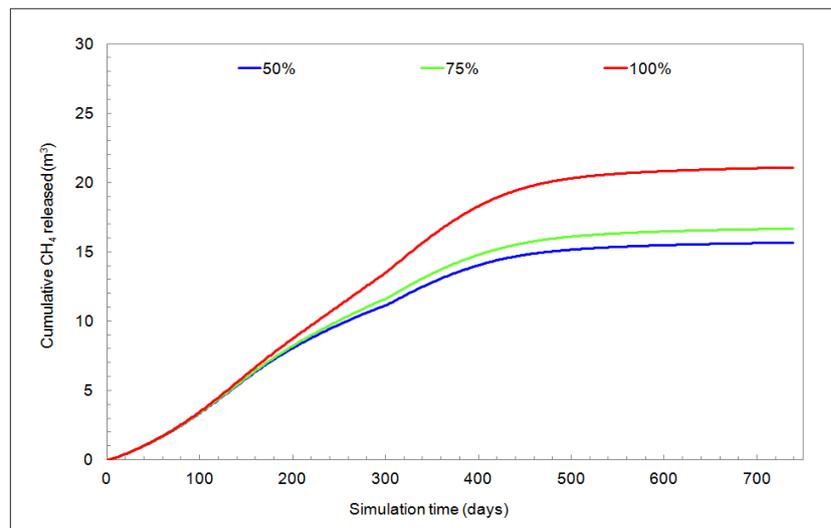
**Figure 4.17** Sensitivity analysis effect of leachate recirculation on VFAs concentration in leachate discharged



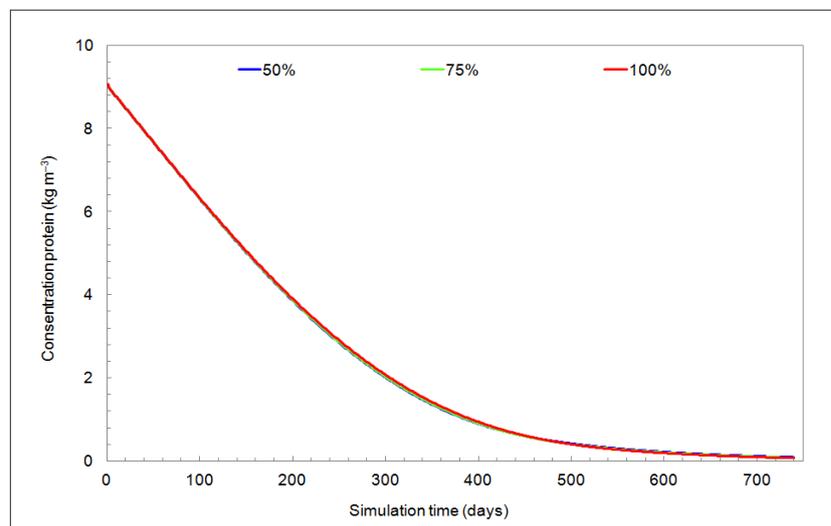
**Figure 4.18** Sensitivity analysis effect of leachate recirculation on cumulative  $\text{CO}_2$  generated

A similar phenomenon was observed in cumulative  $\text{CO}_2$  and  $\text{CH}_4$  released from the model simulation (see Figures 4.18 and 4.19). The final cumulative  $\text{CO}_2$  released at

100% leachate recirculation of about 15.2 m<sup>3</sup> decreased to about 10.9 m<sup>3</sup> when leachate recirculation was reduced to 75%, and finally became about 10.0 m<sup>3</sup> at 50% leachate recirculation, whereas the final cumulative CH<sub>4</sub> released was about 21.1 m<sup>3</sup> at 100% leachate recirculation and decreased to 16.7 m<sup>3</sup> at 75% leachate recirculation; it was finally about 15.7 m<sup>3</sup> at 50% leachate recirculation.



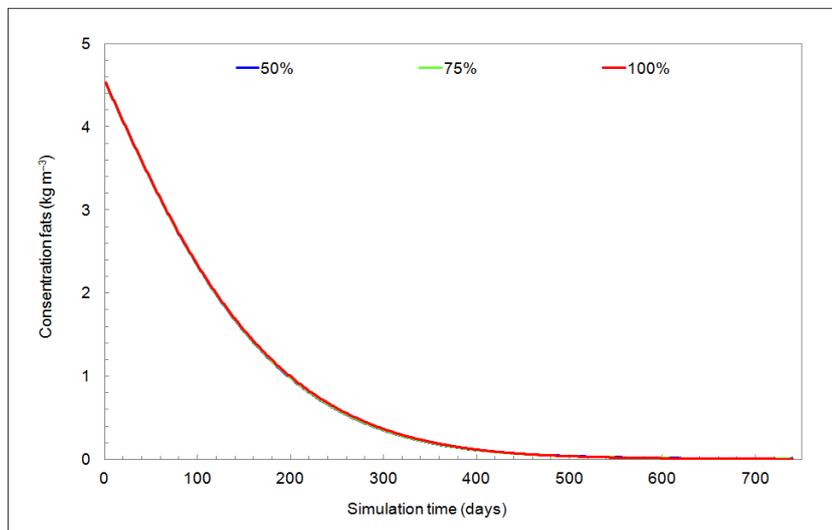
**Figure 4.19** Sensitivity analysis effect of leachate recirculation on cumulative CH<sub>4</sub> generated



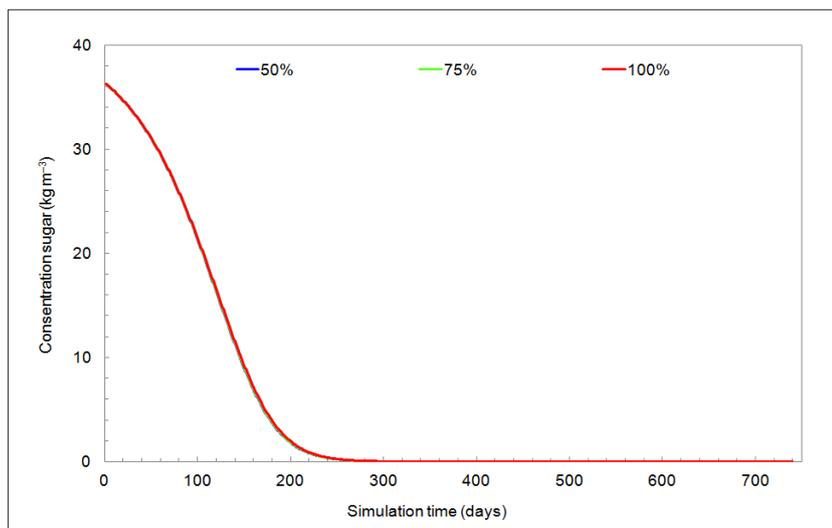
**Figure 4.20** Sensitivity analysis effect of leachate recirculation on protein degradation

These results were only attributed to the methanogenesis step and were not related to the acidogenesis step. VFAs are mainly acetic acid, a substrate for acetotrophic methanogenesis growth. The substrate availability was limited as a consequence of reduction of the leachate recirculation rate. On the other hand, the concentration of

acetotrophic methanogens was equal to that one of a leachate recycling rate of 100%, since the microorganisms were assumed not be washed out by the leachate flow. Hence, the limited substrate coupled with the high concentration of methanogens resulted in a significant decrease of the VFA concentration in the discharged leachate. However, a further reduction in the leachate recycling rate had no significant effect anymore, because the VFA concentration available was not enough to sustain a large methanogenic population.



**Figure 4.21** Sensitivity analysis effect of leachate recirculation on fats degradation



**Figure 4.22** Sensitivity analysis effect of leachate recirculation on sugar degradation

This analysis can be confirmed by the leachate recirculation effects on the biodegradation rate of organic matter results as shown in Figures 4.20, 4.21 and

4.22. The figures show that leachate recirculation does not enhance the biodegradation of sugar, protein and fats. These results were contrary to the one that was observed, where the leachate recirculation was able to reduce the stabilization time, enhance CH<sub>4</sub> production and improve the quality of leachate (Šan and Onay, 2001; Chan et al., 2002; Sponza and Ađdađ, 2004). This difference can be explained by the fact that the biodegradation of organic matter in the landfill site is limited by the heterogeneous nature of the waste (Fellner and Brunner, 2010).

Moreover, the moisture content effect on the biodegradation of organic matter will never increase after it has reached the optimum condition even if more water is added. It is important to note that the leachate recirculation rate used in the LSR experiment of about 30 l week<sup>-1</sup> is equal to 4,000 mm year<sup>-1</sup>, which is nearly five times higher than the average precipitation rate in Delft, the Netherlands, which is about 830 mm year<sup>-1</sup> (KNMI, 2013). Therefore, a reduction of the leachate recirculation rate of down to 50% of the initial rate would still be higher than the optimum moisture content condition that was defined in the moisture content correction factor section (see Chapter 3).

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## **Chapter 5**

### **Model Application**

A numerical model of transformation of degradable and refractory organic carbon in MSW landfills was developed in Chapter 3. The model development was carried out by adopting PBR coupled with the batch reactor concept in order to represent the mobile (i.e. gas and liquid) and immobile (i.e. solid) phases within the landfill. The transformation of degradable and refractory organic carbon was developed based on basic biological concepts associated with chemical concepts to determine the equilibrium conditions of the landfill site, while the mobile phase transport is considered to occur under a physical concept.

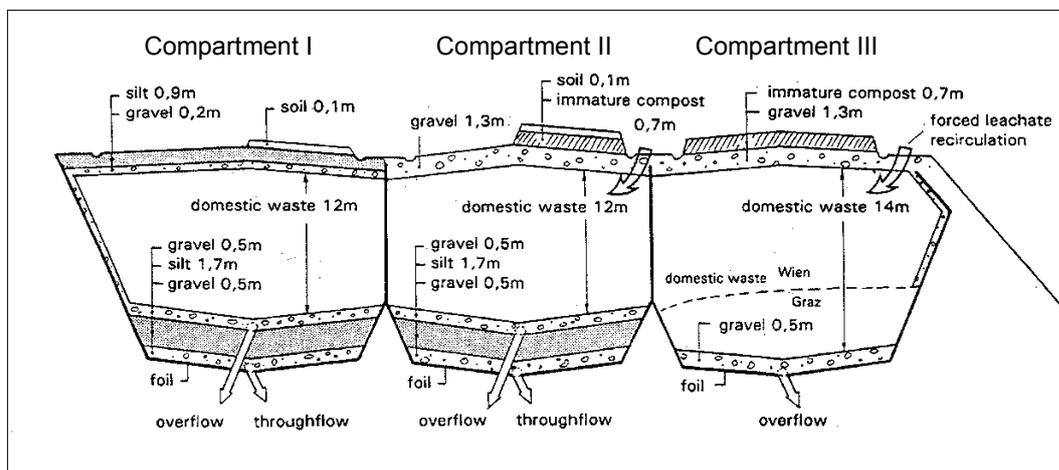
The model calculation results were validated by laboratory experimental results in Chapter 4. The model validation was carried out by comparing the specific parameters of the model calculation to laboratory experimental results from literature. The validation shows that some parameters fit with the laboratory experiment results, while others do not. In addition, several simulations were performed to measure the model sensitivity to the parameters that affect the biodegradation of organic matter in the landfill site. The results show that temperature and pH value had a significant effect on the biodegradation of degradable organic matter in the landfill, while the leachate recirculation to maintain the organic matter fully saturated has an insignificant effect on the acceleration of the degradation of organic matter and therefore expected landfill gas composition.

As the final step of the model development to calculate the degradation of organic matter and predict landfill emissions, this chapter presents the application of the model to a full-scale MSW landfill. The Breitenau landfill in Austria was chosen as the case study for the model application. This landfill is suitable as only MSW is disposed there, and the emissions from this site were monitored between 1988 and 2010. A brief description of the Breitenau landfill and data input preparation is given

in section 5.1, while the results and the discussion are presented in sections 5.2 and 5.3.

## 5.1 Description of the Breitenau Landfill

The Breitenau landfill was constructed in a former gravel quarry located approximately 60 km south–west of Vienna, Austria (47° 44' 37" N, 16° 08' 28" E). The landfill, which was built as an experimental site for numerous research studies conducted by the Vienna University of Technology (Binner et al., 1997; Huber et al., 2004; Döberl et al., 2006; Fellner et al., 2009; Fellner and Brunner, 2010), is divided into three compartments with different capping and sealing systems (Riehl–Herwirsch et al., 1995). Between 1987 and 1988, the three compartments were filled with approximately 95,000 tons of MSW from Vienna. The MSW was placed in layers of approximately 1.0 m and compacted to a wet density of about 1,200 kg m<sup>-3</sup>.



**Figure 5.1** Cross-section of the Breitenau landfill (Riehl–Herwirsch et al., 1995)

In all three compartments, 2 mm HDPE foil was placed over the compacted base to prevent leachate migration to groundwater. The subsequent baseliner in compartments I and II was constructed using a composite system of a 0.5 m gravel layer, a 1.7 m compacted clay layer with hydraulic conductivity of less than 10<sup>-9</sup> m

second<sup>-1</sup>, and lastly a 0.5 m gravel layer as leachate drainage before MSW placement. In compartment III, no additional line besides the HDPE foil was installed, with only a gravel layer of 0.5 m thickness being employed for leachate drainage (see Figure 5.1). The leachate produced was collected separately from each landfill compartment. From the beginning of the landfill operation until 1992, the leachate generated in each compartment was collected in leachate collection tanks, and partly recirculated to the landfill. The volume and duration of the leachate recirculation were different for each compartment. From 1992, all leachate produced and collected was pumped directly to the sewage system without any leachate recirculation. The characteristics and the landfill operation of each compartment are summarized in Table 5.1.

The leachate concentration between 1988 and 2005 was analysed sporadically. In total, only 89 leachate samples were collected and analysed. Moreover, the parameters analysed also vary from one to another leachate analysis. The electrical conductivity, measured by conductivity meters, which were installed at the end of each of the three leachate collection pipes, shows a significant correlation to the leachate discharge rate (Fellner et al., 2009; Laner et al., 2011). This correlation between electric conductivity and the leachate generation rate was used to determine the leachate composition, particularly  $\text{NH}_4\text{-N}$  and chloride concentration.

## **5.2 Estimation of the Breitenau Landfill Emissions**

The application of the model to predict the transformation of readily and refractory organic matter focuses on compartment I of the Breitenau landfill for two reasons. First: only MSW has been deposited in this compartment; and second: previous investigations (e.g. tracer experiments and water flow modeling, solid waste sampling and analysis, continuous measurement of leachate quality) have focused on this compartment. This information is useful and indispensable for both the input data and analysis and the model application results.

Table 5.1 Summary compartment characteristic of the Breitenau landfill

Parameter	Unit	Compartment		
		I	II	III
Surface area	m <sup>2</sup>	4,622	2,929	3,798
Waste volume (wet weight)	t	35,000	25,600	33,200
Waste type and origin	-	- Vienna household w/o preprocessing	- Vienna household w/o preprocessing	- Shredded household from Graz + sewage sludge (67% of total volume) - Vienna household w/o preprocessing (33% of total volume)
Landfilling operation				
- Start	-	Nov 1987	Oct 1987	Jan 1987
- Finish	-	Sep 1988	Oct 1988	Sep 1988
- Period	months	11	12	21
Top cover installation				
- Completion date	-	Jun 1989	Jun-89	Jun-89
- Cover layers construction	-	- 0.1 m soil (half surface) - 0.9 m silt - 0.2 m gravel	- 0.1 m soil (half surface) - 0.7 m silt (half surface) - 1.3 m gravel	- 0.7 m compost - 1.3 m gravel
Total water added to waste saturated	m <sup>3</sup>	32	36	6.5
Total leachate recirculation				
- During landfilling operation	m <sup>3</sup> t <sup>-1</sup> MSW	0.019	0.016	0.0034
- 2 <sup>nd</sup> semester 1989	m <sup>3</sup> t <sup>-1</sup> MSW	no leachate recirculation	no leachate recirculation	no leachate recirculation
- 1 <sup>st</sup> semester 1990	m <sup>3</sup> t <sup>-1</sup> MSW	no leachate recirculation	0.015	0.0064
- 2 <sup>nd</sup> semester 1990	m <sup>3</sup> t <sup>-1</sup> MSW	no leachate recirculation	no leachate recirculation	0.011
- 1 <sup>st</sup> semester 1991	m <sup>3</sup> t <sup>-1</sup> MSW	no leachate recirculation	no leachate recirculation	0.0045
- 2 <sup>nd</sup> semester 1991	m <sup>3</sup> t <sup>-1</sup> MSW	no leachate recirculation	no leachate recirculation	0.0184
Methane stable phase condition				
- pH value > 7.5	months	> 15	> 8	> 8
- BOD/COD < 0.1	months	> 24	> 18	> 16

Source: (Riehl-Herwirsch et al., 1995)

In addition to the landfill characteristics specified in Table 5.1, the composition of waste deposited, daily mean temperature and water infiltration rate in the landfill body are needed as input data of the model to calculate the landfill emissions. For this purpose, this information was collected from various literature sources or direct measurement, and treated in order to meet the model requirements on input data. The preparation of the model input data, namely composition of deposited waste, daily mean temperature and water infiltration rate into the landfill body, are described in the following sections (5.2.1–5.2.3).

### 5.2.1 Composition of Municipal Solid Waste

Approximately 35,000 tons of MSW were disposed into compartment I during the landfilling operation. This amount was dumped in the 4,622 m<sup>2</sup> total footprint area of compartment I with a total height of about 12 m. The composition of the landfilled MSW used in this study refers to the MSW generated from Vienna city, Austria, obtained from Vienna's Municipal Waste Department MA 48. The MSW composition is summarized in Table 5.2.

**Table 5.2** Average composition of the Vienna MSW over 1985–1986 periods

MSW component	Composition <sup>a</sup> (%)	Organic matter (w/w) <sup>b</sup>					
		Protein	Fats	Sugar	Cellulose	Lignin	Other
Biogenic waste	23.3	2.56	1.11	9.11	6.83	1.39	2.28
Paper and cardboard	33.6	0.06	0.40	0.06	14.48	6.11	12.47
Plastic	7.0	–	–	–	–	–	7.00
Textile and rubber	3.1	0.11	0.03	–	1.29	0.08	1.19
Wood	2.1	0.03	0.16	0.02	1.24	0.63	0.02
Glass	10.4	–	–	–	–	–	10.40
Metal	3.7	–	–	–	–	–	3.70
Residual	17.2	–	–	–	–	–	17.20
Total	100.0	2.76	1.71	9.20	23.84	8.22	54.26

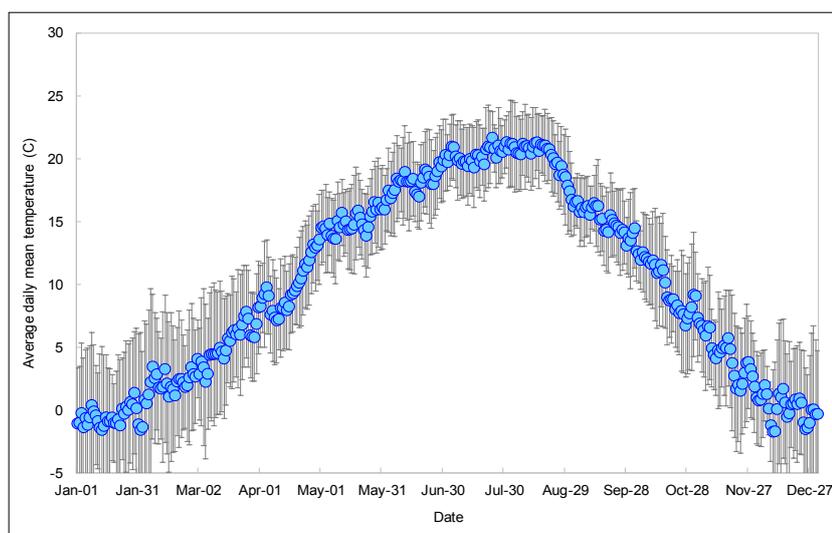
Source: <sup>a</sup> Riehl–Herwirsch et al. (1995); <sup>b</sup> calculated according to Neumayer (1999)

With a similar method to the model validation and sensitivity analysis, the composition of MSW deposited in the Breitenau landfill was treated, and distinguished into its degradability levels as summarized in Table 5.2. The degradable portion of MSW is primarily cellulose with a composition of almost 24% of total dry matter. The composition of simple carbohydrates, proteins and fats was about 9.2, 2.8 and 1.7, respectively. The composition of readily degradable organic

matter was slightly lower than the MSW composition of Wijster, the Netherlands, which has been used in model validation and sensitivity analysis (see Chapter 4).

### 5.2.2 Temperature Input

The temperature used as input data to estimate landfill emissions is the daily mean atmospheric temperature collected from Wr. Neustadt station, the closest meteorology station to the Breitenau landfill. Data are available from 1987 to 2005. These data were subsequently treated to determine the average daily mean atmospheric temperature on a specific date. These figures were used to determine the missing metrological data within the landfill simulation time. Figure 5.2 shows the average daily mean atmospheric temperature from January 1<sup>st</sup> to December 31<sup>st</sup>, applied to all years.



**Figure 5.2** The average daily mean of ambient air temperature over 1987 – 2005 periods

The standard deviation of average daily mean temperature was approximately 3.7 °C. Although the temperature changing affects the degradation of organic matter significantly, this figure is still within the acceptable tolerance level. According to data reported by Langenhoff and Stuckey (2000), a temperature change from 35 to 20 °C reduced the removal efficiency by 25%. However, a further decrease of the temperature to 10 °C resulted in only a 10% reduction of the removal efficiency, whereas the temperature changing from 50 to 65 °C resulted in a slightly lower

acidification yield (Ahring et al., 2001). This indicates that the model results did not differ much despite the temperatures used being a bit different to the actual conditions.

### 5.2.3 Water Input

The leachate emission and the biodegradation of organic matter of deposited waste in the landfill site are controlled by the amount of water input. The amount of water input into the landfill site is equal to the sum of the net water input by precipitation (precipitation deducted by surface run-off and evapotranspiration), moisture content in MSW, and leachate recirculation. A simple method to calculate the water input and content is to perform a water balance. The general water balance equation for MSW landfills as proposed by Baccini et al. (1987) is:

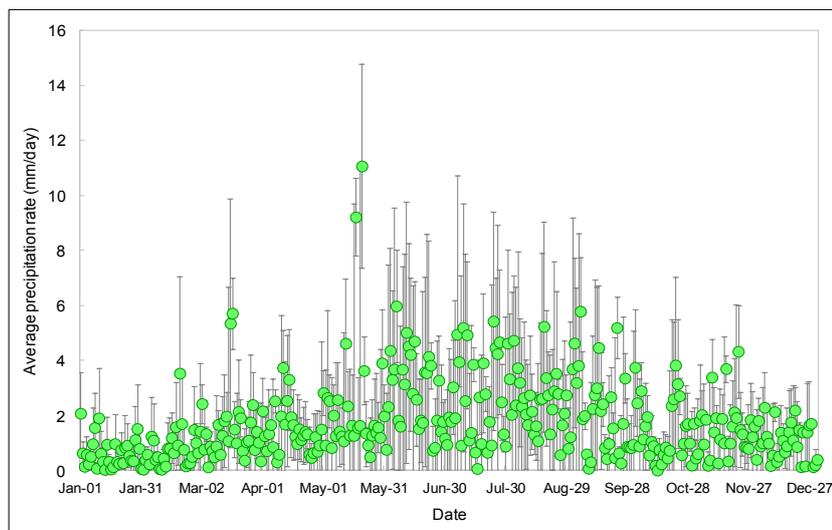
$$q_L^{\text{in}} \pm \sum_{j=1}^n q_{r(j)} - q_L^{\text{out}} - S = 0 \quad \dots\dots\dots (5.1)$$

where  $q_L^{\text{in}}$  is water input and wetting the waste bulk in the landfill body,  $q_{r(i)}$  is water production/consumption by biological process during degradation of organic matter,  $q_L^{\text{out}}$  is leachate outflow from the landfill body, and  $S$  is water storage in the landfill body. All terms are in gram water per kilogram MSW per year and water input as moisture content in MSW refers to the water content of incoming MSW (Baccini et al., 1987).

As the focus in this section is to determine the water input into the landfill (first term) and the last three terms of the above equation are already included in the model (see Chapter 3), this does not have to be considered in this section anymore. The net water input by precipitation to the landfill surface area is determined as follows:

$$q_{L(p)}^{\text{in}} = P - ET - V \quad \dots\dots\dots (5.2)$$

where  $P$  is the precipitation rate ( $\text{mm day}^{-1}$ ),  $ET$  is the evapotranspiration rate ( $\text{mm day}^{-1}$ ), and  $V$  is the surface run-off ( $\text{mm day}^{-1}$ ). The daily precipitation rate data were obtained from the three meteorology stations near the Breitenau landfill together with the daily temperature data, and treated with the similar method. Figure 5.3 shows the average precipitation rate between 1987 and 2005. The standard deviation of 19 years' daily precipitation rate data was approximately  $3.6 \text{ mm day}^{-1}$ .



**Figure 5.3** The average daily precipitation rate over 1987–2005 periods

Numerous empirical methods have been developed to estimate the evapotranspiration rate from different climatic and water storage sources. Some of these derived from Penman's equation (Penman, 1948) to determine evaporation from water surface, bare soil and grass based on a combination of energy balance, and climatic and aerodynamic conditions. This method requires numerous climatic and aerodynamic data such as the net radiation flux, the relative humidity, the wind speed, atmospheric temperature and sensible heat flux in the soil. In practice, not all data are measured and documented. In general, only maximum and minimum values of temperature and precipitation rate are tabulated on a monthly basis. Hence, it was decided to use the simplest and most frequently used method in Europe developed by Haude (1954) based on the Dalton approach for low grass cover on soil according to the deficit of water vapour pressure and written as follows:

$$ET = f(e_s - e)_{14} \dots\dots\dots (5.3)$$

where ET is the evapotranspiration rate (mm day<sup>-1</sup>), *f* is Haude's evapotranspiration proportionality factor (mm mbar<sup>-1</sup>), *e<sub>s</sub>* is the saturated vapour pressure (mbar), *e* is the vapour pressure (mbar), and subscript 14 indicates that both *e<sub>s</sub>* and *e* are measured at 14 pm.

The advantage of this method is that it requires only two meteorological data (daily mean temperature and relative humidity); however, the Haude evapotranspiration proportionality factor is specific to particular regions. Based on a ten-year experiment using lysimeters covered with grass in the north-east of Vienna city, Dobesch (1991) proposed Haude evapotranspiration proportionality factors for the Vienna region as listed in Table 5.3.

**Table 5.3** The original and corrected Haude evapotranspiration factors

<i>f</i>	Month											
	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	Oct	Nov	Dec
DIN 19685 (1997)	0.22	0.22	0.22	0.29	0.29	0.28	0.26	0.25	0.23	0.22	0.22	0.22
Dobesch (1991)	0.14	0.14	0.15	0.24	0.28	0.28	0.23	0.21	0.17	0.15	0.14	0.14

The curve numbers (CNs) method, which has been developed by the Natural Resources Conservation Service of the United States Department of Agriculture (NRCS-USDA), was adopted to calculate the surface run-off. This amount depends on the area, soil group, land use, treatment and hydrologic conditions as follows:

$$V = \frac{(P - I_a)^2}{P - I_a + S} \dots\dots\dots (5.4)$$

where *P* is the precipitation rate (mm day<sup>-1</sup>), *I<sub>a</sub>* is the initial abstraction or the amount of water before run-off (mm day<sup>-1</sup>), and *I<sub>a</sub>* is the function of the maximum potential retention *S* (mm day<sup>-1</sup>). As an approach, the relationship between *I<sub>a</sub>* and *S* can be expressed empirically as *I<sub>a</sub>* = 0.2*S*. The maximum potential retention is determined by the following relation:

$$S = \frac{1,000}{CN} - 10 \dots\dots\dots (5.5)$$

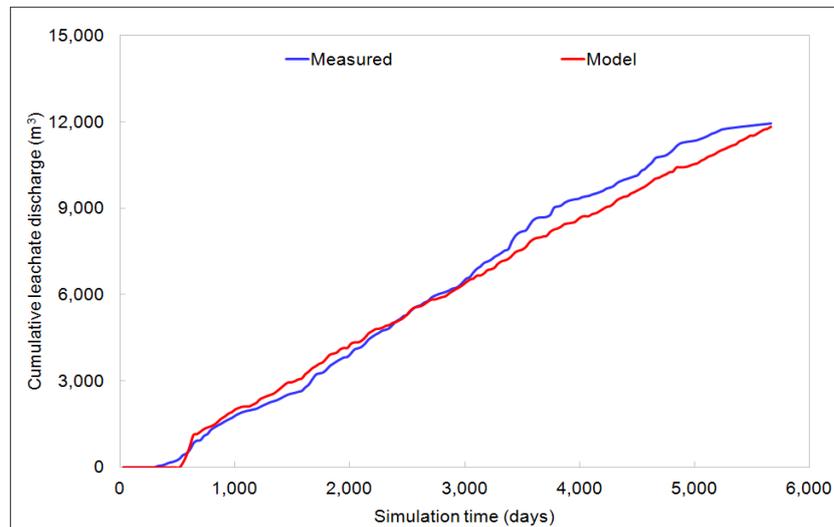
where *CN* is the curve number ranging from 20 to 100 depending on soil type, soil infiltration capability and land use. A lower *CN* indicates that the soil is more permeable. The NRCS has divided soils into four hydrologic soil groups (HSGs): low, moderate, slow and high run-off potential. In this study, the landfill cover is assumed to have slow run-off potential, as it is covered by a combination of wood and grass with fair hydrologic conditions.

Due to the absence of documented measured moisture contents of Vienna MSW deposited in the Breitenau landfill, the moisture content in MSW reported by Brunner et al. (1983) and Ehrig (1989) of about 30% was adopted to calculate the water input by moisture content of MSW. This value corresponds with the moisture content of MSW as reported by Schachermayer et al. (1994). Another assumption was made regarding the water input by leachate recirculation. Although the total amount of leachate recirculation is known, the daily leachate recirculation rate is not documented. Hence, the leachate recirculation rate was assumed to be constant for the entire leachate recirculation period.

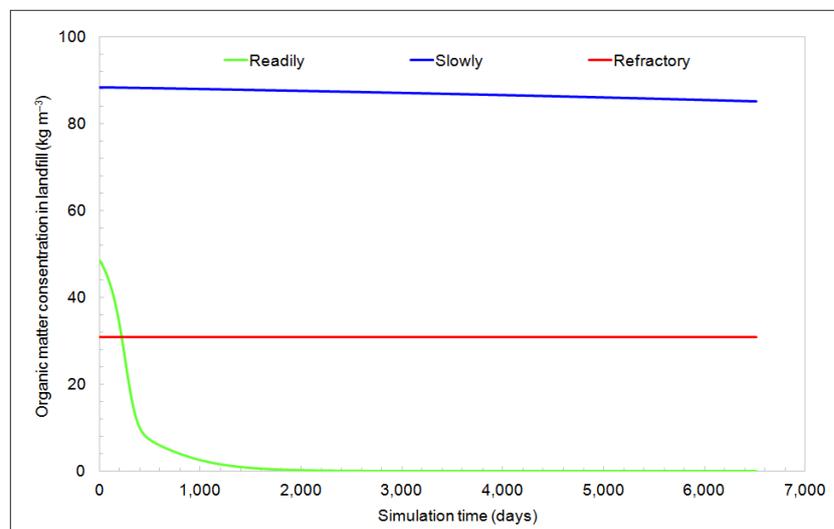
### 5.3 Results and Discussion

Although the Breitenau landfill was designed and built as an experimental site for research studies, some emission parameters were not measured (i.e. composition of landfill gas), while others were not completely recorded and well documented (i.e. leachate discharged). As previously mentioned, approximately 89 samples of the leachate were collected and analysed between 1987 and 2005, while the composition of landfill gas was never measured at all. This condition makes it difficult to select the reference parameters to compare between the model results and the real conditions, and predict the best-fit model calculation results. Since only the

cumulative leachate discharge data are available for the whole time period, it was decided to use them as reference parameters to complete the simulation.



**Figure 5.4** Simulated and filed measured the cumulative discharged leachate of the Breitenau landfill



**Figure 5.5** Simulated the fate organic matter of the Breitenau landfill

Figure 5.4 shows the cumulative leachate discharge of the model calculation and the field-measured data. This figure indicates that the model calculation result for this parameter is generally close to the field-measured data. However, the leachate discharge of the model calculation is low compared to the field-measured data at the beginning of the simulation time. The reason behind this difference is that the water

input by precipitation is stored in the landfill for a certain time until reaching the field capacity. After the total water input reaches the field capacity, the leachate discharge is determined by water balance as presented by Equation 5.1.

Figure 5.5 presents the time profile of readily, slowly and refractory–degradable organic matter in landfills. The readily organic matter decreased immediately from the beginning simulation time, and completely degraded after 1,500 days of simulation time. The slowly organic matter decreased steadily from the beginning until the end of the simulation time, and no degraded refractory organic matter is considered within the simulation.

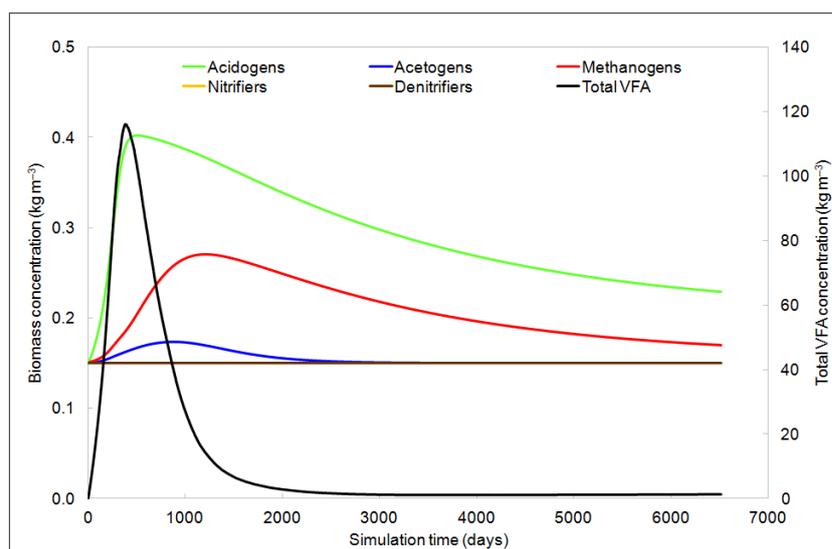
**Table 5.4** Initial and simulated final organic matter of Breitenau landfill

Organic matter	Initial	Final	Degraded
	(x1,000 kg)	(x1,000 kg)	(%)
Readily–degradable	3,348	–	100.0%
Slowly–degradable	5,839	5,634	3.5%
Refractory–degradable	2,013	2,013	0.0%
Total	11,200	7,647	31.7%

Table 5.4 presents initial and simulated final amounts of organic matter from the Breitenau landfill. According to the model simulation results, the total solid organic matter that degraded within the 1987–2005 (i.e. approximately 6,500 days) period was about 32% of the total degradable fraction of MSW disposed. Similar to the LSR results, the readily degradable organic matter from the Breitenau landfill also completely degraded within the bioreactor phase. Although the size of the LSR is smaller than the Breitenau landfill, as shown in Figure 5.5 the bioreactor phase of the Breitenau landfill is almost the same as the LSR. This is indicated by the changing trend of the pH value from decreasing to gradually increasing (see Figure 4.1 and 5.7).

The total solid carbon of degraded organic matters is equivalent to the total carbon of total VFAs, CO<sub>2</sub> and biomass formed. The solid carbon of organic matter is consumed by acidogens and converted to VFAs, CO<sub>2</sub> and acidogenic biomass according to the Monod kinetics model for substrate utilization. Therefore, the total VFA and acidogens concentrations are directly proportional to the decrease of organic matter as shown in Figure 5.6.

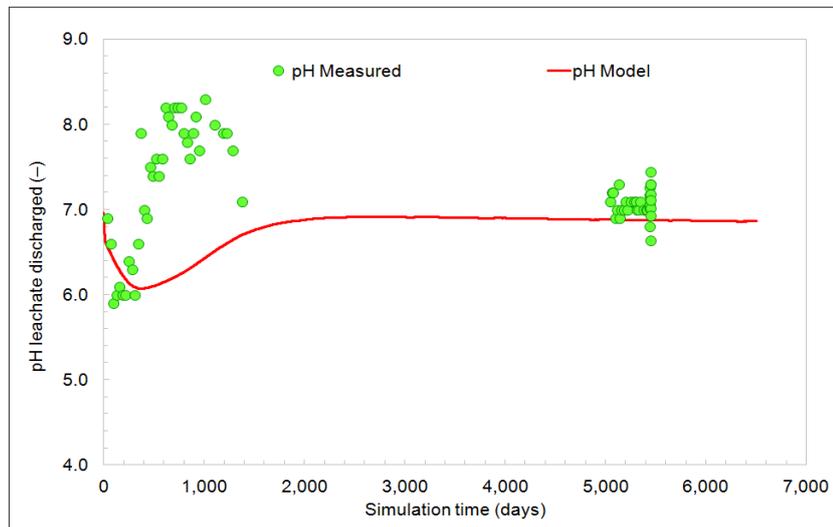
As the VFAs are formed, the pH landfill site decreases (see Figure 5.7), but remains within the range of the optimum condition for acidogens growth. Nevertheless, the acidogens continue to consume the organic matter to produce VFAs and acidogens biomass at a steady rate. It is indicated that the VFAs are closely interlinked to acidogens biomass growth (see Figure 5.6). Immediately after VFAs have been formed, the substrate for methanogens growth is available. However, a low pH value is not the preferred condition for methanogens growth (see Figure 3.5). This can be attributed to the slow growth rate of methanogens in abundant substrate conditions. Therefore, the methanogens growth rate increases at a relatively moderate rate compared to that of acidogens.



**Figure 5.6** Simulated biomass and VFA concentrations of the Breitenau landfill

Figure 5.7 shows the pH value results for generated leachate of the model calculation and the field-measured data. The model calculation result was fits to the field-measured data at the beginning and end of the simulation time, but no in between was observed. The pH value of the model calculation matches well with the VFA concentration. Therefore, the difference between the model calculation and the field-measured data might be caused by other factors not covered in the mass balance of the biological reaction of organic matter degradation. This includes physical processes such as leaching soluble material from the top cover layer

transported by water throughout the preferential flow path in landfills or leachate amendment by soluble materials from the bottom–liner.

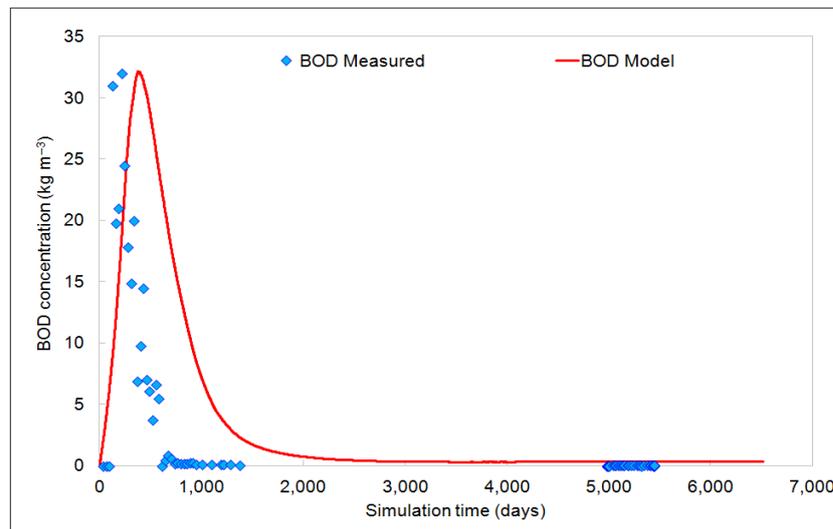


**Figure 5.7** Simulated and field measured pH value of discharged leachate of the Breitenau landfill

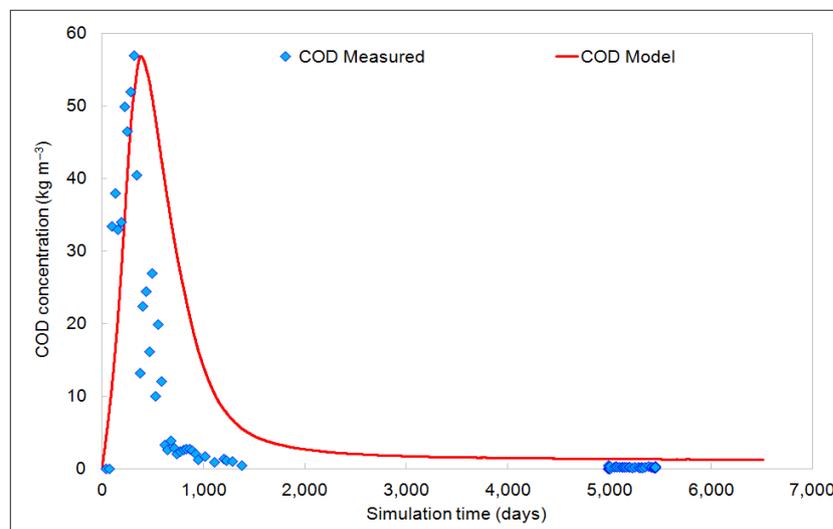
The dramatic increase of the leachate pH value of field–measured data in the early Breitenau landfill operation was evaluated by Döberl et al. (2002). Based on the evaluation results, he concludes that this dramatic increase is caused by the dissolution of  $\text{CaCO}_3$  content in the gravel layers of the top cover and bottom liner. The gravels used for the top cover and bottom liner contain high concentrations of  $\text{CaCO}_3$ . The total  $\text{CaCO}_3$  content in the gravel layers of the top cover and bottom liner were estimated to be about 7,500 tons. This amount is equal to 15 times the  $\text{CaCO}_3$  content in disposed MSW, which is about 500 tons (Döberl et al., 2002).

Figures 5.8 and 5.9 present a comparison of the model calculation and field–measured data of Biological Oxygen Demand (BOD) and Chemical Oxygen Demand (COD) of leachate. These two parameters are commonly used to measure the level of contaminants in water contaminated by organic matter. In general, both figures indicate that the concentrations of BOD and COD of the model calculation have similar trends to the field–measured data. However, the peak of the model calculation result was a bit later than the field–measured data. The reason to judge these differences is that the model is not equipped with a good leachate transport model yet. The leachate transport used in the model is based on the different field

capacity and moisture content in the landfill. Leachate generation from the landfill occurs after the moisture content reaches the field capacity, whilst in reality the leachate flow is also driven by hydrostatic and gravity forces.



**Figure 5.8** Simulated and field measured BOD concentrations discharged leachate of the Breitenau landfill

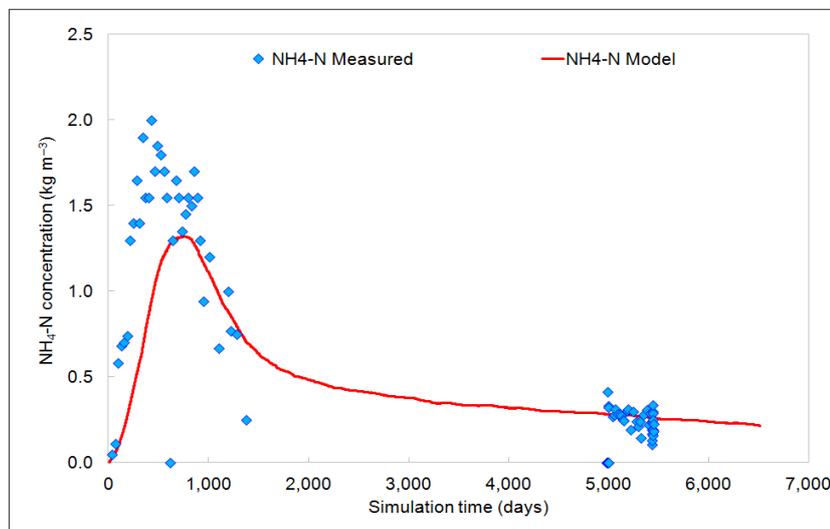


**Figure 5.9** Simulated and field measured COD concentration leachate discharged the Breitenau landfill

Similarly, the peak of ammonium nitrogen ( $\text{NH}_4\text{-N}$ ) concentration of the model calculation is also a bit later than in the field-measured data, which is also due to the aforementioned inappropriate water transport model. In addition, the  $\text{NH}_4\text{-N}$  peak is also bit narrower in the model than in the field-measured data. This difference may be caused by the low nitrogen content in the MSW used in the model compared to

the MSW disposed in the landfill. It is important to note at this point that the protein as the single nitrogen source used in the model is obtained from a literature survey, and not from laboratory analysis results. Since MSW composition is influenced by many factors, for instance economic level, cultural norms, geographical location, energy sources and climate, the protein used in this model may be different to the disposed MSW.

Although the peaks of BOD, COD and  $\text{NH}_4\text{-N}$  concentrations of the field-measured data are not simulated well by the model at the start of the simulation time, the differences between model calculation results and field-measured data are not too big, particularly in view of the lack of data from the Breitenau landfill. Moreover, agreement between the model calculation results and field-measured data increases after the bioreactor landfill period. This indicates that the model can predict the landfill behaviour, particularly in the long run and if the database is sufficient.

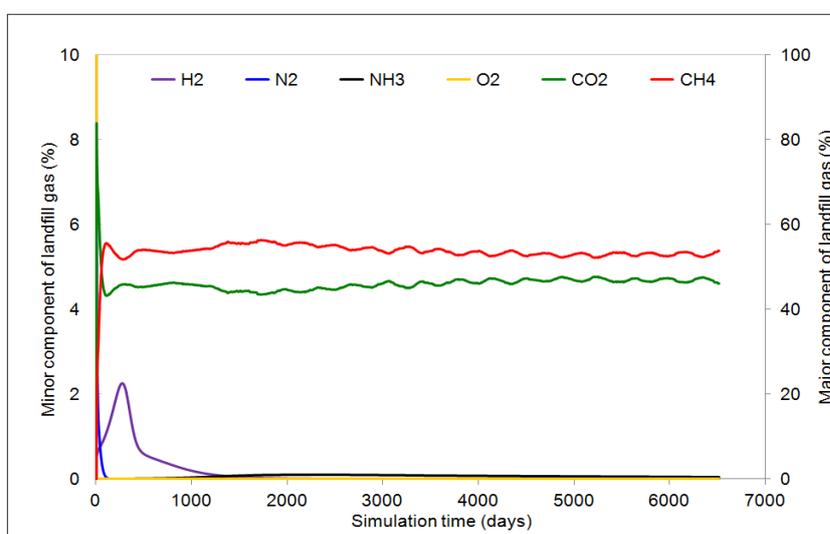


**Figure 5.10** Simulated and field measured  $\text{NH}_4\text{-N}$  concentration leachate discharged of the Breitenau landfill

Figure 5.11 shows the profile of the landfill gas composition of the model simulation. The simulation result shows that  $\text{CH}_4$  and  $\text{CO}_2$  are immediately produced from the beginning of simulation time, but the concentration of  $\text{CH}_4$  is lower than  $\text{CO}_2$  in the early simulation time. This result is closely linked to acidogens and methanogens concentration, where in the early simulation time the

acidogens growth rate is much faster than for methanogens (see Figure 5.6). In addition, a small concentration of  $\text{CO}_2$  is also produced by acidogens from dissolved organic matter degradation. This explains why the  $\text{CO}_2$  is higher in the early degradation of organic matter (El-Fadel et al., 1996b).

$\text{CH}_4$  and  $\text{CO}_2$  are the final products of the organic matter transformation process. They are mainly produced by methanogens of short-chain VFAs (e.g. usually acetic acid) in a similar molar ratio, as parts of  $\text{CO}_2$  together with  $\text{H}_2$  are consumed by hydrogen reducing methanogens to  $\text{CH}_4$ , so that  $\text{CH}_4$  concentration is a bit higher than  $\text{CO}_2$  after the methanogenic phase has been completed (Young, 1989). The  $\text{CH}_4$  concentration in the simulation result is approximately 55% vol. of the total gas released, which is in the range of typical  $\text{CH}_4$  concentration between 40 and 60 % (Reinhart et al., 1992; Kjeldsen et al., 1997; Nastev et al., 2001; Ritzkowski and Stegmann, 2007).

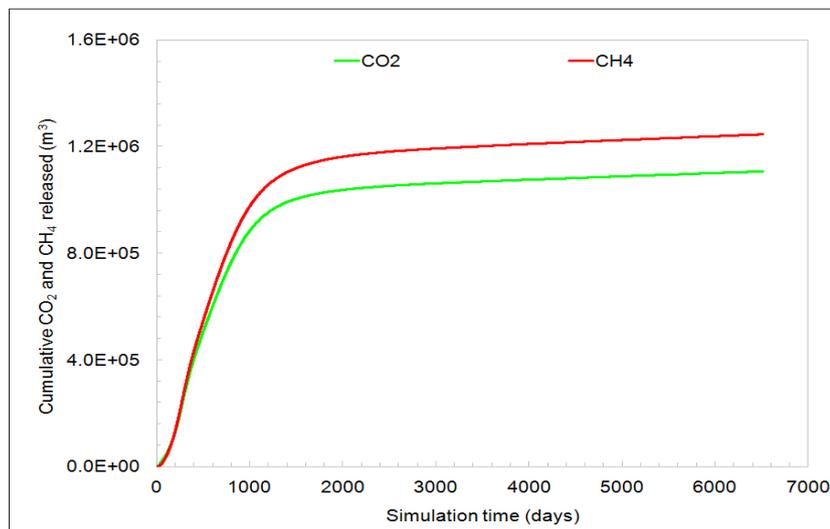


**Figure 5.11** Simulated landfill gas compositions of the Breitenau landfill

Climatic condition will also affect the landfill gas composition, especially in temperate regions. This is mainly due to the microorganism sensitivity to temperature change (see section 4.2.1). As the methanogens are more sensitive to temperature change than acidogens, the  $\text{CO}_2$  concentration increases when the  $\text{CH}_4$  concentration decreases, simply due to this temperature change. This explains why

the concentration of CH<sub>4</sub> and CO<sub>2</sub> fluctuates within the simulation time period. This fluctuation corresponds to seasonal ambient temperature change.

The cumulative CH<sub>4</sub> production is an indicator of landfill performance, meaning its ability to degrade organic matter to a sufficient level in a controlled manner. Thus, these data can be used to estimate the landfill impact on the environment (i.e. greenhouse gas emission) and the remaining CH<sub>4</sub> emission potential. This remaining emission potential can be determined based on the organic matter content of MSW. For example, the potential landfill gas production of each kilogram of cellulose is approximately  $8.29 \times 10^{-3} \text{ m}^3$ , of which 50% is CH<sub>4</sub> (Christensen, 2012).



**Figure 5.12** Simulated cumulative CH<sub>4</sub> and CO<sub>2</sub> released of the Breitenau landfill

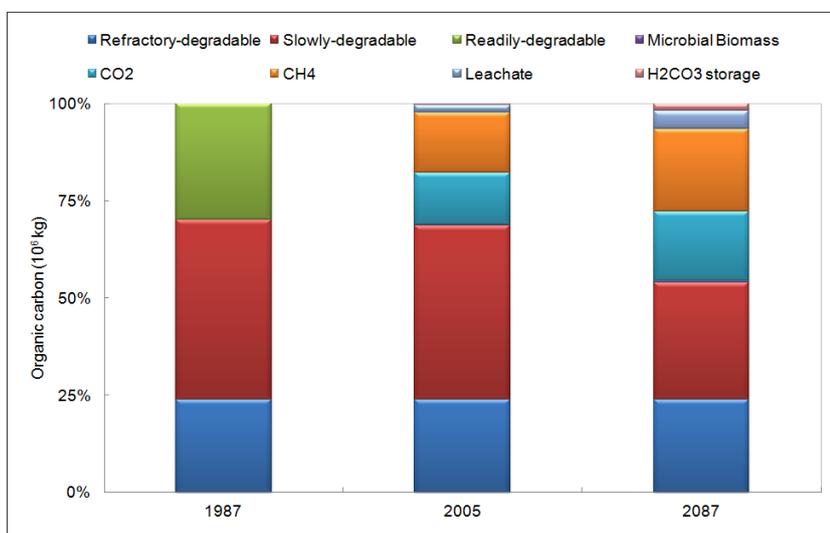
Figure 5.12 shows the cumulative CH<sub>4</sub> and CO<sub>2</sub> production of the model simulation result. The cumulative CH<sub>4</sub> production is lower than the CO<sub>2</sub> production at the beginning of the simulation time. However, it becomes higher due to the steady increase of the methanogens concentration. The peak of CH<sub>4</sub> production occurs between days 1,100 and 1,200, where the maximum methanogens concentration takes place. The CH<sub>4</sub> production is approximately  $258\text{--}322 \text{ m}^3 \text{ day}^{-1}$ . After this period, the CH<sub>4</sub> production and methanogens concentration gradually decrease as the concentration of acetic acid produced from organic matter degradation is not enough to sustain a large methanogenic population (see Figure 5.6). Although the cumulative CH<sub>4</sub> production cannot be validated by field-measured data (i.e. due to

the lack of field-measured data), the cumulative CH<sub>4</sub> production is approximately 1.6 million m<sup>3</sup> is slightly lower compare to the potential CH<sub>4</sub> production of degradation organic matter in Breitenau landfill which is about 1.8 million m<sup>3</sup>. The reason to judging this difference results is that the potential CH<sub>4</sub> production was calculated without taking account organic carbon as organic load in leachate.

The organic carbon of degraded organic matter was calculated by multiplying the amount of degraded organic matter by the ratio of carbon to the molecular weight of organic matter. Thus, the total organic carbon of disposed MSW in the Breitenau landfill is about 5.6 million kg. These amounts consist of 1.7, 2.6 and 1.3 million kg of organic carbon of readily degradable, slowly degradable and refractory organic matter, respectively. From the simulation results, all organic carbon of readily degradable organic matter completely degraded during the first 17 years (i.e. 1987–2005), while only 3.5% of the slowly degradable was degraded and none of the refractory was transformed. Extending the simulation up to 100 years (i.e. 1987–2087) results in further organic carbon degradation of the slowly degradable organic matter for about 0.91 million kg or about 35% of the initial amount. Meanwhile the organic carbon of refractory organic matter still persists in the landfills without any reduction. The persistence of organic carbon of refractory organic matter was also reported by Young and Frazer (1987), who mentioned that the persistence of refractory organic matter due to the recalcitrance of lignite compound under anaerobic conditions.

The mass balance of organic carbon in the Breitenau landfill was drawn based on the cumulative CO<sub>2</sub> and CH<sub>4</sub> released, leachate discharge, and the initial amount of organic carbon of degradable organic matter. The organic carbon of CO<sub>2</sub> and CH<sub>4</sub> was calculated by dividing the cumulative CO<sub>2</sub> and CH<sub>4</sub> by 22.4 (L mole<sup>-1</sup>), and multiplying by the ratio of the atomic mass of carbon to its molecular weight, respectively. The organic carbon discharged as organic load (i.e. acetic, propionic and butyric acids) in leachate was calculated in a similar manner to the organic carbon in the gas phase.

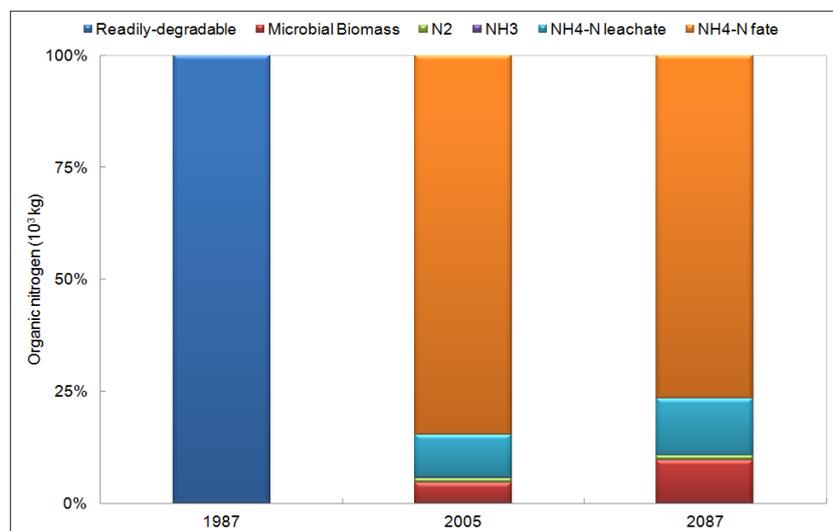
Figure 5.13 shows the mass balance of organic carbon of the Breitenau landfill for 17 and 100 years after the closure of the landfill. By 2005, about 1.7 million kg organic carbon had been degraded and converted to CO<sub>2</sub> (42%), CH<sub>4</sub> (49%), organic carbon load in leachate (6%) and carbon of microbial cell (0.9%). The CH<sub>4</sub> formed is approximately equal to 0.434 m<sup>3</sup> kg<sup>-1</sup> dry solid organic matter. Although this result could not be confirmed by the real condition due to the lack of field-measured data, the CH<sub>4</sub> formed is in the potential methane range of organic matter degradation, which is about 0.373–0.517 m<sup>3</sup> kg<sup>-1</sup> dry organic matter (Barlaz et al., 1989).



**Figure 5.13** Mass balance of simulated organic carbon in the Breitenau landfill

A part of organic carbon is converted to H<sub>2</sub>CO<sub>3</sub>, which is further turned to CaCO<sub>3</sub> when it reacts with Ca<sup>2+</sup> ion, sometimes called “biorock”. The organic carbon of H<sub>2</sub>CO<sub>3</sub> formed accounts for about 1.1% of total degraded organic carbon. The formation of H<sub>2</sub>CO<sub>3</sub> depends on pH, CO<sub>2</sub> partial pressure and ionic strength of the leachate. Moreover, the H<sub>2</sub>CO<sub>3</sub> also acts as a buffer system in the landfill system. When the VFA concentration begins to increase, the H<sub>2</sub>CO<sub>3</sub> will start dissociate to neutralized the pH of landfill through formed bicarbonate ion (McCarty, 1964). Thus, extending the simulation time would result in higher cumulative H<sub>2</sub>CO<sub>3</sub> in landfills as the pH value of landfills is likely to increase. The simulation result of 100 years shows the organic carbon converted to H<sub>2</sub>CO<sub>3</sub> increased to about 3.9% of total degraded organic carbon.

As well as the organic carbon, the nitrogen balance was also calculated. Readily degradable organic matter is the sole nitrogen source of MSW composition used in this model. The initial amount nitrogen was calculated by multiplying the ratio of the atomic mass of nitrogen by the molecular weight of readily degradable organic matter, thus the initial amount of nitrogen was about 61,000 kg. Similarly to organic carbon, the nitrogen leaving the landfill was calculated by multiplying the nitrogen concentration by the flow rate of LFG released and leachate discharged, then multiplying by the ratio of the atomic mass of nitrogen to the molecular weight of the nitrogen compound.



**Figure 5.14** Mass balance of simulated organic nitrogen in the Breitenau landfill

Figure 5.14 shows the mass balance of the simulated nitrogen transformation in the Breitenau landfill. The simulation result shows all nitrogen of readily organic matter has been degraded and converted mainly to NH<sub>3</sub> and utilized as a nitrogen source for new microbial cells. NH<sub>3</sub> could escape from the landfill through either being vaporized or released as LFG or being dissolved in water and discharged as leachate. The simulation results for the year 2005 show about 9.7% of 61,000 kg of degraded nitrogen is dissolved in water and leaves with discharged leachate. This result is confirmed by field-measured data (see Figure 5.10), while 4.6% of degraded nitrogen is utilized as microbial cell nitrogen and about 85% is absorbed by solid waste and remains inside the landfill as fate of nitrogen. These results are reliable

since ammonium is known to be adsorbed easily into various solid organic and inorganic compounds (Nielsen, 1996). The fate of nitrogen concentration is that about 3,380 mg kg<sup>-1</sup> dry remains solid waste. This concentration was slightly lower than the total nitrogen concentration of 15 years' deposited MSW reported by Liao et al. (2013).

The fate of nitrogen can be used as a nitrogen source for other processes such as nitrification before being vaporized as ammonia in landfill gas or slowly dissolved into the water flows within the waste body and discharged as leachate (Heavey, 2003). The NH<sub>4</sub>-N discharge from MSW landfills depends on the water infiltration rate. However, an NH<sub>4</sub>-N concentration change with water infiltration from 140 to 500 mg L<sup>-1</sup> has been observed in the reinstallation of the top cover of the Breitenau landfill (Laner et al., 2011). Extending further simulation for 100 years will result in decreasing the fate of nitrogen in the landfill. By 2087, the fate of nitrogen in the Breitenau landfill will be about 3,350 mg kg<sup>-1</sup> dry weight remaining solid waste.

## **Chapter 6**

### **Conclusion and Recommendation**

The main achievement of this thesis is the development of a numerical model to predict the mass loss of organic matter over time in MSW landfills. The model is based on the coupling of a packed bed reactor (PBR) with a batch reactor concept, and depicts the behaviour of carbon in gaseous, liquid and solid phases in MSW landfills. The model incorporates biological and chemical reactions to simulate the degradation of organic matter under dynamic landfill conditions; in addition, change of internal temperature and pH due to landfill degradation processes, as well as ambient climatic conditions, were included in the model.

The organic fraction of MSW is divided into three categories according to the degradability level (i.e. readily degradable, slowly degradable and refractory– or non–degradable organic matter). The degradation is modeled both parallel and sequentially in three stages. A set of chemical reactions and ordinary differential equations based on the Monod and Contois kinetic substrate utilization concepts was applied. The solid organic matter is broken down by acidogens and converted into short– and long–chain VFAs. Long–chain VFAs are broken down subsequently by acetogens to short–chain VFAs. Once the short chain VFAs are available, the methanogens grow, and CH<sub>4</sub> and CO<sub>2</sub> as the final form of organic matter mineralization are generated.

The model was validated by using landfill simulation reactor (LSR) data. In addition, several simulations were performed to assess the influence of changing landfill conditions (e.g. temperature, pH and leachate recirculation) on microorganism growth as well as on organic matter mineralization rates. Finally, the model was applied to predict the remaining organic matter in the Breitenau landfill, a full–scale MSW landfill situated in Lower Austria, taking into account actual climatic conditions.

## 6.1 Conclusion

Based on the validation, sensitivity analysis and application exercises, the main conclusion of this study is that the model developed based on the coupling of PBR and the batch reactor concept performs well in predicting the degradation of organic matter in MSW landfills. Also, the calculations of landfill gas and leachate emissions of a field-scale MSW landfill were within expected ranges. The classification of organic matter into three categories appeared to be appropriate for representing the heterogeneous organic fraction of MSW. Additionally, the following four conclusions can be drawn.

1. The model validation using the laboratory landfill simulation reactor data provides the information that at least one key parameter exists; this can be used as a reference to define how the model calculation fits to the measured data. This is important since often only a few parameters of landfill emissions from real landfill sites are measured and well documented.
2. The sensitivity analysis shows that within the observed ranges, the temperature change has a greater influence than the pH value and leachate recirculation on the degradation of organic matter. This has never been documented before. Thus, it is important when applying the model for predicting organic matter degradation to take into account the ambient temperature, particularly in temperate regions where the temperature varies widely between seasons. Although the change of pH and leachate recirculation has a much smaller effect than temperature, their influence on the landfill gas and leachate composition is still significant. This is mainly due to the sensitive response of to these parameters.
3. The application of the model to the Breitenau landfill in Austria shows that about 2.9 million kg of a total of 9.3 million kg of degradable organic matter has been degraded within the 17 years since the landfill has been closed. About 94% of degraded organic matter is readily degradable organic matter that degraded in the bioreactor phase and the rest was slowly degradable organic matter, while the refractory organic matter has not degraded.

4. The high concentration of readily degradable organic matter in MSW results in high landfill gas production and DOC loadings in the leachate within the bioreactor phase, and correspondingly lower levels during the aftercare period. During this time period, landfill gas production and organic loads in leachate are low, but the slow degradation rate of organic matter is responsible for the very long post-closure maintenance period.

## 6.2 Recommendations for Future Work

Although the model developed in the present work fitted well with laboratory simulation reactor data and achieved satisfying results when applied to the Breitenau landfill, some expansions are still required to improve the model calculation results as well as the model validation work. Therefore, future work should focus on the following points:

1. The water transport used in this model does not take into account hydrostatic and gravity forces. Hence, the leachate will discharge after the moisture content reaches the field capacity. This assumption would work properly for fully saturated landfills and laboratory simulation reactors, but at the real landfill such a condition can hardly be reached. Therefore, an improved water transport tool should be integrated into the model.
2. Although the biological reaction of organic matter applied in this model is quite dynamic and depends on various parameters (i.e. temperature, pH and leachate recirculation), other factors such as Henry's constant for CO<sub>2</sub> and NH<sub>3</sub>, acids and base dissociation constants, as well as heat conductivity, were held constant at standard values. In fact, these constants are also influenced by temperature changes. It should be tested whether redefining these constants by taking into account the temperature effect can improve the model calculation accuracy or not.
3. The model was validated using a data set of laboratory experimental results (e.g. pH, VFA concentration in leachate, and cumulative CH<sub>4</sub> and CO<sub>2</sub>).

However, the accuracy of these data appeared to be low, particularly regarding cumulative CH<sub>4</sub> and CO<sub>2</sub> generation. Model validation using more accurate experimental data would improve the evaluation and facilitate the optimization of the model.

4. The model application to predict the fate of organic matter and landfill emissions of the Breitenau landfill results in interesting findings that are not covered by the model calculation, but influence the outcomes. For instance, the gravel layers used for the leachate drainage contain a high concentration of CaCO<sub>3</sub>. This CaCO<sub>3</sub> is dissolved when in contact with the low pH value of leachate. This condition results in an increase in the pH value of measured leachate at the beginning of the landfill operation. Future work should pay attention to covering site-specific issues like this.
5. This study shows the crucial influence of the energy balance on the degradation of organic matter in landfills. According to the sensitivity analysis, landfill temperature is more important than leachate recirculation. This result should be further confirmed by (i) combining energy balances of landfills with this model, and (ii) looking into larger ranges of leachate recirculation including nearly “dry” landfills.

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# Appendix A

## Source Code

### Module I: Main Program

```
#include "Cell.h"
double t; // Start calculation time
double dt; // Differential calculation time
double t_end; // End calculation time
double prt_dt; // Interval printout calculation results

char fininame[30], fout1name[30], fout2name[30], fout3name[30];

Global_const CP; // Global constants
Atmospheric_cond atm; // Atmosphere condition
Circumference_media LayM[7];
Heat_param HP; // Heat transfer parameters
Environment_cond env; // Environment condition

Cell * c;

#include <time.h>
clock_t cl_st, cl_lap;
void dbg_start_timer() {
    cl_st = clock();
}

void dbg_end_timer() {
    cout << "Elapsed time: " << (clock() - cl_st) * 1000/CLOCKS_PER_SEC << "msec." <<
endl;
}

int main(void){
int tcount;
double pt;
double tt[8], dti[8], prt_dti[8];
char Landfillname[30], Filename[30];
int days;

// Make output files
cout << "Enter name of Landfill site: ";
cin >> Landfillname;
dbg_start_timer();
strncpy(Filename, Landfillname, sizeof(Filename));
strncpy(fininame, Landfillname, sizeof(fininame));strcat(fininame, "_in.dat");
strncpy(fout1name, Landfillname, sizeof(fout1name));strcat(fout1name, "_out.dat");
strncpy(fout2name, Landfillname, sizeof(fout2name));strcat(fout2name, "_total.dat");
strncpy(fout3name, Landfillname,
sizeof(fout3name));strcat(fout3name, "_leachate.dat");

// Creation of Cell
c = new Cell[1]; // Creation of a Cell object

// Setting calculation time
Cal_time_condition_set(t,dt,t_end,pt,prt_dt,tt,dti,prt_dti);

// Reading parameters from text file
Environment_cond_load(); // Environment condition

// Setting initial condition
c[0].RESET_reaction_Rate(); // Initialization of reaction rate
Cell_circumference_cond_set(); // Setting of the surroundings of Cell
```

```

// Initialization of file
Constoutput(c[0]); // Writing constants & parameters to txt
FoutputHeader(); // Writing out headers to each text file
// Mass balance at t=0
c[0].Massbalance_check(); // Initial check of mass balance

// Print out the results at t=0
Foutput1(c[0]);
Foutput2(c[0]);

//-----
// Start time step calculation
//-----
t = 0;
tcount = 1;
dt = dti[tcount];
prt_dt = prt_dti[tcount];
pt = prt_dt;
days = (int)t;
atm.T = env.Tair[0];
c[0].QLin= env.QRain[0]/1000 * c[0].S;

t_end = env.num_of_days;

while(t < t_end){
  if(t > tt[tcount]){
    tcount= tcount + 1;
    dt = dti[tcount];
    prt_dt= prt_dti[tcount];
  }
  if((int)t >= days + 1){
    days = (int)t;
    atm.T = env.Tair[days];
    c[0].QLin= env.QRain[days]/1000 * c[0].S;
  }

  // Calculation PT and QGout
  c[0].cal_PT();
  c[0].cal_QGout();

  // Starting simulation
  t = t + dt;

  // Calculation of reaction rate
  Cell_reaction_rate(c[0]);

  // Calculation amount of leachate discharged (QLout)
  c[0].cal_QLout();

  // Calculation of TIC, T_NH3, NO3, CH3COOH_T, Ca_plus and Na_plus
  c[0].cal_TIC_step(); // Calculate d[TIC]/dt by Euler's method
  c[0].cal_T_NH3_step(); // Calculate d[TNH3]/dt by Euler's method
  c[0].cal_NO3_step(); // Calculate d[NO3]/dt by Euler's method
  c[0].cal_CH3COOH_T_step(); // Calculate d[CH3COOH_T]/dt by Euler's method
  c[0].cal_CH3CH2COOH_T_step(); // Calculate d[CH3CH2COOH_T]/dt by Euler's method
  c[0].cal_CH3CH2CH2COOH_T_step(); // Calculate d[CH3(CH2)2COOH_T]/dt by Euler's
  method

  c[0].cal_Ca_step(); // Calculate d[Ca]/dt by Euler's method
  c[0].cal_Na_step(); // Calculate d[Na+]/dt by Euler's method
  c[0].cal_Cl_step(); // Calculate d[Cl-]/dt by Euler's method

  // Calculation new pH
  c[0].pH_calculation(); // pH calculation

  // Calculation of S_PRO, S_FAT, S_GLU, S_CEL, ORG_T, and MX
  c[0].cal_SPRO_step(); // Calculate d[S_ORG]/dt by Euler's method
  c[0].cal_SFAT_step(); // Calculate d[S_FAT]/dt by Euler's method
  c[0].cal_SGLU_step(); // Calculate d[S_GLU]/dt by Euler's method
  c[0].cal_SCEL_step(); // Calculate d[S_CEL]/dt by Euler's method
  c[0].cal_SLIG_step(); // Calculate d[S_LIG]/dt by Euler's method
  c[0].cal_X_step(); // Calculate d[X_i]/dt by Euler's method

```

## Edi Munawar

```

c[0].cal_ORG_T_step(); // Calculate total organic substances in a Cell
c[0].cal_H_step(); // Calculate d[H]/dt by Euler's method

// Calculation amount of constituents after equilibrium condition
c[0].cal_IC(); // Inorganic carbon in liquid [IC]
c[0].cal_CH3COOH(); // Acetic acid [CH3COOH]
c[0].cal_CH3COO(); // Acetate ion [CH3COO]
c[0].cal_CH3CH2COOH(); // Propionic acid [CH3CH2COOH]
c[0].cal_CH3CH2COO(); // Propionate ion [CH3CH2COO]
c[0].cal_CH3CH2CH2COOH(); // Butyric acid [CH3CH2CH2COOH]
c[0].cal_CH3CH2CH2COO(); // Butyric acid [CH3CH2CH2COO]
c[0].cal_COD(); // Chemical Organic Demand [COD]

c[0].cal_NH3_T(); // Total Ammonia in liquid phase [NH3]T
c[0].cal_NH3(); // Ammonia concentration [NH3]
c[0].cal_NH4(); // Ammonium ion concentration [NH4]
c[0].cal_PNH3(); // Partial pressure NH3 [P_NH3]
c[0].cal_NH4_Adsorp_inCell(); // Ammonia Adsorbed on solid [NH4_abs]

// Calculation of gas components PCO2, PCH4, PH2, PN2, PNH3, PO2, and water vapor
c[0].cal_PCH4_step(); // Calculate d[P_CH4]/dt by Euler's method
c[0].cal_PH2_step(); // Calculate d[P_H2]/dt by Euler's method
c[0].cal_PN2_step(); // Calculate d[P_N2]/dt by Euler's method
c[0].cal_PO2_step(); // Calculate d[P_O2]/dt by Euler's method
c[0].cal_PH2O_step(); // Calculate d[P_H2O]/dt by Euler's method

// Calculation Accumulated amount of landfill gas constituents
c[0].cal_Acu_QGout(); // Accumulated amount of QGout
c[0].cal_Acu_CO2(); // Accumulated amount of CO2 gas [CO2]
c[0].cal_Acu_CH4(); // Accumulated amount of CH4 gas [CH4]
c[0].cal_Acu_H2(); // Accumulated amount of H2 gas [H2]
c[0].cal_Acu_N2(); // Accumulated amount of N2 gas [N2]
c[0].cal_Acu_PNH3(); // Accumulated amount of NH3 gas [PNH3]
c[0].cal_Acu_O2(); // Accumulated amount of O2 gas [O2]

// Calculation Accumulated amount of leachate constituents
c[0].cal_Acu_QLout(); // Accumulated amount of QLout
c[0].cal_Acu_CH3COOH(); // Accumulated amount of Acetic acid [CH3COOH]
c[0].cal_Acu_CH3CH2COOH(); // Accumulated amount of Propionic acid
[CH3CH2COOH]
c[0].cal_Acu_CH3CH2CH2COOH(); // Accumulated amount of Butyric acid
[CH3(CH2)2COOH]
c[0].cal_Acu_IC(); // Accumulated amount of Total Inorganic Carbon
[IC]
c[0].cal_Acu_NH3(); // Accumulated amount of Ammonia ion [NH4]
c[0].cal_Acu_NO3(); // Accumulated amount of Nitrate [NO3]
c[0].cal_Acu_Caout(); // Accumulated amount of Calcium ion [Ca_plus]

// Calculation of other parameter such as BOD, TOC, and T-N
Other_param_cal(c[0]);

// Check-out of mass balance
c[0].Massbalance_check(); // Mass balance after dt calculation step

// Print out the results-----
if(t >= pt){
printf("t:%5.0f pH:%5.2f Ca2+:%.3e TCa:%.3e H2CO3_T:%.3e CO2:%.3e H2CO3T_out:
%.3e\n",t, c[0].pH, c[0].Ca_plus, c[0].TCa, c[0].H2CO3_T, c[0].P_CO2,
(c[0].xi()*c[0].QLout*c[0].H2CO3_T));

Foutput1(c[0]);
Foutput2(c[0]);

pt = pt + prt_dt;
}
}
cout << "fin!!!!!" << endl;
delete [] c;
Output_file_close();
dbg_end_timer();
return 0;
}

```

## Module II: Program Header

```

#define _CRT_SECURE_NO_WARNINGS
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <iostream>
#include <fstream>
#include <assert.h>
#define PI 3.141592

using namespace std;

enum
RCONST{mOP,mOF,mOG,mOS,mOH,mNP,mNF,mNG,mNS,mNH,mAP,mAB,mMT,mMT2,kAO,kPO,kBO,kNO,kDN};
enum OUTPUT{toFILE,toCON,toBOTH};
enum mediatp{air,waste,cover,soil,grav,none};

#####
#####
// Declaring variables related to the global constants such as gas constant, Henry
// constant, etc. Setting global constants values are conducted in Constructor.cpp
#####
#####
class Global_const{
public:

// -----
// Parameter declaration
// -----
double R;           // Gas constant           [m3*Pa/kmol*K]
double Henry_CO2;  // CO2 Henry constant       [Pa*m3/kmol]
double Henry_NH3;  // NH3 Henry constant       [Pa*m3/kmol]
double Kd_HCO3;    // Bicarbonate acid dissociation constant [kmol/m3]
double Kd_H2CO3;   // Carbonic acid dissociation constant [kmol/m3]
double Kd_NH3;     // NH3 dissociation constant [kmol/m3]
double Kd_C2H4O2;  // Acetic acid dissociation constant [kmol/m3]
double Kd_C3H6O2;  // Propionic acid dissociation constant [kmol/m3]
double Kd_C4H8O2;  // Butyric acid dissociation constant [kmol/m3]
double Ksp_CaCO3;  // Solubility of Calcium Carbonate [kmol/m3]
double Kp_NH3;     // Distribution Coefficient of NH3 [m3/kg]
Global_const();   // Constructor is necessary to initialize these group
                  // parameters
};

#####
#####
// Declaring variables related to atmosphere condition such as temperature, pressure,
// and partial pressure. Setting value of atmosphere condition are in [atm_cond.txt]
#####
#####
class Atmospheric_cond{
public:
double T;           // Atmospheric temperature [K]
double P;           // Atmospheric Pressure [Pa]
double P_CO2;       // Partial Pressure of CO2 in air [Pa]
double P_CH4;       // Partial Pressure of CH4 gas in air [Pa]
double P_H2;        // Partial Pressure of H2 gas in air [Pa]

```

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double P_N2;           // Partial Pressure of N2 gas in air           [Pa]
double P_NH3;         // Partial Pressure of NH3 gas in air          [Pa]
double P_O2;          // Partial Pressure of O2 gas in air           [Pa]
Atmospheric_cond();  // Constructor is necessary to initialize these group
                    // parameters
};

#####
#####
// Declaring variables related to change environment condition such as daily mean
// in [Environment_cond.txt]
#####
#####
class Environment_cond{
public:
int num_of_days;
double Tair[100000]; // Atmospheric temperature           [k]
double QRain[100000]; // Water precipitation                [mm/d]
double QGair[100000]; // Aeration rate                       [m3/d]
Environment_cond(); // Constructor i it's necessary to initialize these
                    // parameters group j
};

#####
#####
// Declaring constants and variables relate to landfill cell such as dimension,
// biodegradation process and its product, etc. Setting value of constants and
// variables are in [Initial_cond.txt] and [reaction_param.txt]
#####
#####
class Cell{
public:
// -----
// Fraction of each phase
// -----
double eL;           // Liquid phase ratio                [m3/m3]
double eS;           // Solid phase ratio                 [m3/m3]
double eG;           // Gas phase ratio                   [m3/m3]
double wcp;          // Field capacity of Cell            [-]

// -----
// Density, Dimension and volume of a landfill Cell
// -----
double H;            // Height of Cell                    [m]
double D;            // Diameter of Cell                  [m]
double S;            // Surface area of Cell              [m2]
double V;            // Volume of Cell                    [m3]
double V_L;          // Volume of liquid phase            [m3]
double V_G;          // Volume of Gas phase               [m3]
double V_S;          // Volume of Solid phase             [m3]
double wc;           // Water content of Cell             [-]
double r_sld;        // Specific weight of solid          [kg/m3-solid]
double r_dry;        // Dry density of Cell               [kg/m3]
double r_wet;        // Wet density of Cell               [kg/m3]

// -----
// Inflow, outflow, and washing-out relationship
// -----
double QLin;         // Water infiltration rate            [mm/d]

```

---

---

```

double QLOut;           // Leachate discharge rate           [mm/d]
double xi0;            // Washout rate (initial)           [-]
double xlmd;          // Washout Acceleration factor       [1/d]
double txi;           // Time constant of wash out         [d]
double QGout;         // Landfill gas discharge from Cell  [kmol/d]
double R_ratio;       // Recycling rate of discharge leachate [-]
double QGin;          // Aeration rate                     [kmol/d]

// -----
// Initial temperature and pressure within Cell
// -----
double Temp;          // Temperature within Cell           [K]
double PT;            // Total Gas Pressure in Cell         [Pa]
double P_CO2;         // Partial Pressure of CO2 in Cell    [Pa]
double P_CH4;         // Partial Pressure of CH4 in Cell    [Pa]
double P_H2;          // Partial Pressure of H2 in Cell     [Pa]
double P_N2;          // Partial Pressure of N2 in Cell     [Pa]
double P_NH3;         // Partial Pressure of NH3 in Cell    [Pa]
double P_O2;          // Partial Pressure of O2 gas within Cell [Pa]
double P_H2O;         // Partial Pressure of water vapor in Cell [Pa]

// -----
// Chemical formula & Molecular Weight of Protein CaHbOcNn
// -----
double S_PRO;         // Protein                           [kg/m3]
double Pro_a;         // Number of atom Carbon in Protein formula [-]
double Pro_b;         // Number of atom H2 in Protein formula [-]
double Pro_c;         // Number of atom O2 in Protein formula [-]
double Pro_n;         // Number of atom N2 in Protein formula [-]
double M_PRO;         // Molecular Weight of Protein        [kg/kmol]

// -----
// Chemical formula & Molecular Weight of Fats CaHbOc
// -----
double S_FAT;         // Fats                               [kg/m3]
double Fat_a;         // Number of atom H2 in Fats formula  [-]
double Fat_b;         // Number of atom O2 in Fats formula  [-]
double Fat_c;         // Number of atom N2 in Fats formula  [-]
double M_FAT;         // Molecular Weight of Fats           [kg/kmol]

// -----
// Chemical formula & Molecular Weight of Carbohydrate (C6H10O5)n, n<=1
// -----
double S_GLU;         // Carbohydrate                       [kg/m3]
double Glu_a;         // Number of atom H2 in Carbohydrate formula [-]
double Glu_b;         // Number of atom O2 in Carbohydrate formula [-]
double Glu_c;         // Number of atom N2 in Carbohydrate formula [-]
double Glu_n;         // Number of repetition in chemical formula [-]
double M_GLU;         // Molecular Weight of Carbohydrate formula [kg/kmol]

// -----
// Chemical formula & Molecular Weight of Cellulose (C6H10O5)n, n=>3
// -----
double S_CEL;         // Cellulose                           [kg/m3]
double Cel_a;         // Number of atom H2 in Cellulose formula [-]
double Cel_b;         // Number of atom O2 in Cellulose formula [-]
double Cel_c;         // Number of atom N2 in Cellulose formula [-]
double Cel_n;         // Number of repetition in chemical formula [-]
double M_CEL;         // Molecular Weight of Cellulose formula [kg/kmol]

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// -----
// Chemical formula & Molecular Weight of Lignin (C10H12O3)
// -----
double S_LIG;           // Lignin [kg/m3]
double Lig_a;          // Number of atom H2 in Lignin formula [-]
double Lig_b;          // Number of atom O2 in Lignin formula [-]
double Lig_c;          // Number of atom N2 in Lignin formula [-]
double M_LIG;          // Molecular Weight of Lignin [kg/kmol]

// -----
// Fraction In-organic matter
// -----
double S_INO;          // In-organic matter [kg/m3]

// -----
// Concentrations in liquid
// -----
double pH;             // pH [-]
double H_plus;         // H2 ion concentration [kmol/m3]
double OH_min;         // H2Oxide ion concentration [kmol/m3]
double TIC;            // Total Inorganic Carbonate including CO2 gas [kmol/m3]
double H2CO3_T;        // Total Carbonate Acid [kmol/m3]
double H2CO3;          // Carbonic Acid concentration [kmol/m3]
double HCO3;           // Bicarbonate ion concentration [kmol/m3]
double CO3;            // Carbonate ion concentration [kmol/m3]
double T_NH3;          // Total NH3 N2 including NH3 gas [kmol/m3]
double NH3_T;          // Total NH3 [kmol/m3]
double NH3;            // NH3 concentration [kmol/m3]
double NH4;            // Ammonium ion concentration [kmol/m3]
double NH4_abs;        // NH3 Absorbed on solid [kmol/m3]
double C2H4O2_T;       // Total Acetic Acid [kmol/m3]
double C2H4O2;         // Acetic Acid concentration [kmol/m3]
double CH3COO;         // Acetate ion concentration [kmol/m3]
double C3H6O2_T;       // Total Propionic acid [kmol/m3]
double C3H6O2;         // Propionic acid concentration [kmol/m3]
double CH3CH2COO;      // Propionate ion concentration [kmol/m3]
double C4H8O2_T;       // Total Butyric acid [kmol/m3]
double C4H8O2;         // Butyric acid concentration [kmol/m3]
double CH3CH2CH2COO;   // Butyrate ion concentration [kmol/m3]
double NaCl;           // Sodium Chloride in solid [kmol/kg]
double Na_plus;        // Alkali ions [kmol/m3]
double Cl_min;         // Chlorine ion [kmol/m3]
double NO3;            // Nitrate ion concentration [kmol/m3]
double Ca_plus;        // Calcium ion concentration [kmol/m3]
double CaCO3;          // Calcium Carbonate in solid [kmol/kg]
double TCa;            // Total Calcium in Cell [kmol/m3]
double TOC;            // TOC in leachate [mg-C/L]
double BOD;            // Biological Organic Carbon in leachate [mg-O2/L]
double COD;            // Chemical Organic Carbon in leachate [mg-O2/L]
double IC;             // Inorganic carbon in liquid [mg-C/L]
double TN;             // Total N2 [mg-N/L]
double HUMUS;          // Humus (degradable organic component of COD) [kmol/m3]

// -----
// Fraction in solid phase [kg-C/kg-s]
// -----
double FOC;

```

---

```

// -----
// Reaction rate for the decomposition of organic matter
// -----
// OP Aerobic decomposition of Protein [kmol/m3-d]
double R_X_OP;           // OP : Net Biomass growth rate
double R_PRO_OP;        //   : Protein organic substances consumption rate
double R_O2_OP;         //   : O2 consumption rate
double R_CO2_OP;        //   : CO2 generation rate
double R_NH3_OP;        //   : NH3 generation rate
double R_H2O_OP;        //   : Water generation rate
double R_C2H4O2_OP;     //   : Acetic acid generation rate
double R_H2_OP;         //   : H2 generation rate
// OF Aerobic decomposition of Fats [kmol/m3-d]
double R_X_OF;           // OF : Net Biomass growth rate
double R_FAT_OF;        //   : Fats consumption rate
double R_O2_OF;         //   : O2 consumption rate
double R_CO2_OF;        //   : CO2 generation rate
double R_NH3_OF;        //   : NH3 generation rate
double R_H2O_OF;        //   : Water generation rate
double R_C2H4O2_OF;     //   : Acetic acid generation rate
double R_H2_OF;         //   : H2 generation rate
// OG Aerobic decomposition of Carbohydrate [kmol/m3-d]
double R_X_OG;           // OG : Net Biomass growth rate
double R_GLU_OG;        //   : Carbohydrate consumption rate
double R_O2_OG;         //   : O2 consumption rate
double R_CO2_OG;        //   : CO2 generation rate
double R_NH3_OG;        //   : NH3 generation rate
double R_H2O_OG;        //   : Water generation rate
double R_C2H4O2_OG;     //   : Acetic acid generation rate
double R_H2_OG;         //   : H2 generation rate
// OS Aerobic decomposition of Cellulose [kmol/m3-d]
double R_X_OS;           // OS : Net Biomass growth rate
double R_CEL_OS;        //   : Cellulose organic substances consumption rate
double R_O2_OS;         //   : O2 consumption rate
double R_CO2_OS;        //   : CO2 generation rate
double R_NH3_OS;        //   : NH3 generation rate
double R_H2O_OS;        //   : Water generation rate
double R_C2H4O2_OS;     //   : Acetic acid generation rate
double R_H2_OS;         //   : H2 generation rate
// OH Aerobic decomposition of Lignin [kmol/m3-d]
double R_X_OH;           // OH : Net Biomass growth rate
double R_LIG_OH;        //   : Lignin organic substances consumption rate
double R_O2_OH;         //   : O2 consumption rate
double R_CO2_OH;        //   : CO2 generation rate
double R_NH3_OH;        //   : NH3 generation rate
double R_H2O_OH;        //   : Water generation rate
double R_C2H4O2_OH;     //   : Acetic acid generation rate
double R_H2_OH;         //   : H2 generation rate
// NP Anaerobic fermentation of Protein [kmol/m3-d]
double R_X_NP;           // NP : Net Biomass growth rate
double R_PRO_NP;        //   : Protein organic substances consumption rate
double R_H2O_NP;        //   : Water generation rate
double R_C2H4O2_NP;     //   : Acetic acid generation rate
double R_C3H6O2_NP;     //   : Propionic acid generation rate
double R_C4H8O2_NP;     //   : Butyric acid generation rate
double R_CO2_NP;        //   : CO2 generation rate
double R_H2_NP;         //   : H2 generation rate
double R_NH3_NP;        //   : NH3 generation rate
double R_O2_NP;         //   : O2 generation rate
// NF Anaerobic fermentation of Fats [kmol/m3-d]
double R_X_NF;           // NF : Net Biomass growth rate
double R_FAT_NF;        //   : Fats organic substances consumption rate

```

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```

double R_C2H4O2_NF;      //      : Acetic acid generation rate
double R_CO2_NF;        //      : CO2 generation rate
double R_H2_NF;         //      : H2 generation rate
double R_NH3_NF;        //      : NH3 generation rate
double R_H2O_NF;        //      : Water generation rate
double R_O2_NF;         //      : O2 generation rate
// NG Anaerobic fermentation of Carbohydrate [kmol/m3-d]
double R_X_NG;          // NG  : Net Biomass growth rate
double R_GLU_NG;        //      : Carbohydrate organic substances consumption rate
double R_C2H4O2_NG;     //      : Acetic acid generation rate
double R_CO2_NG;        //      : CO2 generation rate
double R_H2_NG;         //      : H2 generation rate
double R_NH3_NG;        //      : NH3 generation rate
double R_H2O_NG;        //      : Water generation rate
double R_O2_NG;         //      : O2 generation rate
// NS Anaerobic fermentation of Cellulose [kmol/m3-d]
double R_X_NS;          // NS  : Net Biomass growth rate
double R_CEL_NS;        //      : Cellulose consumption rate
double R_C2H4O2_NS;     //      : Acetic acid generation rate
double R_CO2_NS;        //      : CO2 generation rate
double R_NH3_NS;        //      : NH3 generation rate
double R_H2O_NS;        //      : Water generation rate
double R_H2_NS;         //      : H2 generation rate
double R_O2_NS;         //      : O2 generation rate
// NH Anaerobic fermentation of Lignin [kmol/m3-d]
double R_X_NH;          // NH  : Net Biomass growth rate
double R_LIG_NH;        //      : Lignin consumption rate
double R_C2H4O2_NH;     //      : Acetic acid generation rate
double R_CO2_NH;        //      : CO2 generation rate
double R_NH3_NH;        //      : NH3 generation rate
double R_H2O_NH;        //      : Water generation rate
double R_H2_NH;         //      : H2 generation rate
double R_O2_NH;         //      : O2 generation rate
// AP Acetogenesis of Propionic acid [kmol/m3-d]
double R_X_AP;          // AP  : Net Biomass growth rate
double R_C3H6O2_AP;     //      : Propionic acid consumption rate
double R_C2H4O2_AP;     //      : Acetic acid generation rate
double R_CO2_AP;        //      : CO2 generation rate
double R_NH3_AP;        //      : NH3 generation rate
double R_H2O_AP;        //      : Water generation rate
double R_H2_AP;         //      : H2 generation rate
double R_O2_AP;         //      : O2 generation rate
// AB Acetogenesis of Butyric acid [kmol/m3-d]
double R_X_AB;          // AB  : Net Biomass growth rate
double R_C4H8O2_AB;     //      : Butyric acid consumption rate
double R_C2H4O2_AB;     //      : Acetic acid generation rate
double R_CO2_AB;        //      : CO2 generation rate
double R_NH3_AB;        //      : NH3 generation rate
double R_H2O_AB;        //      : Water generation rate
double R_H2_AB;         //      : H2 generation rate
double R_O2_AB;         //      : O2 generation rate
// MT CH4 formation from Acetic acid [kmol/m3-d]
double R_X_MT;          // MT  : Net Biomass growth rate
double R_C2H4O2_MT;     //      : Acetic acid consumption rate
double R_CH4_MT;        //      : CH4 generation rate
double R_CO2_MT;        //      : CO2 generation rate
double R_NH3_MT;        //      : NH3 generation rate
double R_H2O_MT;        //      : Water generation rate
double R_H2_MT;         //      : H2 generation rate
double R_O2_MT;         //      : O2 generation rate

```

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```

// MT2 CH4 formation from CO2+H2 [kmol/m3-d]
double R_X_MT2;           // MT2 : Net Biomass growth rate
double R_C2H4O2_MT2;     //      : Acetic acid consumption rate
double R_CH4_MT2;        //      : CH4 generation rate
double R_CO2_MT2;        //      : CO2 generation rate
double R_NH3_MT2;        //      : NH3 generation rate
double R_H2O_MT2;        //      : Water generation rate
double R_H2_MT2;         //      : H2 consumption rate
double R_O2_MT2;         //      : O2 generation rate
// AO Aerobic oxidation of Acetic acid [kmol/m3-d]
double R_X_AO;           // AO  : Net Biomass growth rate
double R_C2H4O2_AO;     //      : Acetic acid consumption rate
double R_O2_AO;          //      : O2 consumption rate
double R_NH3_AO;         //      : NH3 consumption rate
double R_CO2_AO;         //      : CO2 generate rate
double R_H2O_AO;         //      : Water generation rate
double R_H2_AO;          //      : H2 consumption rate
// PO Aerobic oxidation of Propionic acid [kmol/m3-d]
double R_X_PO;           // PO  : Net Biomass growth rate
double R_C3H6O2_PO;     //      : Propionic acid consumption rate
double R_O2_PO;          //      : O2 consumption rate
double R_NH3_PO;         //      : NH3 consumption rate
double R_C2H4O2_PO;     //      : Acetic acid generate rate
double R_CO2_PO;         //      : CO2 generate rate
double R_H2O_PO;         //      : Water generation rate
double R_H2_PO;          //      : H2 consumption rate
// BO Aerobic oxidation of Butyric acid [kmol/m3-d]
double R_X_BO;           // BO  : Net Biomass growth rate
double R_C4H8O2_BO;     //      : Butyric acid consumption rate
double R_O2_BO;          //      : O2 consumption rate
double R_NH3_BO;         //      : NH3 consumption rate
double R_C2H4O2_BO;     //      : Acetic acid generate rate
double R_CO2_BO;         //      : CO2 generate rate
double R_H2O_BO;         //      : Water generation rate
double R_H2_BO;          //      : H2 consumption rate
// NO Aerobic nitrification of NH3 [kmol/m3-d]
double R_X_NO;           // NO  : Net Biomass growth rate
double R_NH3_NO;         //      : NH3 consumption rate
double R_O2_NO;          //      : O2 consumption rate
double R_C2H4O2_NO;     //      : Acetic acid consumption rate
double R_NO3_NO;         //      : Nitrate generate rate
double R_H2O_NO;         //      : Water generation rate
double R_CO2_NO;         //      : CO2 generate rate
double R_H2_NO;          //      : H2 consumption rate
// DN Anaerobic denitrification of Nitrate [kmol/m3-d]
double R_X_DN;           // DN  : Net Biomass growth rate
double R_NO3_DN;         //      : Nitric acid generation rate
double R_C2H4O2_DN;     //      : Acetic acid generation rate
double R_N2_DN;          //      : N2 formation rate
double R_CO2_DN;         //      : CO2 generation rate
double R_H2O_DN;         //      : Water generation rate
double R_H2_DN;          //      : H2 consumption rate
double R_NH3_DN;         //      : NH3 consumption rate
double R_O2_DN;          //      : O2 generation rate

// -----
// Effective diffusion coefficient of i component in gas
// -----
double Dif;              // Diffusion Coefficient of Gas           [m2/d]

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// -----
// Production rate of humus by Biomass reaction
// -----
double RFC;           // Rate of fomic acid conversion           [kmol/m3-d]

// -----
// Heat transfer by heat conduction flux
// -----
double qe[7];         // Heat transfer by conduction           [KJ/(m2*d)]

// -----
// Heat production by biological reactions
// -----
double dH_O2_OP;      // heat value of R_O2_OP               [kJ/kmol]
double dH_C2H4O2_OP; // heat value of R_C2H4O2_OP           [kJ/kmol]
double dH_O2_OF;      // heat value of R_O2_OF               [kJ/kmol]
double dH_C2H4O2_OF; // heat value of R_C2H4O2_OF           [kJ/kmol]
double dH_O2_OG;      // heat value of R_O2_OG               [kJ/kmol]
double dH_C2H4O2_OG; // heat value of R_C2H4O2_OG           [kJ/kmol]
double dH_O2_OS;      // heat value of R_O2_OS               [kJ/kmol]
double dH_C2H4O2_OS; // heat value of R_C2H4O2_OS           [kJ/kmol]
double dH_O2_OH;      // heat value of R_O2_OH               [kJ/kmol]
double dH_C2H4O2_OH; // heat value of R_C2H4O2_OH           [kJ/kmol]
double dH_C2H4O2_NP; // heat value of R_C2H4O2_NP           [kJ/kmol]
double dH_C3H6O2_NP; // heat value of R_C3H6O2_NP           [kJ/kmol]
double dH_C4H8O2_NP; // heat value of R_C4H8O2_NP           [kJ/kmol]
double dH_O2_NF;      // heat value of R_O2_NF               [kJ/kmol]
double dH_C2H4O2_NF; // heat value of R_C2H4O2_NF           [kJ/kmol]
double dH_O2_NG;      // heat value of R_O2_NG               [kJ/kmol]
double dH_C2H4O2_NG; // heat value of R_C2H4O2_NG           [kJ/kmol]
double dH_O2_NS;      // heat value of R_O2_NS               [kJ/kmol]
double dH_C2H4O2_NS; // heat value of R_C2H4O2_NS           [kJ/kmol]
double dH_O2_NH;      // heat value of R_O2_NH               [kJ/kmol]
double dH_C2H4O2_NH; // heat value of R_C2H4O2_NH           [kJ/kmol]
double dH_O2_NH;      // heat value of R_O2_NH               [kJ/kmol]
double dH_C2H4O2_AP; // heat value of R_C2H4O2_AP           [kJ/kmol]
double dH_O2_AP;      // heat value of R_O2_AP               [kJ/kmol]
double dH_C2H4O2_AB; // heat value of R_C2H4O2_AB           [kJ/kmol]
double dH_O2_AB;      // heat value of R_O2_AB               [kJ/kmol]
double dH_CH4_MT;     // heat value of R_CH4_MT              [kJ/kmol]
double dH_C2H4O2_MT; // heat value of R_C2H4O2_MT           [kJ/kmol]
double dH_O2_MT;      // heat value of R_O2_MT               [kJ/kmol]
double dH_CH4_MT2;    // heat value of R_CH4_MT2             [kJ/kmol]
double dH_C2H4O2_MT2; // heat value of R_C2H4O2_MT2         [kJ/kmol]
double dH_O2_MT2;     // heat value of R_O2_MT2              [kJ/kmol]
double dH_O2_AO;      // heat value of R_O2_AO               [kJ/kmol]
double dH_C2H4O2_AO; // heat value of R_C2H4O2_AO           [kJ/kmol]
double dH_O2_PO;      // heat value of R_O2_PO               [kJ/kmol]
double dH_C2H4O2_PO; // heat value of R_C2H4O2_PO           [kJ/kmol]
double dH_O2_BO;      // heat value of R_O2_BO               [kJ/kmol]
double dH_C2H4O2_BO; // heat value of R_C2H4O2_BO           [kJ/kmol]
double dH_NH3_NO;     // heat value of R_O2_NO               [kJ/kmol]
double dH_C2H4O2_NO; // heat value of R_C2H4O2_NO           [kJ/kmol]
double dH_C2H4O2_DN; // heat value of R_C2H4O2_DN           [kJ/kmol]
double dH_NO3_DN;     // heat value of R_NO3_DN              [kJ/kmol]

// -----
// Old values required for calculation
// -----
double oldV_G;        // Old values required for gas phase   [-]
double oldV_L;        // Old values required for liquid phase [-]
double oldTemp;       // Old values required for Temperature [-]

```

```

// -----
// Accumulated amount
// -----
double Acu_QGout; // Accumulated amount of QGout [kmol]
double Acu_CO2; // Accumulated amount of CO2 gas [kmol]
double Acu_CH4; // Accumulated amount of CH4 gas [kmol]
double Acu_H2; // Accumulated amount of H2 gas [kmol]
double Acu_N2; // Accumulated amount of N2 gas [kmol]
double Acu_PNH3; // Accumulated amount of NH3 gas [kmol]
double Acu_O2; // Accumulated amount of O2 gas [kmol]

double Acu_QLout; // Accumulated amount of QLout [m3]
double Acu_C2H4O2; // Accumulated amount of Acetate [kmol]
double Acu_C3H6O2; // Accumulated amount of Propionate [kmol]
double Acu_C4H8O2; // Accumulated amount of Butyrate [kmol]
double Acu_IC; // Accumulated amount of IC [mg-C]
double Acu_NH3; // Accumulated amount of NH3 [kmol]
double Acu_NO3; // Accumulated amount of Nitrate [kmol]
double Acu_Caout; // Accumulated amount of Ca [kmol]

#####
#####
// Parameters relating to biological reactions
// Attention variables and constants coexist!!!!
#####
#####
// -----
// Biomass growth rate
// -----
double R_OP_G; // Biomass growth rate of Protein OP [kmol/m3-d]
double R_OF_G; // Biomass growth rate of Fats OF [kmol/m3-d]
double R_OG_G; // Biomass growth rate of Carbohydrate OG [kmol/m3-d]
double R_OS_G; // Biomass growth rate of Cellulose OS [kmol/m3-d]
double R_OH_G; // Biomass growth rate of Lignin OH [kmol/m3-d]
double R_NP_G; // Biomass growth rate of Protein NP [kmol/m3-d]
double R_NF_G; // Biomass growth rate of Fats NF [kmol/m3-d]
double R_NG_G; // Biomass growth rate of Carbohydrate NG [kmol/m3-d]
double R_NS_G; // Biomass growth rate of Cellulose NS [kmol/m3-d]
double R_NH_G; // Biomass growth rate of Lignin NH [kmol/m3-d]
double R_AP_G; // Biomass growth rate of Propionic acids AP [kmol/m3-d]
double R_AB_G; // Biomass growth rate of Butyric acids AB [kmol/m3-d]
double R_MT_G; // Biomass growth rate of Methanogens MT [kmol/m3-d]
double R_MT2_G; // Biomass growth rate of Methanogens MT2 [kmol/m3-d]
double R_AO_G; // Biomass growth rate of Acetic acids AO [kmol/m3-d]
double R_PO_G; // Biomass growth rate of Propionic acids PO [kmol/m3-d]
double R_BO_G; // Biomass growth rate of Butyric acids BO [kmol/m3-d]
double R_NO_G; // Biomass growth rate of Nitrification NO [kmol/m3-d]
double R_DN_G; // Biomass growth rate of Denitrification DN [kmol/m3-d]

// -----
// Biomass decay rate
// -----
double R_OP_D; // Biomass growth rate of Protein OP [kmol/m3-d]
double R_OF_D; // Biomass growth rate of Fats OF [kmol/m3-d]
double R_OG_D; // Biomass growth rate of Carbohydrate OG [kmol/m3-d]
double R_OS_D; // Biomass growth rate of Cellulose OS [kmol/m3-d]
double R_OH_D; // Biomass growth rate of Lignin OH [kmol/m3-d]
double R_NP_D; // Biomass growth rate of Protein NP [kmol/m3-d]
double R_NF_D; // Biomass growth rate of Fats NF [kmol/m3-d]
double R_NG_D; // Biomass growth rate of Carbohydrate NG [kmol/m3-d]
double R_NS_D; // Biomass growth rate of Cellulose NS [kmol/m3-d]

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double R_NH_D;           // Biomass growth rate of Lignin NH           [kmol/m3-d]
double R_AP_D;           // Biomass growth rate of Propionic acids AP           [kmol/m3-d]
double R_AB_D;           // Biomass growth rate of Butyric acids AB           [kmol/m3-d]
double R_MT_D;           // Biomass growth rate of Methanogens MT           [kmol/m3-d]
double R_MT2_D;          // Biomass growth rate of Methanogens MT2           [kmol/m3-d]
double R_AO_D;           // Biomass growth rate of Acetic acids AO           [kmol/m3-d]
double R_PO_D;           // Biomass growth rate of Propionic acids PO           [kmol/m3-d]
double R_BO_D;           // Biomass growth rate of Butyric acids BO           [kmol/m3-d]
double R_NO_D;           // Biomass growth rate of Nitrification NO           [kmol/m3-d]
double R_DN_D;           // Biomass growth rate of Denitrification DN           [kmol/m3-d]

// Chemical formula & Molecule weight of Biomass (CxHuOvNw)
double Bio_x;           // Number of atom Carbon in Biomass formula           [-]
double Bio_u;           // Number of atom H2 in Biomass formula           [-]
double Bio_v;           // Number of atom O2 in Biomass formula           [-]
double Bio_w;           // Number of atom N2 in Biomass formula           [-]
double MX;              // Molecule weight of Biomass                       [kg/kmol]

// -----
// The ranges of partial pressure of O2 to determine the reaction type
// -----
double jdgP_O2_1;       // Lower limit of aerobic condition                   [Pa]
double jdgP_O2_2;       // Upper limit of anaerobic condition                 [Pa]
double jdgP_O2_3;       // Lower limit of anaerobic condition                 [Pa]

// -----
// Constants of biological decomposition
// -----
// OP Aerobic decomposition Protein
double Y_OP;            // Yield coefficient Protein                           [-]
double mu_OP;           // Maximum specific growth rate constant               [1/d]
double K_OP_S;          // Substrate saturation constant                       [-]
double K_OP_O;          // Saturation constant for partial pressure O2         [Pa]
double K_OP_D;          // Decay rate coefficient                              [1/d]
// OF Aerobic decomposition Fats
double Y_OF;            // Yield coefficient Fats                              [-]
double mu_OF;           // Maximum specific growth rate constant               [1/d]
double K_OF_S;          // Substrate saturation constant                       [-]
double K_OF_O;          // Saturation constant for partial pressure O2         [Pa]
double K_OF_D;          // Decay rate coefficient                              [1/d]
// OG Aerobic decomposition Carbohydrate
double Y_OG;            // Yield coefficient Carbohydrate                      [-]
double mu_OG;           // Maximum specific growth rate constant               [1/d]
double K_OG_S;          // Contois saturation constant                         [-]
double K_OG_O;          // Saturation constant for partial pressure O2         [Pa]
double K_OG_D;          // Decay rate coefficient                              [1/d]
// OS Aerobic decomposition Cellulose
double Y_OS;            // Yield coefficient Cellulose                         [-]
double mu_OS;           // Maximum specific growth rate constant               [1/d]
double K_OS_S;          // Substrate saturation constant                       [-]
double K_OS_O;          // Saturation constant for partial pressure O2         [Pa]
double K_OS_D;          // Decay rate coefficient                              [1/d]
// OH Aerobic decomposition Lignin
double Y_OH;            // Yield coefficient Lignin                            [-]
double mu_OH;           // Maximum specific growth rate constant               [1/d]
double K_OH_S;          // Substrate saturation constant                       [-]
double K_OH_O;          // Saturation constant for partial pressure O2         [Pa]
double K_OH_D;          // Decay rate coefficient                              [1/d]
// Acetic acid production rate of anaerobic fermentation organic matter
// The mole coefficient of Acetic acid is determined based on the atomic balance as
// described in Model Organic Decomposition.docx and calculate in Balance Check
// Organic Degradation.xml
double R_NP;            // Acetic acid production of Protein

```

```

double R_NF;           // Acetic acid production of Fats
double R_NG;           // Acetic acid production of Carbohydrate
double R_NS;           // Acetic acid production of Cellulose
double R_NH;           // Acetic acid production of Lignin
double R_AP;           // Acetic acid production of Propionate
double R_AB;           // Acetic acid production of Butyrate
double R_NX;           // Acetic acid production of Decayed micro-organism
// NP Anaerobic fermentation Protein
double Y_NF;           // Yield coefficient Protein           [-]
double mu_NP;          // Maximum specific growth rate constant           [1/d]
double K_NP_D;         // Decay rate coefficient                               [1/d]
double K_NP_S;         // Substrate saturation constant                       [kg/m3]
// NF Anaerobic fermentation Fats
double Y_NF;           // Yield coefficient Fats                               [-]
double mu_NF;          // Maximum specific growth rate constant           [1/d]
double K_NF_D;         // Decay rate coefficient                               [1/d]
double K_NF_S;         // Substrate saturation constant                       [kg/m3]
// NG Anaerobic fermentation Carbohydrate
double Y_NG;           // Yield coefficient Carbohydrate                     [-]
double mu_NG;          // Maximum specific growth rate constant           [1/d]
double K_NG_D;         // Decay rate coefficient                               [1/d]
double K_NG_S;         // Substrate saturation constant                       [kg/m3]
// NS Anaerobic fermentation Cellulose
double Y_NS;           // Yield coefficient Cellulose                         [-]
double mu_NS;          // Maximum specific growth rate constant           [1/d]
double K_NS_S;         // Substrate saturation constant                       [kg/m3]
double K_NS_D;         // Decay rate coefficient                               [1/d]
// NH Anaerobic fermentation Lignin
double Y_NH;           // Yield coefficient Lignin                           [-]
double mu_NH;          // Maximum specific growth rate constant           [1/d]
double K_NH_S;         // Substrate saturation constant                       [kg/m3]
double K_NH_D;         // Decay rate coefficient                               [1/d]
// AP Acetogenesis Propionic acid
double Y_AP;           // Yield coefficient Propionate                       [-]
double mu_AP;          // Maximum specific growth rate constant           [1/d]
double K_AP_S;         // Substrate saturation constant                       [kg/m3]
double K_AP_D;         // Decay rate coefficient                               [1/d]
// AB Acetogenesis Butyric acid
double Y_AB;           // Yield coefficient Butyrate                         [-]
double mu_AB;          // Maximum specific growth rate constant           [1/d]
double K_AB_S;         // Substrate saturation constant                       [kg/m3]
double K_AB_D;         // Decay rate coefficient                               [1/d]
// MT CH4 formation from Acetic acid
double Y_MT;           // Yield coefficient Methanogens                      [-]
double mu_MT;          // Maximum specific growth rate constant           [1/d]
double K_MT_S;         // Saturation constant for C2H4O2                     [kmol/m3]
double K_MT_D;         // Decay rate coefficient of CH4 bacteria              [1/d]
// MT2 CH4 formation from CO2+H2
double Y_MT2;          // Yield coefficient Methanogens                      [-]
double mu_MT2;         // Maximum specific growth rate constant           [1/d]
double K_MT2_S;        // Saturation constant for CO2 + H2                   [kg/m3]
double K_MT2_D;        // Decay rate coefficient of CH4 bacteria              [1/d]
// AO Acetic acid aerobic oxidation
double Y_AO;           // Yield coefficient Acetic acid oxidation            [-]
double mu_AO;          // Maximum specific growth rate constant           [1/d]
double K_AO_S;         // Substrate saturation constant                       [-]
double K_AO_O;         // Saturation constant for partial pressure O2        [Pa]
double K_AO_D;         // Decay rate coefficient                               [1/d]
// PO Propionic acid aerobic oxidation
double Y_PO;           // Yield coefficient Propionic acid oxidation          [-]
double mu_PO;          // Maximum specific growth rate constant           [1/d]
double K_PO_S;         // Substrate saturation constant                       [-]

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double K_PO_O;           // Saturation constant for partial pressure O2 [Pa]
double K_PO_D;           // Decay rate coefficient [1/d]
// BO Butyric acid aerobic oxidation
double Y_BO;             // Yield coefficient Butyric acid oxidation [-]
double mu_BO;            // Maximum specific growth rate constant [1/d]
double K_BO_S;           // Substrate saturation constant [-]
double K_BO_O;           // Saturation constant for partial pressure O2 [Pa]
double K_BO_D;           // Decay rate coefficient [1/d]
// NO Nitrification of NH3
double Y_NO;             // Yield coefficient NH3 oxidation [-]
double mu_NO;            // Maximum specific growth rate constant [1/d]
double K_NO_S;           // Substrate saturation constant [-]
double K_NO_O;           // Saturation constant for partial pressure O2 [Pa]
double K_NO_D;           // Decay rate coefficient [1/d]
// DN Denitrification
double Y_DN;             // Yield coefficient Denitrification [-]
double mu_DN;            // Maximum specific growth rate constant [1/d]
double K_DN_S;           // Saturation constant for C2H4O2 [kmol/m3]
double K_DN_D;           // Decay rate coefficient of CH4 bacteria [1/d]
// Critical amount of acetic acid
double C2H4O2_Tcri;     // Critical amount of acetic acid [kmol/m3]

// -----
// Initial amount of bacteria [kg/m3]
// -----
double X_OPini;          // Aerobic decomposition bacteria of Protein
double X_OFini;          // Aerobic decomposition bacteria of Fats
double X_OGini;          // Aerobic decomposition bacteria of Carbohydrate
double X_OSini;          // Aerobic decomposition bacteria of Cellulose
double X_OHini;          // Aerobic decomposition bacteria of Lignin
double X_NPini;          // Anaerobic fermentation bacteria of Protein
double X_NFini;          // Anaerobic fermentation bacteria of Fats
double X_NGini;          // Anaerobic fermentation bacteria of Carbohydrate
double X_NSini;          // Anaerobic fermentation bacteria of Cellulose
double X_NHini;          // Anaerobic fermentation bacteria of Lignin
double X_APini;          // Acetogenesis bacteria of Propionate
double X_ABini;          // Acetogenesis bacteria of Butyrate
double X_MTini;          // CH4 formation bacteria of Acetic acid
double X_MT2ini;         // CH4 formation bacteria of CO2+H2
double X_AOini;          // Acetic acid oxidation bacteria
double X_POini;          // Propionic acid oxidation bacteria
double X_BOini;          // Butyric acid oxidation bacteria
double X_NOini;          // NH3 nitrification bacteria
double X_DNini;          // Nitrate denitrification bacteria

// -----
// Amount of bacteria [kg/m3]
// -----
double X_OP;             // Aerobic decomposition bacteria of Protein
double X_OF;             // Aerobic decomposition bacteria of Fats
double X_OG;             // Aerobic decomposition bacteria of Carbohydrate
double X_OS;             // Aerobic decomposition bacteria of Cellulose
double X_OH;             // Aerobic decomposition bacteria of Lignin
double X_NP;             // Anaerobic fermentation bacteria of Protein
double X_NF;             // Anaerobic fermentation bacteria of Fats
double X_NG;             // Anaerobic fermentation bacteria of Carbohydrate
double X_NS;             // Anaerobic fermentation bacteria of Cellulose
double X_NH;             // Anaerobic fermentation bacteria of Lignin
double X_AP;             // Acetogenesis of Propionate
double X_AB;             // Acetogenesis of Butyrate
double X_MT;             // CH4 formation bacteria of Acetic acid
double X_MT2;           // CH4 formation bacteria of CO2+H2
double X_AO;             // Acetic acid oxidation bacteria

```

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```

double X_PO;           // Propionic acid oxidation bacteria
double X_BO;           // Butyric acid oxidation bacteria
double X_NO;           // NH3 nitrification bacteria
double X_DN;           // Nitrate denitrification bacteria

// -----
// Amount of organic matter
// -----
double ORG_T;          // Total of organic matter           [kg/m3]

// -----
// Variables for Total Carbon and Total N2 Mass balance check
// -----
double C_in_Solid;     // Total Carbon in Solid phase           [kmol-C]
double C_in_Liquid;    // Total Carbon in Liquid phase           [kmol-C]
double C_in_Gas;       // Total Carbon in Gas phase             [kmol-C]
double C_in_Total;     // Total Carbon in Cell                   [kmol-C]
double N_in_Solid;     // Total N2 in Solid phase               [kmol-N]
double N_in_Liquid;    // Total N2 in Liquid phase             [kmol-N]
double N_in_Gas;       // Total N2 in Gas phase                 [kmol-N]
double N_in_Total;     // Total N2 in Cell                       [kmol-N]

// -----
// Constructor
// -----
Cell();                // Constructor is necessary to initialize these group
parameters

#####
#####
// The functions used in Cell class
#####
#####
// -----
// Sub-routine for reaction rate calculation
// -----
void Const_param_set(void);      // parameter setting from txt file
void Inicond_set(void);         // initial condition setting from txt file
void RESET_reaction_Rate(void); // Initialization of reaction rate

// 1) Aerobic degradation of Protein & dead OP biomass
void AerobicDecompositionProtein(double fx);
void OP_AnaerobicFermentationBiomass(double fx);

// 2) Aerobic degradation of Fats & dead OF biomass
void AerobicDecompositionFats(double fx);
void OF_AnaerobicFermentationBiomass(double fx);

// 3) Aerobic degradation of Carbohydrate & dead OG biomass
void AerobicDecompositionCarbohydrate(double fx);
void OG_AnaerobicFermentationBiomass(double fx);

// 4) Aerobic degradation of Cellulose & dead OS biomass
void AerobicDecompositionCellulose(double fx);
void OS_AnaerobicFermentationBiomass(double fx);

// 5) Aerobic degradation of ligni & dead OH biomass
void AerobicDecompositionLignin(double fx);
void OH_AnaerobicFermentationBiomass(double fx);

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```
// 6) Anaerobic degradation of Protein & dead NP biomass
void AnaerobicFermentationProtein(double fx);
void NP_AerobicDecompositionBiomass(double fx);

// 7) Anaerobic degradation of Fats & dead NF biomass
void AnaerobicFermentationFats(double fx);
void NF_AerobicDecompositionBiomass(double fx);

// 8) Anaerobic degradation of Carbohydrate & dead NG biomass
void AnaerobicFermentationCarbohydrate(double fx);
void NG_AerobicDecompositionBiomass(double fx);

// 9) Anaerobic degradation of Cellulose & dead NS biomass
void AnaerobicFermentationCellulose(double fx);
void NS_AerobicDecompositionBiomass(double fx);

// 10) Anaerobic degradation of Lignin & dead NH biomass
void AnaerobicFermentationLignin(double fx);
void NH_AerobicDecompositionBiomass(double fx);

// 11) Anaerobic degradation of Propionic acids & dead AP biomass
void AcetogenesisPropionicAcid(double fx);
void AP_AerobicDecompositionBiomass(double fx);

// 12) Anaerobic degradation of Butyric acids & dead AB biomass
void AcetogenesisButyricAcid(double fx);
void AB_AerobicDecompositionBiomass(double fx);

// 13) Methane formation of Acetic acids & dead MT biomass
void CH4FormationAceticAcid(double fx);
void MT_AnaerobicDeg.Biomass(double fx);
void MT_AerobicDecompositionBiomass(double fx);

// 14 ) Methane formation of H2 & CO2 & dead MT2 biomass
void CH4FormationCO2andH2(double fx);
void MT2_AnaerobicFermentationBiomass(double fx);
void MT2_AerobicDecompositionBiomass(double fx);

// 15 ) Oxidation of Acetic acids & & dead AO biomass
void AerobicOxidationAceticAcid(double fx);
void AO_AnaerobicFermentationBiomass(double fx);

// 16 ) Oxidation of Propionic acids & dead PO biomass
void AerobicOxidationPropionicAcid(double fx);
void PO_AnaerobicFermentationBiomass(double fx);

// 17 ) Oxidation of Butyric acids & dead BO biomass
void AerobicOxidationButyricAcid(double fx);
void BO_AnaerobicFermentationBiomass(double fx);

// 18 ) Nitrification of NH3 & dead NO biomass
void AerobicNitrificationNH3(double fx);
void NO_AnaerobicFermentationBiomass(double fx);

// 19 ) Denitrification of Nitrate & dead DN biomass
void AnaerobicDenitrificationNitrate(double fx);
void DN_AerobicDecompositionBiomass(double fx);

// -----
// Sub-routine for calculation
// -----
double sqr(double x){
return pow(x, 2.0);
```

```

    }
void push_Hplus(double setpH){
H_plus = pow(10.0,-setpH);
}

// -----
// Sub-routine for washing-out calculation
// -----
double xi(void);

// -----
// Sub-routine for pressure equilibrium calculation
// -----
void Cell_press_equilibrium(void);

// -----
// Sub-routine for mass balance calculation
// -----
void Massbalance_check();

// -----
// Sub-routine for calculations concentration at dt step
// -----
void cal_PT(void);           // Total Gas Pressure in Cell           [Pa]
void cal_QGout(void);       // Landfill gas discharge gas from Cell [kmol/d]
void cal_PCO2_step(void);   // Partial Pressure CO2 in landfill gas [Pa]
void cal_PCH4_step(void);   // Partial Pressure CH4 in landfill gas [Pa]
void cal_PH2_step(void);    // Partial Pressure H2 in landfill gas  [Pa]
void cal_PN2_step(void);    // Partial Pressure N2 in landfill gas  [Pa]
void cal_PNH3_step(void);   // Partial Pressure NH3 in landfill gas [Pa]
void cal_PO2_step(void);    // Partial Pressure O2 in landfill gas  [Pa]
void cal_PH2O_step(void);   // Partial Pressure H2O in landfill gas [Pa]

void cal_QLout(void);       // Rate leachate discharge of Cell     [m3/d]
void cal_TIC_step(void);    // Total Carbonate including CO2 gas    [kmol/m3]
void cal_T_NH3_step(void);  // Total NH3 including NH3 gas         [kmol/m3]
void cal_NO3_step(void);    // Nitrate ion concentration           [kmol/m3]
void cal_C2H4O2_T_step(void); // Total Acetic Acid                   [kmol/m3]
void cal_C3H6O2_T_step(void); // Total Propionic acid                 [kmol/m3]
void cal_C4H8O2_T_step(void); // Total Butyric acid                   [kmol/m3]
void cal_Ca_step(void);     // Calcium ion concentration            [kmol/m3]
void cal_Na_step(void);     // Alkali ions                          [kmol/m3]
void cal_Cl_step(void);     // Chlorine ion                         [kmol/m3]

void cal_SPRO_step(void);   // Protein                              [kg/m3]
void cal_SFAT_step(void);   // Fats                                  [kg/m3]
void cal_SGLU_step(void);   // Carbohydrate                         [kg/m3]
void cal_SCEL_step(void);   // Cellulose                             [kg/m3]
void cal_SLIG_step(void);   // Lignin                                [kg/m3]
void cal_X_step(void);      // Biomass                              [kg/m3]
void cal_ORG_T_step(void);  // Total of organic matter              [kg/m3]
void cal_H_step(void);     // Volume waste at dt step              [m3]

// -----
// Sub-routine for equilibrium calculation
// -----
void cal_H2CO3_T(void);     // Total Carbonate Acid                 [kmol/m3]
void cal_H2CO3(void);      // Carbonic Acid concentration          [kmol/m3]
void cal_HCO3(void);       // Bicarbonate ion concentration        [kmol/m3]
void cal_CO3(void);        // Carbonate ion concentration          [kmol/m3]
void cal_PCO2(void);       // Partial Pressure of CO2              [Pa]

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```

void cal_IC(void);           // Total Inorganic carbon in liquid      [mg-C/L]

void cal_NH3_T(void);       // Total NH3 [kmol/m3]
void cal_NH3(void);        // NH3 concentration [kmol/m3]
void cal_NH4(void);        // Ammonium ion concentration [kmol/m3]
void cal_PNH3(void);       // NH3 gas [kmol/m3]
void cal_NH4_Adsorp(void);  // NH3 Adsorbed on solid [kmol/m3]
void cal_C2H4O2(void);     // Acetic Acid concentration [kmol/m3]
void cal_CH3COO(void);     // Acetate ion concentration [kmol/m3]
void cal_C3H6O2(void);     // Propionic acid concentration [kmol/m3]
void cal_CH3CH2COO(void);  // Propionate ion concentration [kmol/m3]
void cal_C4H8O2(void);     // Butyric acid concentration [kmol/m3]
void cal_CH3CH2CH2COO(void); // Butyrate ion concentration [kmol/m3]
void cal_COD(void);        // COD in leachate [mg-O2/L]

// -----
// Sub-routine for Accumulated calculation
// -----
void cal_Acu_QGout(void);   // Accumulated amount of QGout [kmol]
void cal_Acu_CO2(void);    // Accumulated amount of CO2 gas [kmol]
void cal_Acu_CH4(void);    // Accumulated amount of CH4 gas [kmol]
void cal_Acu_H2(void);     // Accumulated amount of N2gas [kmol]
void cal_Acu_N2(void);     // Accumulated amount of N2gas [kmol]
void cal_Acu_PNH3(void);   // Accumulated amount of NH3 gas [kmol]
void cal_Acu_O2(void);     // Accumulated amount of O2 gas [kmol]

void cal_Acu_QLout(void);  // Accumulated amount of QLout [m3/d]
void cal_Acu_C2H4O2(void); // Accumulated amount of Acetate [kmol]
void cal_Acu_C3H6O2(void); // Accumulated amount of Propionate [kmol]
void cal_Acu_C4H8O2(void); // Accumulated amount of Butyrate [kmol]
void cal_Acu_IC(void);     // Accumulated amount of IC [mg-C]
void cal_Acu_NH3(void);    // Accumulated amount of NH3 [kmol]
void cal_Acu_NO3(void);    // Accumulated amount of Nitrate [kmol]
void cal_Acu_Caout(void);  // Accumulated amount of Ca [kmol]

// -----
// Sub-routine for pH calculation
// -----
void pH_calculation();
double Ion_Balance(double);
};

#####
#####
// Declaring variables relating to heat calculation
// These values are different depending on the type of Cell
#####
#####
class Heat_param{
public:
double Ua;           // Overall heat-transfer coefficient [kJ/(m*d*K)]
double Tsoil_const; // Temperature of soil is constant [k]

// Thermal conductivity of waste [kJ/(m*d*K)]
double K_waste(double cwc){
return(11.9568257792 + exp(cwc * 5.809821));
}
double K_cover;     // Thermal conductivity of cover [kJ/(m*d*K)]
double K_grav;      // Thermal conductivity of gravel [kJ/(m*d*K)]
double K_soil;       // Thermal conductivity of soil [kJ/(m*d*K)]
double K_water;     // Thermal conductivity of water [kJ/(m*d*K)]

```

---

```

// Specific heat capacity of waste [kJ/(kg*°K)]
double cp_waste(double cwc){
return(-0.2 + exp (cwc * 0.52));
}
double cp_cover;           // Specific heat capacity of cover           [kJ/ (kg*°K)]
double cp_grav;           // Specific heat capacity of gravel       [kJ/ (kg*°K)]
double cp_soil;           // Specific heat capacity of soil         [kJ/ (kg*°K)]
double cp_water;          // Specific heat capacity of water        [kJ/ (kg*°K)]

// Apparent density of waste [kg/m3]
double re_waste(double cwc){
return(pRa * cwc + pRb);
}
double pRa;               // Apparent density of waste           [kg/m3]
double pRb;               // Apparent density of waste           [kg/m3]
double re_cover;         // Apparent density of cover           [kg/m3]
double re_grav;          // Apparent density of gravel          [kg/m3]
double re_soil;          // Apparent density of soil            [kg/m3]
double re_water;         // Apparent density of water           [kg/m3]

Heat_param();

// Constructor it's necessary to initialize these parameters group
};

#####
#####
// Setting the conditions in the vicinity of Cell (for the calculation of
// temperature)
#####
#####
class Circumference_media{
public:
// -----
// Parameter declaration
// -----
mediatp media;
double temp;           // Temperature within Cell           [K]
double H;              // Height of Cell                     [m]
double wc;             // Water content of Cell              [-]

// -----
// DEFAULT VALUE
// -----
Circumference_media(){
media = none;
temp = 0.0;           // Temperature within Cell           [K]
H = 0.0;             // Height of Cell                     [m]
wc = 0.0;            // Water content of Cell              [-]
};
};
void Cell_circumference_cond_set(void);

```

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---

```
#####  
#####  
// Implementation of global functions  
#####  
#####  
int Initial_cal_time_set(double &t,double &dt,double &t_end,double &pt,double  
    &prt_dt,double tt[],double dti[],double prt_dti[]);  
void Euler_step_cal(Cell& ce);  
void New_conc_after_dt(Cell& ce);  
void Cell_reaction_rate(Cell& ce);  
void pH_cal(Cell& ce);  
int Heat_flux_cal(Cell& ce);  
int Temp_step_cal(Cell& ce);  
void Constoutput(Cell& ce);  
void FoutputHeader(void);  
void Foutput1(Cell& ce);  
void Foutput2(Cell& ce);  
void Output_file_close(void);  
void Other_param_cal(Cell& ce);  
int Cal_time_condition_set(double &t,double &dt,double &t_end,double &pt,double  
    &prt_dt,double tt[],double dti[],double prt_dti[]);  
int Environment_cond_load(void);
```

## Module III: Constructor

```

#include "Cell.h"
extern Global_const CP; // Global constants
extern Atmospheric_cond atm; // Atmosphere condition
extern Heat_param HP; // Heat transfer parameters
extern Environment_cond env; // Environment condition
extern Circumference_media LayM[7];

#####
#####
// Setting the interval of calculation time
// Declaration of variables relating to the time was done in [main.cpp]
#####
#####
int Initial_cal_time_set(double &t,double &dt,double &t_end,double &pt,double
&prt_dt,
double tt[],double dti[],double prt_dti[]){
t = 0.0;
t_end = 750;

#define DT_IS_CHECK1
#ifndef DT_IS_ORIG
tt[1]= 0.3; dti[1]= 0.0001; prt_dti[1]= 0.03;
tt[2]= 3.0; dti[2]= 0.001; prt_dti[2]= 0.3;
tt[3]= 30.0; dti[3]= 0.01; prt_dti[3]= 3.0;
tt[4]= 300; dti[4]= 0.1; prt_dti[4]= 30.0;
tt[5]= 3000; dti[5]= 1; prt_dti[5]= 300;
tt[6]= 30000; dti[6]= 5.0; prt_dti[6]= 1500;
tt[7]= 300000; dti[7]= 10.0; prt_dti[7]= 3000;
#endif
#ifdef DT_IS_CHECK1
tt[1]= 0.3; dti[1]= 0.0001; prt_dti[1]= 0.03;
tt[2]= 3.0; dti[2]= 0.0005; prt_dti[2]= 0.3;
tt[3]= 30.0; dti[3]= 0.002; prt_dti[3]= 3.0;
tt[4]= 300; dti[4]= 0.01; prt_dti[4]= 30.0;
tt[5]= 3000; dti[5]= 0.05; prt_dti[5]= 300;
tt[6]= 30000; dti[6]= 0.2; prt_dti[6]= 1500;
tt[7]= 300000; dti[7]= 1.0; prt_dti[7]= 3000;
#endif
#ifdef DT_IS_CHECK2
tt[1]= 0.3; dti[1]= 0.0001; prt_dti[1]= 0.03;
tt[2]= 3.0; dti[2]= 0.0003; prt_dti[2]= 0.3;
tt[3]= 30.0; dti[3]= 0.001; prt_dti[3]= 3.0;
tt[4]= 300; dti[4]= 0.003; prt_dti[4]= 30.0;
tt[5]= 3000; dti[5]= 0.01; prt_dti[5]= 300;
tt[6]= 30000; dti[6]= 0.03; prt_dti[6]= 1500;
tt[7]= 300000; dti[7]= 1.0; prt_dti[7]= 3000;
#endif
#ifdef DT_IS_CHECK3
tt[1]= 0.3; dti[1]= 0.0001; prt_dti[1]= 0.03;
tt[2]= 3.0; dti[2]= 0.0002; prt_dti[2]= 0.3;
tt[3]= 30.0; dti[3]= 0.0005; prt_dti[3]= 3.0;
tt[4]= 300; dti[4]= 0.001; prt_dti[4]= 30.0;
tt[5]= 3000; dti[5]= 0.002; prt_dti[5]= 300;
tt[6]= 30000; dti[6]= 0.005; prt_dti[6]= 1500;
tt[7]= 300000; dti[7]= 0.01; prt_dti[7]= 3000;
#endif

dt=dti[1];
prt_dt=prt_dti[1];
pt=prt_dt;

return 0;
}

```

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```

#####
#####
// Setting values variable related to the global constants
#####
#####
Global_const::Global_const() {
R          = 8.314E+3;      // Gas constant          [Pa*m3/kmol*K]
Henry_CO2  = 3.015E+6;     // CO2 Henry constant    [Pa*m3/kmol]
Henry_NH3  = 5.635E+3;     // Ammonia Henry constant [Pa*m3/kmol]
Kd_H2CO3   = 4.295E-7;     // Carbonic acid dissociation constant [kmol/m3]
Kd_HCO3    = 4.786E-11;    // Bicarbonate dissociation constant [kmol/m3]
Kd_NH3     = 3.162E-11;    // Ammonia dissociation constant [kmol/m3]
Kd_CH3COOH = 1.738E-5;     // Acetic acid dissociation constant [kmol/m3]
Kd_CH3CH2COOH = 1.34E-5; // Propionic acid dissociation constant [kmol/m3]
Kd_CH3CH2CH2COOH = 1.52E-5; // Butyric acid dissociation constant [kmol/m3]
Ksp_CaCO3  = 4.80E-8;     // Solubility of Calcium Carbonate [kmol/m3]
Kp_NH3     = 0.01;       // Distribution Coefficient of Ammonia [m3/kg]
};

#####
#####
// Setting initial value for variables related to atmosphere condition
#####
#####
Atmospheric_cond::Atmospheric_cond() {
T          = 303.15;      // Atmospheric temperature [K]
P          = 0.1013 * 1E+6; // Atmospheric Pressure [Pa]
P_CO2     = 0.0003 * P;   // Partial Pressure of CO2 in air [Pa]
P_CH4     = 0 * P;       // Partial Pressure of CH4 in air [Pa]
P_H2      = 0 * P;       // Partial Pressure of H2 in air [Pa]
P_N2      = 0.7897 * P;  // Partial Pressure of N2 in air [Pa]
P_NH3     = 0 * P;       // Partial Pressure of NH3 in air [Pa]
P_O2      = 0.21 * P;    // Partial Pressure of O2 in air [Pa]
};

#####
#####
// Initial setting value for variables related to environment condition
#####
#####
Environment_cond::Environment_cond() {
int i;
num_of_days = 99999;
for(i=1;i<=num_of_days;i++){
    Tair[i] = 303.15;      // Atmospheric temperature [k]
    QRain[i] = 10.825;    // Water precipitation [mm/d]
}
}

#####
#####
// Setting initial value for constants and variables relate to landfill Cell
#####
#####
int i;
// -----
// Fraction of each phase
// -----
eL      = 0.410;          // Liquid phase ratio [m3/m3]
eS      = 0.436;          // Solid phase ratio [m3/m3]
eG      = 1.0 - (eL + eS); // Gas phase ratio [m3/m3]
wcp     = 0.350;         // Field capacity of Cell [-]

// -----
// Density, Dimension and Volume of a Landfill Cell
// -----
H       = 2.0;           // Height of Cell [m]
D       = 0.71;         // Width of Cell [m]

```

```

S      = 0.25 * PI * pow(D,2); // Surface area of Cell[m2]
V      = H * S;                // Volume of Cell [m3]
V_L    = eL * V;              // Volume of liquid phase [m3]
V_G    = eG * V;              // Volume of Gas phase [m3]
V_S    = eS * V;              // Volume of Solid phase [m3]
wc     = V_L/V;               // Water content of Cell [-]

r_sld  = 1040;                // Specific weight of solid [kg/m3]
r_dry  = (r_sld * V_S)/V;     // Dry density of Cell [kg/m3]
r_wet  = (r_sld * V_S + 1000 * V_L)/V; // Wet density of Cell [kg/m3]

// -----
// Inflow, Outflow, and washing-out relationship
// -----
QLin   = 505.154/1000 * S;    // Rate water infiltration into Cell [mm/d]
QLout  = 0.0;                // Rate leachate discharge of Cell [m3/d]
xi0    = 0.3;                // Washout rate (initial) [-]
xlmd   = 0.2;                // Washout Acceleration factor [1/d]
txi    = 365 * 2.0;          // Time constant of wash out [d]
QGout  = 0.0;                // Landfill gas release from Cell [kmol/d]

R_ratio = 1.0;                // Ratio leachate recycle to discharge [-]
QGIN    = 0.0;                // Aeration rate [kmol/d]

// -----
// Fraction organic and inorganic matter in solid phase
// -----
S_PRO  = 0.02;                // Protein fraction in MSW [% in solid]
S_FAT  = 0.01;                // Fats fraction in MSW [% in solid]
S_GLU  = 0.08;                // Carbohydrate fraction in MSW [% in solid]
S_CEL  = 0.20;                // Cellulose fraction in MSW [% in solid]
S_LIG  = 0.07;                // Lignin fraction in MSW [% in solid]

// -----
// Inorganic fraction in MSW
// -----
S_INO  = 1.0 - (S_PRO + S_FAT + S_GLU + S_CEL + S_LIG); // [% in solid]

// -----
// Mass organic and inorganic matter in landfill
// -----
S_PRO  = S_PRO * r_sld * V_S/V; // Protein mass in MSW [kg/m3]
S_FAT  = S_FAT * r_sld * V_S/V; // Fats mass in MSW [kg/m3]
S_GLU  = S_GLU * r_sld * V_S/V; // Carbohydrate mass in MSW [kg/m3]
S_CEL  = S_CEL * r_sld * V_S/V; // Cellulose mass in MSW [kg/m3]
S_LIG  = S_LIG * r_sld * V_S/V; // Lignin mass in MSW [kg/m3]
S_INO  = S_INO * r_sld * V_S/V; // Inorganic mass in MSW [kg/m3]

// -----
// Chemical formula & Molecular Weight of Protein CaHbOcNn
// -----
Pro_a  = 46.0;                // Number of atom carbon in Protein formula [-]
Pro_b  = 77.0;                // Number of atom hydrogen in Protein formula [-]
Pro_c  = 17.0;                // Number of atom oxygen in Protein formula [-]
Pro_n  = 12.0;                // Number of atom nitrogen in Protein formula [-]
M_PRO  = 12.01 * Pro_a + 1.01 * Pro_b + 15.99 * Pro_c + 14.0 * Pro_n;

// -----
// Chemical formula & Molecular Weight of Fats CaHbOc
// -----
Fat_a  = 55.0;                // Number of atom carbon in Cellulose formula [-]
Fat_b  = 104;                // Number of atom oxygen in Cellulose formula [-]
Fat_c  = 6.00;                // Number of atom nitrogen in Cellulose formula [-]
M_FAT  = 12.01 * Fat_a + 1.01 * Fat_b + 15.99 * Fat_c;

// -----
// Chemical formula & Molecular Weight of Carbohydrate (C6H10O5)n, n=1
// -----
Glu_a  = 6.00;                // Number of atom carbon in Carbohydrate [-]
Glu_b  = 10.0;               // Number of atom oxygen in Carbohydrate [-]
Glu_c  = 5.00;                // Number of atom nitrogen in Carbohydrate [-]
Glu_n  = 1.00;                // Number of repetition in chemical formula [-]
M_GLU  = (12.01 * Glu_a + 1.01 * Glu_b + 15.99 * Glu_c) * Glu_n;

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// -----
// Chemical formula & Molecular Weight of Cellulose (C6H10O5)n, n=3
// -----
Cel_a = 6.00; // Number of atom carbon in Cellulose formula [-]
Cel_b = 10.0; // Number of atom oxygen in Cellulose formula [-]
Cel_c = 5.00; // Number of atom nitrogen in Cellulose formula [-]
Cel_n = 3.00; // Number of repetition in chemical formula [-]
M_CEL = (12.01 * Cel_a + 1.01 * Cel_b + 15.99 * Cel_c) * Cel_n;

// -----
// Chemical formula & Molecular Weight of Lignin (C10H12O3)
// -----
Lig_a = 10.0; // Number of atom carbon in Lignin formula [-]
Lig_b = 12.0; // Number of atom oxygen in Lignin formula [-]
Lig_c = 3.00; // Number of atom nitrogen in Lignin formula [-]
M_LIG = 12.01 * Lig_a + 1.01 * Lig_b + 15.99 * Lig_c;

// -----
// Initial temperature and pressure within Cell
// -----
PT = 0.1013 * 1E+6; // Total Gas Pressure [Pa]
Temp = 303.15; // Temperature within Cell [K]
P_H2O = EXP(20.386 - 5132/Temp) // Partial Pressure of water [Pa]

P_CO2 = 0.0004 * (PT-P_H2O); // Partial Pressure of CO2 [Pa]
P_CH4 = 0 * (PT-P_H2O); // Partial Pressure of CH4 [Pa]
P_H2 = 0 * (PT-P_H2O); // Partial Pressure of H2 [Pa]
P_N2 = 0.7896 * (PT-P_H2O); // Partial Pressure of N2 [Pa]
P_NH3 = 0 * (PT-P_H2O); // Partial Pressure of NH3 [Pa]
P_O2 = 0.21 * (PT-P_H2O); // Partial Pressure of O2 [Pa]

// -----
// Concentrations in liquid phase
// -----
pH = 6.0; // pH [-]
H_plus = pow(10.0, -pH); // Hydrogen ion concentration [kmol/m3]
OH_min = pow(10.0, pH-14); // HydrogenOxide ion concentration [kmol/m3]

// -----
// Carbonate groups [kmol/m3]
// -----
// Carbonic Acid concentration [kmol/m3]
H2CO3 = (P_CO2/CP.Henry_CO2);

// Bicarbonate ion concentration [kmol/m3]
HCO3 = H2CO3 * (CP.Kd_H2CO3/H_plus);

// Carbonate ion concentration [kmol/m3]
CO3 = H2CO3 * (CP.Kd_H2CO3 * CP.Kd_HCO3/sqr(H_plus));

// Total Carbonate [kmol/m3]
H2CO3_T = H2CO3 * (1.0 + (CP.Kd_H2CO3/H_plus) + (CP.Kd_H2CO3 *
CP.Kd_HCO3/sqr(H_plus)));

// -----
// Acetate groups
// -----
// Total Acetic Acid [kmol/m3]
CH3COOH_T = 0.15;

// Acetate ion concentration [kmol/m3]
CH3COOH = CH3COOH_T/(1 + (CP.Kd_CH3COOH/H_plus));
// Acetic acid concentration [kmol/m3]
CH3COO = CH3COOH_T/(1 + (CP.Kd_CH3COOH/H_plus)) * (CP.Kd_CH3COOH/H_plus);

// -----
// Propionate groups
// -----
// Total Propionic acid [kmol/m3]
CH3CH2COOH_T = 0.0;

```

```

// Propionate ion concentration [kmol/m3]
CH3CH2COOH = CH3CH2COOH_T/(1 + (CP.Kd_CH3CH2COOH/H_plus));

// Propionic acid concentration [kmol/m3]
CH3CH2COO = CH3CH2COOH_T/(1 + (CP.Kd_CH3CH2COOH/H_plus)) * (CP.Kd_CH3CH2COOH/H_plus);

// -----
// Butyrate groups
// -----
// Total Butyric acid [kmol/m3]
CH3CH2CH2COOH_T = 0.0;

// Butyrate ion concentration [kmol/m3]
CH3CH2CH2COOH = CH3CH2CH2COOH_T/(1 + (CP.Kd_CH3CH2CH2COOH/H_plus));

// Butyric acid concentration [kmol/m3]
CH3CH2CH2COO = CH3CH2CH2COOH_T/(1 + (CP.Kd_CH3CH2CH2COOH/H_plus)) *
                (CP.Kd_CH3CH2CH2COOH/H_plus);

// -----
// Ammonia groups
// -----
// Total Ammonia in liquid phase [kmol/m3]
NH3_T = 0.0;// 0.035;

// Ammonia concentration [kmol/m3]
NH3 = NH3_T/(1.0 + (CP.Kd_NH3/OH_min));

// Ammonium ion concentration [kmol/m3]
NH4 = NH3_T/(1.0 + (CP.Kd_NH3/OH_min)) * (CP.Kd_NH3/OH_min);

// Ammonia Absorbed on solid [kmol/m3]
NH4_abs = CP.Kp_NH3 * r_sld * (V_S/V_L) * NH4;

// Total Ammonia in Cell including NH3 gas [kmol/m3]
T_NH3 = NH3_T + CP.Kp_NH3 * r_sld * (V_S/V_L) * NH4;

// -----
// Other compound in liquid phase
// -----
CaCO3 = 0.0004; // Calcium Carbonate in solid [kmol/kg]
NaCl = 0.1353; // Sodium Chloride in solid [kmol/kg]
Ca_plus = 0.0; // Calcium ion concentration [kmol/m3]
Na_plus = 0.0; // Sodium ion [kmol/m3]
Cl_min = 0.0; // Chlorine ion [kmol/m3]
NO3 = 0.0; // Nitrate ion concentration [kmol/m3]

// -----
// Total Calcium in Cell [kmol/m3]
// -----
TCa = Ca_plus + CaCO3 * r_sld * (V_S /V_L);

// -----
// Total Inorganic Carbonate in Cell including CO2 gas [kmol/m3]
// -----
TIC = H2CO3 * (1.0 + (CP.Kd_H2CO3/H_plus)) + (CP.Kd_H2CO3 *
        CP.Kd_HCO3/sqr(H_plus));

// -----
// other compound in liquid phase
// -----
TOC = 24000 * CH3COOH_T; // TOC in leachate [mg-C/L]
BOD = 0.4 * (32/12) * TOC; // BOD in leachate [mg-O2/L]
COD = 0.0; // COD in leachate [mg-O2/L]
IC = 12000 * H2CO3_T; // Inorganic carbon in liquid [mg-C/L]
TN = 14000 * NH3_T; // Total Nitrogen [mg-N/L]
HUMUS = 0.0; // Humus [kmol/m3]
FOC = 0.0; // Initialize OC in solid phase [kg-C/kg-s]

```

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// -----
// Reaction rate for the decomposition of organic matter
// -----
// OP Aerobic decomposition of Protein [kmol/m3-d]
R_X_OP      = 0.0;      // OP : Net Biomass growth rate
R_PRO_OP    = 0.0;      //      : Protein organic consumption rate
R_O2_OP     = 0.0;      //      : Oxygen consumption rate
R_CO2_OP    = 0.0;      //      : CO2 generation rate
R_NH3_OP    = 0.0;      //      : Ammonia generation rate
R_H2O_OP    = 0.0;      //      : Water generation rate
R_CH3COOH_OP = 0.0;     //      : Acetic acid generation rate
R_H2_OP     = 0.0;      //      : Hydrogen generation rate
// OF Aerobic decomposition of Fats [kmol/m3-d]
R_X_OF      = 0.0;      // OF : Net Biomass growth rate
R_FAT_OF    = 0.0;      //      : Fats organic consumption rate
R_O2_OF     = 0.0;      //      : Oxygen consumption rate
R_CO2_OF    = 0.0;      //      : CO2 generation rate
R_NH3_OF    = 0.0;      //      : Ammonia generation rate
R_H2O_OF    = 0.0;      //      : Water generation rate
R_CH3COOH_OF = 0.0;     //      : Acetic acid generation rate
R_H2_OF     = 0.0;      //      : Hydrogen generation rate
// OG Aerobic decomposition of Carbohydrate [kmol/m3-d]
R_X_OG      = 0.0;      // OG : Net Biomass growth rate
R_GLU_OG    = 0.0;      //      : Carbohydrate organic consumption rate
R_O2_OG     = 0.0;      //      : Oxygen consumption rate
R_CO2_OG    = 0.0;      //      : CO2 generation rate
R_NH3_OG    = 0.0;      //      : Ammonia generation rate
R_H2O_OG    = 0.0;      //      : Water generation rate
R_CH3COOH_OG = 0.0;     //      : Acetic acid generation rate
R_H2_OG     = 0.0;      //      : Hydrogen generation rate
// OS Aerobic decomposition of Cellulose [kmol/m3-d]
R_X_OS      = 0.0;      // OS : Net Biomass growth rate
R_CEL_OS    = 0.0;      //      : Cellulose organic consumption rate
R_O2_OS     = 0.0;      //      : Oxygen consumption rate
R_CO2_OS    = 0.0;      //      : CO2 generation rate
R_NH3_OS    = 0.0;      //      : Ammonia generation rate
R_H2O_OS    = 0.0;      //      : Water generation rate
R_CH3COOH_OS = 0.0;     //      : Acetic acid generation rate
R_H2_OS     = 0.0;      //      : Hydrogen generation rate
// OH Aerobic decomposition of Lignin [kmol/m3-d]
R_X_OH      = 0.0;      // OH : Net Biomass growth rate
R_LIG_OH    = 0.0;      //      : Lignin organic consumption rate
R_O2_OH     = 0.0;      //      : Oxygen consumption rate
R_CO2_OH    = 0.0;      //      : CO2 generation rate
R_NH3_OH    = 0.0;      //      : Ammonia generation rate
R_H2O_OH    = 0.0;      //      : Water generation rate
R_CH3COOH_OH = 0.0;     //      : Acetic acid generation rate
R_H2_OH     = 0.0;      //      : Hydrogen generation rate
// NP Anaerobic fermentation of Protein [kmol/m3-d]
R_X_NP      = 0.0;      // NP : Net Biomass growth rate
R_PRO_NP    = 0.0;      //      : Protein organic consumption rate
R_CH3COOH_NP = 0.0;     //      : Acetic acid generation rate
R_CH3CH2COOH_NP = 0.0; //      : Propionic acid generation rate
R_CH3CH2CH2COOH_NP = 0.0; //      : Butyric acid generation rate
R_CO2_NP    = 0.0;      //      : CO2 generation rate
R_H2_NP     = 0.0;      //      : Hydrogen generation rate
R_NH3_NP    = 0.0;      //      : Ammonia generation rate
R_H2O_NP    = 0.0;      //      : Water generation rate
R_O2_NP     = 0.0;      //      : Oxygen generation rate
// NF Anaerobic fermentation of Fats [kmol/m3-d]
R_X_NF      = 0.0;      // NF : Net Biomass growth rate
R_FAT_NF    = 0.0;      //      : Fats organic consumption rate
R_CH3COOH_NF = 0.0;     //      : Acetic acid generation rate
R_CO2_NF    = 0.0;      //      : CO2 generation rate
R_NH3_NF    = 0.0;      //      : Ammonia generation rate
R_H2O_NF    = 0.0;      //      : Water generation rate
R_H2_NF     = 0.0;      //      : Hydrogen generation rate
R_O2_NF     = 0.0;      //      : Oxygen generation rate
// NG Anaerobic fermentation of Carbohydrate [kmol/m3-d]
R_X_NG      = 0.0;      // NG : Net Biomass growth rate
R_GLU_NG    = 0.0;      //      : Carbohydrate organic consumption rate
R_CH3COOH_NG = 0.0;     //      : Acetic acid generation rate

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R_CO2_NG      = 0.0;      //      : CO2 generation rate
R_NH3_NG      = 0.0;      //      : Ammonia generation rate
R_H2O_NG      = 0.0;      //      : Water generation rate
R_H2_NG       = 0.0;      //      : Hydrogen generation rate
R_O2_NG       = 0.0;      //      : Oxygen generation rate
// NS Anaerobic fermentation of Cellulose [kmol/m3-d]
R_X_NS        = 0.0;      // NS: Net Biomass growth rate
R_CEL_NS      = 0.0;      //      : Cellulose organic consumption rate
R_CH3COOH_NS  = 0.0;      //      : Acetic acid generation rate
R_CO2_NS      = 0.0;      //      : CO2 generation rate
R_NH3_NS      = 0.0;      //      : Ammonia generation rate
R_H2O_NS      = 0.0;      //      : Water generation rate
R_H2_NS       = 0.0;      //      : Hydrogen generation rate
R_O2_NS       = 0.0;      //      : Oxygen generation rate
// NH Anaerobic fermentation of Lignin [kmol/m3-d]
R_X_NH        = 0.0;      // NH: Net Biomass growth rate
R_LIG_NH      = 0.0;      //      : Lignin organic consumption rate
R_CH3COOH_NH  = 0.0;      //      : Acetic acid generation rate
R_CO2_NH      = 0.0;      //      : CO2 generation rate
R_NH3_NH      = 0.0;      //      : Ammonia generation rate
R_H2O_NH      = 0.0;      //      : Water generation rate
R_H2_NH       = 0.0;      //      : Hydrogen generation rate
R_O2_NH       = 0.0;      //      : Oxygen generation rate
// AP Acetogenesis of Propionic acid [kmol/m3-d]
R_X_AP        = 0.0;      // AP : Net Biomass growth rate
R_CH3CH2COOH_AP = 0.0;    //      : Propionic acids consumption rate
R_H2O_AP      = 0.0;      //      : Water generation rate
R_NH3_AP      = 0.0;      //      : Ammonia generation rate
R_CH3COOH_AP  = 0.0;      //      : Acetic acid generation rate
R_CO2_AP      = 0.0;      //      : CO2 generation rate
R_H2_AP       = 0.0;      //      : Hydrogen generation rate
R_O2_AP       = 0.0;      //      : Oxygen generation rate
// AB Acetogenesis of Butyric acid [kmol/m3-d]
R_X_AB        = 0.0;      // AB : Net Biomass growth rate
R_CH3CH2CH2COOH_AB = 0.0; //      : Butyric acids consumption rate
R_H2O_AB      = 0.0;      //      : Water generation rate
R_NH3_AB      = 0.0;      //      : Ammonia generation rate
R_CH3COOH_AB  = 0.0;      //      : Acetic acid generation rate
R_CO2_AB      = 0.0;      //      : CO2 generation rate
R_H2_AB       = 0.0;      //      : Hydrogen generation rate
R_O2_AB       = 0.0;      //      : Oxygen generation rate
// MT Methane formation from Acetic acid [kmol/m3-d]
R_X_MT        = 0.0;      // MT : Net Biomass growth rate
R_CH3COOH_MT  = 0.0;      //      : Acetic acid consumption rate
R_CH4_MT      = 0.0;      //      : Methane generation rate
R_CO2_MT      = 0.0;      //      : CO2 generation rate
R_NH3_MT      = 0.0;      //      : Ammonia generation rate
R_H2O_MT      = 0.0;      //      : Water generation rate
R_H2_MT       = 0.0;      //      : Hydrogen generation rate
R_O2_MT       = 0.0;      //      : Oxygen generation rate
// MT2 Methane formation from CO2 + H2 [kmol/m3-d]
R_X_MT2       = 0.0;      // MT2: Net Biomass growth rate
R_CH3COOH_MT2 = 0.0;      //      : Acetic acid consumption rate
R_CH4_MT2     = 0.0;      //      : Methane generation rate
R_CO2_MT2     = 0.0;      //      : CO2 generation rate
R_NH3_MT2     = 0.0;      //      : Ammonia generation rate
R_H2O_MT2     = 0.0;      //      : Water generation rate
R_H2_MT2      = 0.0;      //      : Hydrogen consumption rate
R_O2_MT2      = 0.0;      //      : Oxygen generation rate
// AO Oxidation of Acetic acid [kmol/m3-d]
R_X_AO        = 0.0;      // AO : Net Biomass growth rate
R_CH3COOH_AO  = 0.0;      //      : Acetic acid consumption rate
R_O2_AO       = 0.0;      //      : Oxygen consumption rate
R_NH3_AO      = 0.0;      //      : Ammonia consumption rate
R_CO2_AO      = 0.0;      //      : CO2 generate rate
R_H2O_AO      = 0.0;      //      : Water generation rate
R_H2_AO       = 0.0;      //      : Water generation rate
// PO Oxidation of Propionic acid [kmol/m3-d]
R_X_PO        = 0.0;      // PO : Net Biomass growth rate
R_CH3CH2COOH_PO = 0.0;    //      : Propionic acid consumption rate
R_O2_PO       = 0.0;      //      : Oxygen consumption rate
R_NH3_PO      = 0.0;      //      : Ammonia consumption rate

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R_CH3COOH_PO      = 0.0;    //      : Acetic acid generate rate
R_CO2_PO          = 0.0;    //      : CO2 generate rate
R_H2O_PO         = 0.0;    //      : Water generation rate
R_H2_PO          = 0.0;    //      : Water generation rate
// BO Oxidation of Butyric acid [kmol/m3-d]
R_X_BO           = 0.0;    // BO : Net Biomass growth rate
R_CH3CH2CH2COOH_BO = 0.0; //      : Butyric acid consumption rate
R_O2_BO         = 0.0;    //      : Oxygen consumption rate
R_NH3_BO        = 0.0;    //      : Ammonia consumption rate
R_CH3COOH_BO    = 0.0;    //      : Acetic acid generate rate
R_CO2_BO        = 0.0;    //      : CO2 generate rate
R_H2O_BO        = 0.0;    //      : Water generation rate
R_H2_BO         = 0.0;    //      : Water generation rate
// NO Nitrification of Ammonia [kmol/m3-d]
R_X_NO          = 0.0;    // NO : Net Biomass growth rate
R_NH3_NO        = 0.0;    //      : Ammonia consumption rate
R_O2_NO         = 0.0;    //      : Oxygen consumption rate
R_CH3COOH_NO    = 0.0;    //      : Acetic acid consumption rate
R_NO3_NO        = 0.0;    //      : Nitrate generate rate
R_H2O_NO        = 0.0;    //      : Water generation rate
R_CO2_NO        = 0.0;    //      : CO2 generate rate
R_H2_NO         = 0.0;    //      : Hydrogen consumption rate
// DN Denitrification of Nitrate [kmol/m3-d]
R_X_DN          = 0.0;    // DN : Net Biomass growth rate
R_NO3_DN        = 0.0;    //      : Nitric acid generation rate
R_CH3COOH_DN    = 0.0;    //      : Acetic acid generation rate
R_N2_DN         = 0.0;    //      : Nitrogen formation rate
R_CO2_DN        = 0.0;    //      : CO2 generation rate
R_H2O_DN        = 0.0;    //      : Water generation rate
R_H2_DN         = 0.0;    //      : Hydrogen consumption rate
R_NH3_DN        = 0.0;    //      : Ammonia consumption rate
R_O2_DN         = 0.0;    //      : Oxygen generation rate

// -----
// Effective diffusion coefficient of i component in gas
// -----
Dif              = 0.0001;    // Diffusion Coefficient of Gas          [m2/d]

// -----
// Production rate of humus by Biomass reaction
// -----
RFC              = 0.05;     // Fumic acid conversion                [kmol/m3-d]

// -----
// Heat transfer by heat conduction flux
// -----
for(i=0;i<=6;i++)qe[i]=0.0;    // heat flux unit                        [KJ/(m2*d)]

// -----
// Heat production by biological reactions [kJ/kmol]
// -----
dH_O2_OP        = 460000;    // heat value of R_O2_OP
dH_CH3COOH_OP   = 36200;    // heat value of R_CH3COOH_OP
dH_O2_OF        = 460000;    // heat value of R_O2_OF
dH_CH3COOH_OF   = 36200;    // heat value of R_CH3COOH_OF
dH_O2_OG        = 460000;    // heat value of R_O2_OG
dH_CH3COOH_OG   = 36200;    // heat value of R_CH3COOH_OG
dH_O2_OS        = 460000;    // heat value of R_O2_OS
dH_CH3COOH_OS   = 36200;    // heat value of R_CH3COOH_OS
dH_O2_OH        = 460000;    // heat value of R_O2_OH
dH_CH3COOH_OH   = 36200;    // heat value of R_CH3COOH_OH
dH_CH3COOH_NP   = 36200;    // heat value of R_CH3COOH_NP
dH_CH3CH2COOH_NP = 36200;    // heat value of R_CH3CH2COOH_NP
dH_O2_NP        = 460000;    // heat value of R_O2_NP
dH_CH3COOH_NF   = 36200;    // heat value of R_CH3COOH_NF
dH_O2_NF        = 460000;    // heat value of R_O2_NF
dH_CH3COOH_NG   = 36200;    // heat value of R_CH3COOH_NG
dH_O2_NG        = 460000;    // heat value of R_O2_NG
dH_CH3COOH_NS   = 36200;    // heat value of R_CH3COOH_NS
dH_O2_NS        = 460000;    // heat value of R_O2_NS
dH_CH3COOH_NH   = 36200;    // heat value of R_CH3COOH_NH

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dH_O2_NH          = 460000;      // heat value of R_O2_NH
dH_CH3COOH_AP     = 36200;       // heat value of R_CH3COOH_AP
dH_O2_AP          = 460000;      // heat value of R_O2_AP
dH_CH3COOH_AB     = 36200;       // heat value of R_CH3COOH_AB
dH_O2_AB          = 460000;      // heat value of R_O2_AB
dH_CH4_MT         = -15900;      // heat value of R_CH4_MT
dH_CH3COOH_MT     = 36200;       // heat value of R_CH3COOH_MT
dH_O2_MT         = 460000;      // heat value of R_O2_MT
dH_CH4_MT2        = 253000;      // heat value of R_CH4_MT2
dH_CH3COOH_MT2    = 36200;       // heat value of R_CH3COOH_MT2
dH_O2_MT2         = 460000;      // heat value of R_O2_MT2
dH_O2_AO          = 460000;      // heat value of R_O2_AO
dH_CH3COOH_AO     = 36200;       // heat value of R_CH3COOH_AO
dH_O2_PO          = 460000;      // heat value of R_O2_PO
dH_CH3COOH_PO     = 36200;       // heat value of R_CH3COOH_PO
dH_O2_BO          = 460000;      // heat value of R_O2_BO
dH_CH3COOH_BO     = 36200;       // heat value of R_CH3COOH_BO
dH_NH3_NO         = 361000;      // heat value of R_O2_NO
dH_CH3COOH_NO     = 36200;       // heat value of R_CH3COOH_NO
dH_CH3COOH_DN     = 36200;       // heat value of R_CH3COOH_DN
dH_NO3_DN         = -46000;      // heat value of R_NO3_DN

// -----
// Old values required for calculation
// -----
oldV_G             = V_G;         // Old values for gas phase          [-]
oldV_L             = V_L;         // Old values for liquid phase       [-]
oldTemp            = Temp;        // Old values for temperature        [-]

// -----
// Accumulated amount
// -----
Acu_QGout          = 0.0;        // Accumulated amount of QGout       [kmol]
Acu_CO2            = 0.0;        // Accumulated amount of CO2 gas     [kmol]
Acu_CH4            = 0.0;        // Accumulated amount of CH4 gas     [kmol]
Acu_H2             = 0.0;        // Accumulated amount of H2 gas      [kmol]
Acu_N2             = 0.0;        // Accumulated amount of N2 gas      [kmol]
Acu_PNH3           = 0.0;        // Accumulated amount of NH3 gas     [kmol]
Acu_O2             = 0.0;        // Accumulated amount of O2 gas      [kmol]

Acu_QLout          = 0.0;        // Accumulated amount of QGout       [kmol]
Acu_CH3COOH        = 0.0;        // Accumulated amount of Acetate     [kmol]
Acu_CH3CH2COOH     = 0.0;        // Accumulated amount of Propionate  [kmol]
Acu_CH3CH2CH2COOH = 0.0;        // Accumulated amount of Butyrate    [kmol]
Acu_IC             = 0.0;        // Accumulated amount of IC          [mg-C]
Acu_NH3            = 0.0;        // Accumulated amount of Ammonia     [kmol]
Acu_NO3            = 0.0;        // Accumulated amount of Nitrate     [kmol]
Acu_Caout          = 0.0;        // Accumulated amount of Ca          [kmol]

#####
#####
// Parameters relating to biological reactions
// Attention variables and constants coexist!!!!
#####
#####
// -----
// Biomass growth rate [kmol/m3-d]
// -----
R_OP_G             = 0.0;        // Biomass growth rate of Protein OP
R_OF_G             = 0.0;        // Biomass growth rate of Fats OF
R_OG_G             = 0.0;        // Biomass growth rate of Carbohydrate OG
R_OS_G             = 0.0;        // Biomass growth rate of Cellulose OS
R_OH_G             = 0.0;        // Biomass growth rate of Lignin OH
R_NP_G             = 0.0;        // Biomass growth rate of Protein NP
R_NF_G             = 0.0;        // Biomass growth rate of Fats NF
R_NG_G             = 0.0;        // Biomass growth rate of Carbohydrate NG
R_NS_G             = 0.0;        // Biomass growth rate of Cellulose NS
R_NH_G             = 0.0;        // Biomass growth rate of Lignin NH
R_AP_G             = 0.0;        // Biomass growth rate of Propionic acids AP
R_AB_G             = 0.0;        // Biomass growth rate of Butyric acids AB
R_MT_G             = 0.0;        // Biomass growth rate of Methanogens MT

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R_MT2_G = 0.0; // Biomass growth rate of Methanogens MT2
R_AO_G = 0.0; // Biomass growth rate of Acetic acids AO
R_PO_G = 0.0; // Biomass growth rate of Propionic acids PO
R_BO_G = 0.0; // Biomass growth rate of Butyric acids BO
R_NO_G = 0.0; // Biomass growth rate of Nitrification NO
R_DN_G = 0.0; // Biomass growth rate of Denitrification DN

// -----
// Biomass decay rate [kmol/m3-d]
// -----
R_OP_D = 0.0; // Biomass growth rate of Protein OP
R_OF_D = 0.0; // Biomass growth rate of Fats OF
R_OG_D = 0.0; // Biomass growth rate of Carbohydrate OG
R_OS_D = 0.0; // Biomass growth rate of Cellulose OS
R_OH_D = 0.0; // Biomass growth rate of Lignin OH
R_NP_D = 0.0; // Biomass growth rate of Protein NP
R_NF_D = 0.0; // Biomass growth rate of Fats NF
R_NG_D = 0.0; // Biomass growth rate of Carbohydrate NG
R_NS_D = 0.0; // Biomass growth rate of Cellulose NS
R_NH_D = 0.0; // Biomass growth rate of Lignin NH
R_AP_D = 0.0; // Biomass growth rate of Propionic acids AP
R_AB_D = 0.0; // Biomass growth rate of Butyric acids AB
R_MT_D = 0.0; // Biomass growth rate of Methanogens MT
R_MT2_D = 0.0; // Biomass growth rate of Methanogens MT2
R_AO_D = 0.0; // Biomass growth rate of Acetic acids AO
R_PO_D = 0.0; // Biomass growth rate of Propionic acids PO
R_BO_D = 0.0; // Biomass growth rate of Butyric acids BO
R_NO_D = 0.0; // Biomass growth rate of Nitrification NO
R_DN_D = 0.0; // Biomass growth rate of Denitrification DN

// -----
// Chemical formula & Molecular Weight of Biomass (CxHuOvNw)
// -----
Bio_x = 5.00; // Number of atom C in Biomass formula [-]
Bio_u = 7.00; // Number of atom H in Biomass formula [-]
Bio_v = 2.00; // Number of atom O in Biomass formula [-]
Bio_w = 1.00; // Number of atom N in Biomass formula [-]
MX = 12.01 * Bio_x + 1.01 * Bio_u + 15.99 * Bio_v + 14.0 * Bio_w;

// -----
// The ranges of partial pressure of O2 to determine the reaction type [Pa]
// -----
jdgP_O2_1 = 0.10 * atm.P; // Lower limit of aerobic condition
jdgP_O2_2 = 0.001 * atm.P; // Upper limit of anaerobic condition
jdgP_O2_3 = 0.0001 * atm.P; // Lower limit of anaerobic condition

// -----
// Constants of biological decomposition
// -----
// OP Aerobic decomposition of Protein
Y_OP = 0.10; // Yield coefficient Protein [-]
mu_OP = 5.00; // Maximum specific growth rate constant [1/d]
K_OP_S = 0.015; // Substrate saturation constant [-]
K_OP_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_OP_D = 0.05 * mu_OP; // Decay rate coefficient [1/d]
// OF Aerobic decomposition of Fats
Y_OF = 0.10; // Yield coefficient Fats [-]
mu_OF = 5.00; // Maximum specific growth rate constant [1/d]
K_OF_S = 0.015; // Substrate saturation constant [-]
K_OF_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_OF_D = 0.05 * mu_OF; // Decay rate coefficient [1/d]
// OG Aerobic decomposition of Carbohydrate
Y_OG = 0.10; // Yield coefficient Carbohydrate [-]
mu_OG = 5.00; // Maximum specific growth rate constant [1/d]
K_OG_S = 10/Y_OG; // Contois saturation constant [-]
K_OG_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_OG_D = 0.05 * mu_OG; // Decay rate coefficient [1/d]
// OS Aerobic decomposition of Cellulose
Y_OS = 0.10; // Yield coefficient Cellulose [-]
mu_OS = 1.00; // Maximum specific growth rate constant [1/d]
K_OS_S = 0.15; // Substrate saturation constant [-]
K_OS_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]

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K_OS_D = 0.05 * mu_OS; // Decay rate coefficient [1/d]
// OH Aerobic decomposition of Lignin
Y_OH = 0.10; // Yield coefficient Lignin [-]
mu_OH = 1.00; // Maximum specific growth rate constant [1/d]
K_OH_S = 0.15; // Substrate saturation constant [-]
K_OH_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_OH_D = 0.05 * mu_OH; // Decay rate coefficient [1/d]
// R_NP, R_NF, R_NG, R_NS & R_NX are mole ratio of Acetic acid to CO2 gas from
// carbon of organic matter. These figure are determined based on atomic balance of
// chemical reaction organic matter degradation. The following value are use in this
// model, for other combination the figure should refer to complete chemical reaction
// equation.
// Anaerobic Protein : Y_NP = 0.150, R_NP <= 4.650;
// Anaerobic Fats : Y_NF = 0.150, R_NF <= 27.10;
// Anaerobic Carbohydrate : Y_NG = 0.150, R_NG <= 2.625;
// Anaerobic Cellulose : Y_NS = 0.150, R_NS <= 8.625;
// Anaerobic Lignin : Y_NH = 0.150, R_NH <= 4.625;
// Anaerobic Propionic : Y_AP = 0.150, R_AP <= 1.125;
// Anaerobic Butyric : Y_AB = 0.150, R_AB <= 1.625;
// Anaerobic Biomass : R_NX <= 2.500;
// At above this value, all C is converted to be CH3COOH. Beyond this value, the
// atomic balance will not equal any more. For other Y_XX value, the R_XX, value must
// be recalculate using "Balance Check Organic Biodegradation 2012.06.02" file.
R_NP = 3.650; // Acetic acid production of Protein degradation
R_NF = 20.10; // Acetic acid production of Fats degradation
R_NG = 2.025; // Acetic acid production of Carbohydrate degradation
R_NS = 8.625; // Acetic acid production of Cellulose degradation
R_NH = 4.625; // Acetic acid production of Lignin degradation
R_AP = 1.125; // Acetic acid production of Propionate Acetogenesis
R_AB = 1.625; // Acetic acid production of Butyrate Acetogenesis
R_NX = 2.500; // Acetic acid production of Decayed biomass
// NP Anaerobic fermentation of Protein
Y_NP = 0.20; // Yield coefficient Protein [-]
mu_NP = 0.001; // Maximum specific growth rate constant [1/d]
K_NP_S = 25.00; // Substrate saturation constant [kg/m3]
K_NP_D = 0.05 * mu_NP; // Decay rate coefficient [1/d]
// NF Anaerobic fermentation of Fats
Y_NF = 0.20; // Yield coefficient Fats [-]
mu_NF = 0.002; // Maximum specific growth rate constant [1/d]
K_NF_S = 25.00; // Substrate saturation constant [kg/m3]
K_NF_D = 0.05 * mu_NF; // Decay rate coefficient [1/d]
// NG Anaerobic fermentation of Carbohydrate
Y_NG = 0.05; // Yield coefficient Carbohydrate [-]
mu_NG = 0.002; // Maximum specific growth rate constant [1/d]
K_NG_S = 25.00; // Substrate saturation constant [kg/m3]
K_NG_D = 0.05 * mu_NG; // Decay rate coefficient [1/d]
// NS Anaerobic fermentation of Cellulose
Y_NS = 0.150; // Yield coefficient Cellulose [-]
mu_NS = 0.000; // Maximum specific growth rate constant [1/d]
K_NS_S = 250.0; // Substrate saturation constant [kg/m3]
K_NS_D = 0.05 * mu_NS; // Decay rate coefficient [1/d]
// NH Anaerobic fermentation of Lignin
Y_NH = 0.150; // Yield coefficient Lignin [-]
mu_NH = 0.000; // Maximum specific growth rate constant [1/d]
K_NH_S = 500.0; // Substrate saturation constant [kg/m3]
K_NH_D = 0.05 * mu_NH; // Decay rate coefficient [1/d]
// AP Acetogenesis of Propionic acid
Y_AP = 0.050; // Yield coefficient Propionic acid [-]
mu_AP = 0.100; // Maximum specific growth rate constant [1/d]
K_AP_S = 10.00; // Substrate saturation constant [kg/m3]
K_AP_D = 0.05 * mu_AP; // Decay rate coefficient [1/d]
// AB Acetogenesis of Butyric acid
Y_AB = 0.050; // Yield coefficient Butyric acid [-]
mu_AB = 0.100; // Maximum specific growth rate constant [1/d]
K_AB_S = 10.00; // Substrate saturation constant [kg/m3]
K_AB_D = 0.05 * mu_AB; // Decay rate coefficient [1/d]
// MT Methane formation from Acetic acid
Y_MT = 0.005; // Yield coefficient Methanogens [-]
mu_MT = 0.009; // Maximum specific growth rate constant [1/d]
K_MT_S = 30.00; // Saturation constant for CH3COOH [kg/m3]
K_MT_D = 0.05 * mu_MT; // Decay rate coefficient [1/d]

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// MT2 Methane formation from CO2+H2
Y_MT2 = 0.005; // Yield coefficient Methanogens [-]
mu_MT2 = 0.750; // Maximum specific growth rate constant [1/d]
K_MT2_S = 15.00; // Saturation constant for CO2 + H2 [kg/m3]
K_MT2_D = 0.05 * mu_MT2; // Decay rate coefficient [1/d]
// AO Aerobic oxidation of Acetic acid
Y_AO = 0.20; // Yield coefficient Acetic acid decomposition [-]
mu_AO = 1.00; // Maximum specific growth rate constant [1/d]
K_AO_S = 0.02; // Substrate saturation constant [-]
K_AO_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_AO_D = 0.05 * mu_AO; // Decay rate coefficient [1/d]
// PO Aerobic oxidation of Propionic acid
Y_PO = 0.20; // Yield coefficient Propionic decomposition [-]
mu_PO = 1.00; // Maximum specific growth rate constant [1/d]
K_PO_S = 0.02; // Substrate saturation constant [-]
K_PO_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_PO_D = 0.05 * mu_PO; // Decay rate coefficient [1/d]
// BO Aerobic oxidation of Butyric acid
Y_BO = 0.20; // Yield coefficient Butyric acid decomposition [-]
mu_BO = 1.00; // Maximum specific growth rate constant [1/d]
K_BO_S = 0.02; // Substrate saturation constant [-]
K_BO_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_BO_D = 0.05 * mu_BO; // Decay rate coefficient [1/d]
// NO Aerobic nitrification of Ammonia
Y_NO = 0.20; // Yield coefficient Ammonia oxidation [-]
mu_NO = 1.00; // Maximum specific growth rate constant [1/d]
K_NO_S = 0.02; // Substrate saturation constant [-]
K_NO_O = 0.02*0.1013*1E6; // Saturation constant partial pressure O2 [Pa]
K_NO_D = 0.05 * mu_NO; // Decay rate coefficient [1/d]
// DN Anaerobic denitrification of Nitrate
Y_DN = 0.050; // Yield Methane formation from acetic acid [-]
mu_DN = 0.001; // Maximum specific growth rate methanogens [1/d]
K_DN_S = 0.30; // Substrate saturation constant [kg/m3]
K_DN_D = 0.05 * mu_DN; // Decay rate coefficient of methane bacteria [1/d]
// Critical amount of acetic acid
CH3COOH_Tcri= 2.0E-3; // Critical amount of acetic acid [kg/m3]

// -----
// Initial amount of bacteria [kg/m3]
// -----
X_OPini = 0.150; // Aerobic decomposition bacteria of Protein
X_OFini = 0.150; // Aerobic decomposition bacteria of Fats
X_OGini = 0.150; // Aerobic decomposition bacteria of Carbohydrate
X_OSini = 0.150; // Aerobic decomposition bacteria of Cellulose
X_OHini = 0.150; // Aerobic decomposition bacteria of Lignin
X_NPini = 0.150; // Anaerobic fermentation bacteria of Protein
X_NFini = 0.150; // Anaerobic fermentation bacteria of Fats
X_NGini = 0.150; // Anaerobic fermentation bacteria of Carbohydrate
X_NSini = 0.150; // Anaerobic fermentation bacteria of Cellulose
X_NHini = 0.150; // Anaerobic fermentation bacteria of Lignin
X_APini = 0.150; // Acetogenesis Propionic acid bacteria
X_ABini = 0.150; // Acetogenesis Propionic acid bacteria
X_MTini = 0.150; // Methane formation of Acetic acid bacteria
X_MT2ini = 0.150; // Methane formation bacteria of CO2+H2 bacteria
X_AOini = 0.150; // Acetic acid oxidation bacteria
X_POini = 0.150; // Propionic acid oxidation bacteria
X_BOini = 0.150; // Butyric acid oxidation bacteria
X_NOini = 0.150; // Ammonia nitrification bacteria
X_DNini = 0.150; // Nitrate denitrification bacteria

// -----
// Amount of bacteria [kg/m3]
// -----
X_OP = X_OPini; // Aerobic decomposition bacteria of Protein
X_OF = X_OFini; // Aerobic decomposition bacteria of Fats
X_OG = X_OGini; // Aerobic decomposition bacteria of Carbohydrate
X_OS = X_OSini; // Aerobic decomposition bacteria of Cellulose
X_OH = X_OHini; // Aerobic decomposition bacteria of Lignin
X_NP = X_NPini; // Anaerobic fermentation bacteria of Protein
X_NF = X_NFini; // Anaerobic fermentation bacteria of Fats

```

```

X_NG      = X_NGini;           // Anaerobic fermentation bacteria of Carbohydrate
X_NS      = X_NSini;           // Anaerobic fermentation bacteria of Cellulose
X_NH      = X_NHini;           // Anaerobic fermentation bacteria of Lignin
X_AP      = X_APini;           // Acetogenesis Propionic acid bacteria
X_AB      = X_ABini;           // Acetogenesis Butyric acid bacteria
X_MT      = X_MTini;           // Methane formation of Acetic acid bacteria
X_MT2     = X_MT2ini;          // Methane formation bacteria of CO2+H2 bacteria
X_AO      = X_AOini;           // Acetic acid oxidation bacteria
X_PO      = X_POini;           // Propionic acid oxidation bacteria
X_BO      = X_BOini;           // Butyric acid oxidation bacteria
X_NO      = X_NOini;           // Ammonia nitrification bacteria
X_DN      = X_DNini;           // Nitrate denitrification bacteria

// -----
// Total of organic matter [kg/m3]
// -----
ORG_T     = S_PRO + S_FAT + S_GLU + S_CEL + S_LIG
          + X_OP + X_OF + X_OG + X_OS + X_OH + X_NP + X_NF + X_NG + X_NS + X_NH
          + X_AP + X_AB + X_MT + X_MT2 + X_AO + X_PO + X_BO + X_NO + X_DN
          - X_OPini - X_OFini - X_OGini - X_OSini - X_OHini - X_NPini - X_NFini
          - X_NGini - X_NSini - X_NHini - X_APini - X_ABini - X_MTini - X_MT2ini
          - X_AOini - X_POini - X_BOini - X_NOini - X_DNini;

// -----
// Variables for Total Carbon and Total Nitrogen Mass balance check
// -----
C_in_Solid = 0.0;              // Total Carbon in Solid phase           [kmol-C]
C_in_Liquid = 0.0;             // Total Carbon in Liquid phase          [kmol-C]
C_in_Gas    = 0.0;             // Total Carbon in Gas phase             [kmol-C]
C_in_Total  = 0.0;             // Total Carbon in Cell                   [kmol-C]

N_in_Solid  = 0.0;              // Total Nitrogen in Solid phase          [kmol-N]
N_in_Liquid = 0.0;             // Total Nitrogen in Liquid phase         [kmol-N]
N_in_Gas    = 0.0;             // Total Nitrogen in Gas phase            [kmol-N]
N_in_Total  = 0.0;             // Total Nitrogen in Cell                 [kmol-N]

#####
#####
// Constants and initial values for heat calculation
#####
#####
Heat_param::Heat_param() {
Ua      = 100;                  // Overall heat-transfer coefficient     [kJ/(m2*d*K)]
Tsoil_const = 303.15;          // Homo-thermal Temperature of soil     [K]

// double K_waste(double cwc);
K_cover   = 145.76;             // Thermal conductivity of cover        [kJ(m*d*K)]
K_grav    = 60.465;            // Thermal conductivity of gravel       [kJ(m*d*K)]
K_soil    = 145.76;            // Thermal conductivity of soil         [kJ(m*d*K)]
K_water   = 50.10;             // Thermal conductivity of water        [kJ(m*d*K)]

// cp_waste(double cwc)
cp_cover  = 1.48;               // Specific heat capacity of cover       [kJ/(kg*K)]
cp_grav   = 1.48;               // Specific heat capacity of gravel      [kJ/(kg*K)]
cp_soil   = 1.48;               // Specific heat capacity of soil        [kJ/(kg*K)]
cp_water  = 4.18;               // Specific heat capacity of water       [kJ/(kg*K)]

// re_waste(double cwc);
pRa      = 495;                 // Apparent density of waste            [-]
pRb      = 1000;                // Apparent density of waste            [-]

re_cover  = 1300;               // Apparent density of cover            [kg/m3]
re_grav   = 1300;               // Apparent density of gravel           [kg/m3]
re_soil   = 1300;               // Apparent density of soil             [kg/m3]
re_water  = 1300;               // Apparent density of water            [kg/m3]
}

```

```
//#####  
//#####  
// Setting the vicinity conditions of a landfill Cell for temperature calculation  
//#####  
//#####  
void Cell_circumference_cond_set(void){  
LayM[1].media = cover; LayM[1].temp = 303.15; LayM[1].H = 1.0; LayM[1].wc = 0.0;  
LayM[2].media = grav; LayM[2].temp = 303.15; LayM[2].H = 15.0; LayM[2].wc = 0.5;  
LayM[3].media = air; LayM[3].temp = 303.15; LayM[3].H = 0.1; LayM[3].wc = 0.0;  
LayM[4].media = none; LayM[4].temp = -999; LayM[4].H = -999; LayM[4].wc = -999;  
LayM[5].media = none; LayM[5].temp = -999; LayM[5].H = -999; LayM[5].wc = -999;  
LayM[6].media = none; LayM[6].temp = -999; LayM[6].H = -999; LayM[6].wc = -999;  
}
```

## Module IV: Calculation Step

```

#include "Cell.h" // Header file
extern double t; // Start calculation time
extern double dt; // Differential calculation time
extern double t_end; // End calculation time
extern double prt_dt; // Interval printout calculation results
extern Global_const CP; // Global constants
extern Atmospheric_cond atm; // Atmosphere condition
extern Environment_cond env; // Environment condition

#####
#####
// Calculating gas production and the amount of leachate
#####
#####
//-----
// Calculation of total pressure within the Cell [Pa]
//-----
void Cell::cal_PT(void) {
PT = P_CO2
  + P_NH3
  + P_O2
  + P_N2
  + P_H2
  + P_CH4
  + P_H2O;
}

//-----
// Calculation Gas production [QGout] [kmol/d]
//-----
void Cell::cal_QGout(void) {
QGout = (PT-atm.P)*V_G/(CP.R*Temp)/dt;

  if (PT <= atm.P) {
    QGout = 0.0;
  }

}

//-----
// Calculation The amount of leachate [QLout]
//-----
void Cell::cal_QLout(void) {
double A,B,C,D;

A = QLin;
B = (R_H2O_OP+R_H2O_OF+R_H2O_OG+R_H2O_OS+R_H2O_OH
  + R_H2O_NP+R_H2O_NF+R_H2O_NG+R_H2O_NS+R_H2O_NH
  + R_H2O_AP+R_H2O_AB+R_H2O_MT+R_H2O_MT2
  + R_H2O_AO+R_H2O_PO+R_H2O_BO
  + R_H2O_NO+R_H2O_DN) *V;
C = -QGout*P_H2O/PT;

D = A+(B+C) *18/1000

oldV_G = V_G;
oldV_L = V_L;

V_L = V_L+D*dt;

if (V_L > V*wcp) {
  QLout = (V_L-V*wcp)/dt;
  V_L = V*wcp;
  wc = V_L/V;
}
else{

```

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---

```

    QLout   = 0.0;
    wc      = V_L/V;
  }
  V_G      = V-V_S-V_L;
}

//#####
//#####
// Calculating the pressure in Cell to to make it be in equilibrium with the
// atmospheric pressure
// after the discharge of QGout. Each partial pressure is obtained by multiplying the
// atm.P/PT.
//#####
//#####
void Cell::Cell_press_equilibrium(void){
P_CO2   = P_CO2 * atm.P/PT;
P_CH4   = P_CH4 * atm.P/PT;
P_H2    = P_H2  * atm.P/PT;
P_N2    = P_N2  * atm.P/PT;
P_NH3   = P_NH3*atm.P/PT;
P_O2    = P_O2  * atm.P/PT;
P_H2O   = P_H2O*atm.P/PT;
PT      = atm.P;
}

//#####
//#####
// Mass Balance for Carbon and Nitrogen
//#####
//#####
void Cell::Massbalance_check(){
//-----
// Calculation of Carbon balance within Cell
//-----
C_in_Gas      = (P_CO2+P_CH4)*V_G/(CP.R*Temp);

C_in_Liquid   = (H2CO3_T+CH3COOH_T*2.0+CH3CH2COOH_T*3.0+CH3CH2CH2COOH_T*4.0)*V_L;

C_in_Solid    = (S_PRO/M_PRO*Pro_a+S_FAT/M_FAT*Fat_a+S_GLU/M_GLU*Glu_a+S_CEL/M_CEL
* Cel_a+S_LIG/M_LIG*Lig_a)*V
+ (X_OP+X_OF+X_OG+X_OS+X_OH+X_NP+X_NF+X_NG+X_NS+X_NH
+ X_AP+X_AB+X_MT+X_MT2+ X_AO+X_PO+X_BO+ X_NO+X_DN)/MX*Bio_x*V
+ CaCO3*V_S*r_sld;

C_in_Total   = (P_CH4)*V_G/(CP.R*Temp)
+ (TIC+CH3COOH_T*2.0+CH3CH2COOH_T*3.0+CH3CH2CH2COOH_T*4.0)*V_L
+ (S_PRO/M_PRO*Pro_a+S_FAT/M_FAT*Fat_a+S_GLU/M_GLU*Glu_a+S_CEL/M_CEL
* Cel_a + S_LIG/M_LIG*Lig_a)*V
+ (X_OP+X_OF+X_OG+X_OS+X_OH+X_NP+X_NF+X_NG+X_NS+X_NH
+ X_AP+X_AB+X_MT+X_MT2+ X_AO+X_PO+X_BO+ X_NO+X_DN)/MX*Bio_x*V;

//-----
// Fraction of OC calculation [kg-C/kg-S]
//-----
FOC           = (C_in_Solid-CaCO3*V_S*r_sld)*12/(V_S*r_sld);

//-----
// Calculation of Nitrogen balance within Cell
//-----
N_in_Gas      = (P_NH3+P_N2*2.0)*V_G/(CP.R*Temp);

N_in_Liquid   = (NH3_T+NO3)*V_L;

N_in_Solid    = (S_PRO)/M_PRO*Pro_n*V
+ NH4_abs*V_L
+ (X_OP+X_OF+X_OG+X_OS+X_OH+X_NP+X_NF+X_NG+X_NS+X_NH
+ X_AP+X_AB+X_MT+X_MT2+ X_AO+X_PO+X_BO+ X_NO+X_DN)/MX*Bio_w*V;

N_in_Total   = (P_NH3+P_N2*2.0)*V_G/(CP.R*Temp)
+ (NH3_T+NO3)*V_L

```

```

+ (S_PRO)/M_PRO*Pro_n*V
+ NH4_abs*V_L
+ (X_OP+X_OF+X_OG+X_OS+X_OH+X_NP+X_NF+X_NG+X_NS+X_NH
+ X_AP+X_AB+X_MT+X_MT2+ X_AO+X_PO+X_BO+ X_NO+X_DN)/MX*Bio_w*V;
}

#####
#####
// Calculation at dt step (Euler's method)
#####
//-----
// The rate of washing-out Debugging
//-----
double Cell::xi(void){
    return(1.0);
}

#####
#####
// Calculating aqueous concentrations at dt step
#####
//-----
// Euler's method for Total Inorganic Carbonate [d(TIC)/dt]
//-----
void Cell::cal_TIC_step(void){
double C,D,E,F,G,H;
C  =-QGout*P_CO2/PT;
    if(QGout < 0.0){
        C  = 0.0;
    }
D  =(R_CO2_OP+R_CO2_OF+R_CO2_OG+R_CO2_OS+R_CO2_OH
+ R_CO2_NP+R_CO2_NF+R_CO2_NG+R_CO2_NS+R_CO2_NH
+ R_CO2_AP+R_CO2_AB+R_CO2_MT+R_CO2_MT2
+ R_CO2_AO+R_CO2_PO+R_CO2_BO
+ R_CO2_NO+R_CO2_DN)*V;

E  = (C+D)*dt*(CP.R*Temp)/V_G;

F  = (E/CP.Henry_CO2)*(1.0+(CP.Kd_H2CO3/H_plus)
+ (CP.Kd_H2CO3*CP.Kd_HCO3)/sqr(H_plus));

G  =-xi()*QLout*H2CO3_T;
H  = R_ratio*(-G);

TIC = F+(oldV_L*TIC+(G+H)*dt)/V_L;

if(TIC < 0.0) {
    cout << "***** TIC minus!! *****" << endl;
    TIC  = 0.0;
}
}

//-----
// Euler's method for Total Ammonia [d(T_NH3)/dt]
//-----
void Cell::cal_T_NH3_step(void){
double C,D,E,F,G,H;

C  =-QGout*P_NH3/PT;
    if(QGout < 0.0){
        C  = 0.0;
    }
}

D  =(R_NH3_OP+R_NH3_OF+R_NH3_OG+R_NH3_OS+R_NH3_OH
+ R_NH3_NP+R_NH3_NF+R_NH3_NG+R_NH3_NS+R_NH3_NH
+ R_NH3_AP+R_NH3_AB+R_NH3_MT+R_NH3_MT2
+ R_NH3_AO+R_NH3_PO+R_NH3_BO
+ R_NH3_NO+R_NH3_DN)*V;

```

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E = (C+D)*dt*(CP.R*Temp)/V_G;

F = (E/CP.Henry_NH3)*(1.0+(CP.Kd_NH3/OH_min));

G = -xi()*QLout*NH3_T;
H = R_ratio*(-G);

T_NH3 = F+(oldV_L*T_NH3+(G+H)*dt)/V_L;
if(T_NH3 < 0.0){
  cout << "***** T_NH3 minus!! *****" << endl;
  T_NH3 = 0.0;
}

//-----
// Euler's method for Total Acetic acid [d(CH3COOH_T)/dt]
//-----
void Cell::cal_CH3COOH_T_step(void){
double A,B,C;

A = -xi()*QLout*CH3COOH_T;
B = R_ratio*(-A);

C = (R_CH3COOH_OP+R_CH3COOH_OF+R_CH3COOH_OG+R_CH3COOH_OS+R_CH3COOH_OH
+ R_CH3COOH_NP+R_CH3COOH_NF+R_CH3COOH_NG+R_CH3COOH_NS+R_CH3COOH_NH
+ R_CH3COOH_AP+R_CH3COOH_AB+R_CH3COOH_MT+R_CH3COOH_MT2
+ R_CH3COOH_AO+R_CH3COOH_PO+R_CH3COOH_BO
+ R_CH3COOH_NO+R_CH3COOH_DN)*V;

CH3COOH_T = (oldV_L*CH3COOH_T+(A+B+C)*dt)/V_L;
if(CH3COOH_T < 0.0){
  cout << "***** CH3COOH_T minus!! *****" << endl;
  CH3COOH_T = 0.0;
}

//-----
// Euler's method for Total Propionate [d(CH3CH2COOH_T)/dt]
//-----
void Cell::cal_CH3CH2COOH_T_step(void){
double A,B,C;

A = -xi()*QLout*CH3CH2COOH_T;
B = R_ratio*(-A);

C = (R_CH3CH2COOH_NP+R_CH3CH2COOH_AP+R_CH3CH2COOH_PO)*V;

CH3CH2COOH_T = (oldV_L*CH3CH2COOH_T+(A+B+C)*dt)/V_L;
if(CH3CH2COOH_T < 0.0){
  cout << "***** CH3CH2COOH_T minus!! *****" << endl;
  CH3CH2COOH_T = 0.0;
}

//-----
// Euler's method for Total Butyrate [d(CH3CH2CH2COOH_T)/dt]
//-----
void Cell::cal_CH3CH2CH2COOH_T_step(void){
double A,B,C;

A = -xi()*QLout*CH3CH2CH2COOH_T;
B = R_ratio*(-A);

C = (R_CH3CH2CH2COOH_NP+R_CH3CH2CH2COOH_AB+R_CH3CH2CH2COOH_BO)*V;

CH3CH2CH2COOH_T = (oldV_L*CH3CH2CH2COOH_T+(A+B+C)*dt)/V_L;
if(CH3CH2CH2COOH_T < 0.0){
  cout << "***** CH3CH2CH2COOH_T minus!! *****" << endl;
  CH3CH2CH2COOH_T = 0.0;
}
}

```

```

//-----
// Euler's method for Nitrate [d(NO3)/dt]
//-----
void Cell::cal_NO3_step(void) {
double A,B,C;

A  =-xi()*QLout*NO3;
B  = R_ratio*(-A);

C  = (R_NO3_NO+R_NO3_DN)*V;

NO3 = (oldV_L*NO3+(A+B+C)*dt)/V_L;
if(NO3 < 0.0){
cout << "***** NO3 minus!! *****" << endl;
NO3  = 0.0;
}
}

//-----
// Euler's method for Calculation of Total Calcium [d(Ca)/dt]
//-----
void Cell::cal_Ca_step(void) {
double A,B;

A  =-xi()*QLout*Ca_plus;
B  = R_ratio*(-A);

Ca_plus = (oldV_L*Ca_plus+(A+B)*dt)/V_L;

TCa = Ca_plus+CaCO3*r_sld*(V_S/V_L);
if(TCa < 0.0){
cout << "***** TCa minus!! *****" << endl;
TCa  = 0.0;
}
}

//-----
// Euler's method for Alkaline concentration such as Na+ [d(Na_plus)/dt]
//-----
void Cell::cal_Na_step(void) {
double A,B,C;

A  =-xi()*QLout*Na_plus;
B  = R_ratio*(-A);

C  =-(R_PRO_OP+R_FAT_OF+R_GLU_OG+R_CEL_OS+R_LIG_OH
+ R_PRO_NP+R_FAT_NF+R_GLU_NG+R_CEL_NS+R_LIG_NH) * NaCl*r_sld*(V_S /V_L);

Na_plus = (oldV_L*Na_plus+(A+B+C)*dt)/V_L;
if(Na_plus < 0.0){
cout << "***** Na_plus minus!! *****" << endl;
Na_plus  = 0.0;
}
}

//-----
// Euler's method for Chloride [d(Cl)/dt]
//-----
void Cell::cal_Cl_step(void) {
double A,B,C;

A  =-xi()*QLout*Cl_min;
B  = R_ratio*(-A);

C  =-(R_PRO_OP+R_FAT_OF+R_GLU_OG+R_CEL_OS+R_LIG_OH
+ R_PRO_NP+R_FAT_NF+R_GLU_NG+R_CEL_NS+R_LIG_NH) * NaCl*r_sld*(V_S /V_L);

Cl_min = (oldV_L*Cl_min+(A+B+C)*dt)/V_L;
if(Cl_min < 0.0){
cout << "***** Cl_min minus!! *****" << endl;
Cl_min  = 0.0;
}
}

```

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```

    }
}

//#####
//#####
// Calculation of gaseous concentrations at dt step
//#####
//#####
//-----
// Euler's method for partial pressure Methane [d(P_CH4)/dt]
//-----
void Cell::cal_PCH4_step(void){
double C,D;
double oldP_CH4;

C   =-QGout*P_CH4/PT;
    if(QGout < 0.0){
        C       = 0.0;
    }

D   = (R_CH4_MT+R_CH4_MT2)*V;

oldP_CH4 = P_CH4;
P_CH4    = (oldV_G*P_CH4/(CP.R*oldTemp)+(C+D)*dt)*((CP.R*Temp)/V_G);
    if(P_CH4 < 0.0){
        cout << "***** P_CH4 minus!! *****" << endl;
        P_CH4 = 0.0;
    }
}

//-----
// Euler's method for partial pressure Hydrogen [d(P_H2)/dt]
//-----
void Cell::cal_PH2_step(void){
double C,D;
double oldP_H2;

C   = -QGout*P_H2/PT;
    if(QGout < 0.0){
        C       = 0.0;
    }

D   =(R_H2_OP+R_H2_OF+R_H2_OG+R_H2_OS+R_H2_OH
+ R_H2_NP+R_H2_NF+R_H2_NG+R_H2_NS+R_H2_NH
+ R_H2_AP+R_H2_AB+R_H2_MT+R_H2_MT2
+ R_H2_AO+R_H2_PO+R_H2_BO
+ R_H2_NO+R_H2_DN)*V;

oldP_H2 = P_H2;
P_H2    = (oldV_G*P_H2/(CP.R*oldTemp)+(C+D)*dt)*((CP.R*Temp)/V_G);
    if(P_H2 < 0.0){
        cout << "***** P_H2 minus!! *****" << endl;
        P_H2 = 0.0;
    }
}

//-----
// Euler's method for partial pressure Nitrogen [d(P_N2)/dt]
//-----
void Cell::cal_PN2_step(void){
double C,D;
double oldP_N2;

C   =-QGout*P_N2/PT;
    if(QGout < 0.0){
        C       = 0.0;
    }

D   = (R_N2_DN)*V;

oldP_N2 = P_N2;

```

```

P_N2 = (oldV_G*P_N2/(CP.R*oldTemp)+(C+D)*dt)*((CP.R*Temp)/V_G);
    if(P_N2 < 0.0){
        cout << "***** P_N2 minus!! *****" << endl;
        P_N2 = 0.0;
    }
}

//-----
// Euler's method for partial pressure Oxygen [d(P_O2)/dt]
//-----
void Cell::cal_PO2_step(void){
double C,D;
double oldP_O2;

C = -QGout*P_O2/PT;
    if(QGout < 0.0){
        C = 0.0;
    }

D = (R_O2_OP+R_O2_OF+R_O2_OG+R_O2_OS+R_O2_OH
    + R_O2_NP+R_O2_NF+R_O2_NG+R_O2_NS+R_O2_NH
    + R_O2_AP+R_O2_AB+R_O2_MT+R_O2_MT2
    + R_O2_AO+R_O2_PO+R_O2_BO
    + R_O2_NO+R_O2_DN)*V;

oldP_O2 = P_O2;
P_O2 = (oldV_G*P_O2/(CP.R*oldTemp)+(C+D)*dt)*(CP.R*Temp)/V_G;
    if(P_O2 < 0.0){
        cout << "***** P_O2 minus!! *****" << endl;
        P_O2 = 0.0;
    }
}

//-----
// Euler's method for partial pressure of Water vapor [d(P_H2O)/dt]
//-----
void Cell::cal_PH2O_step(void){

P_H2O = exp(20.386-5132/Temp)*133.32239/1000;
}

#####
#####
// Calculating the amount of organic substances at dt step
#####
#####
//-----
// Euler's method for Protein [d(S_PRO)/dt]
//-----
void Cell::cal_SPRO_step(void){
S_PRO = S_PRO+(R_PRO_OP+R_PRO_NP)*M_PRO*dt;
}

//-----
// Euler's method for Fats [d(S_FAT)/dt]
//-----
void Cell::cal_SFAT_step(void){
S_FAT = S_FAT+(R_FAT_OF+R_FAT_NF)*M_FAT*dt;
}

//-----
// Euler's method for Carbohydrate [d(S_GLU)/dt]
//-----
void Cell::cal_SGLU_step(void){
S_GLU = S_GLU+(R_GLU_OG+R_GLU_NG)*M_GLU*dt;
}

```

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```
//-----
// Euler's method for Cellulose [d(S_CEL)/dt]
//-----
void Cell::cal_SCEL_step(void){
S_CEL = S_CEL+(R_CEL_OS+R_CEL_NS)*M_CEL*dt;
}

//-----
// Euler's method for Lignin [d(S_LIG)/dt]
//-----
void Cell::cal_SLIG_step(void){
S_LIG = S_LIG+(R_LIG_OH+R_LIG_NH)*M_LIG*dt;
}

//-----
// Calculating the amount of biomass at dt step
//-----
void Cell::cal_X_step(void){
X_OP = X_OP + R_X_OP*MX*dt; // Euler's method for [d(X_OP)/dt]
X_OF = X_OF + R_X_OF*MX*dt; // Euler's method for [d(X_OF)/dt]
X_OG = X_OG + R_X_OG*MX*dt; // Euler's method for [d(X_OG)/dt]
X_OS = X_OS + R_X_OS*MX*dt; // Euler's method for [d(X_OS)/dt]
X_OH = X_OH + R_X_OH*MX*dt; // Euler's method for [d(X_OH)/dt]
X_NP = X_NP + R_X_NP*MX*dt; // Euler's method for [d(X_NP)/dt]
X_NF = X_NF + R_X_NF*MX*dt; // Euler's method for [d(X_NF)/dt]
X_NG = X_NG + R_X_NG*MX*dt; // Euler's method for [d(X_NG)/dt]
X_NS = X_NS + R_X_NS*MX*dt; // Euler's method for [d(X_NS)/dt]
X_NH = X_NH + R_X_NH*MX*dt; // Euler's method for [d(X_NH)/dt]
X_AP = X_AP + R_X_AP*MX*dt; // Euler's method for [d(X_AP)/dt]
X_AB = X_AB + R_X_AB*MX*dt; // Euler's method for [d(X_AB)/dt]
X_MT = X_MT + R_X_MT*MX*dt; // Euler's method for [d(X_MT)/dt]
X_MT2 = X_MT2 + R_X_MT2*MX*dt; // Euler's method for [d(X_MT2)/dt]
X_AO = X_AO + R_X_AO*MX*dt; // Euler's method for [d(X_AO)/dt]
X_PO = X_PO + R_X_PO*MX*dt; // Euler's method for [d(X_PO)/dt]
X_BO = X_BO + R_X_BO*MX*dt; // Euler's method for [d(X_BO)/dt]
X_NO = X_NO + R_X_NO*MX*dt; // Euler's method for [d(X_NO)/dt]
X_DN = X_DN + R_X_DN*MX*dt; // Euler's method for [d(X_DN)/dt]
}

//-----
// Total amount of organic substances in a Cell [kg/m3]
//-----
void Cell::cal_ORG_T_step(void){
ORG_T = S_PRO+S_FAT+S_GLU+S_CEL+S_LIG
+ X_OP+X_OF+X_OG+X_OS+X_OH+ X_NP+X_NF+X_NG+X_NS+X_NH
+ X_AP+X_AB+X_MT+X_MT2+X_AO+X_PO+X_BO+X_NO+X_DN
- X_OPini-X_OFini-X_OGini-X_OSini-X_OHini
- X_NPini-X_NPini-X_NGini-X_NSini-X_NHini
- X_APini-X_ABini-X_MTini-X_MT2ini
- X_AOini-X_POini-X_BOini-X_NOini-X_DNini;
}

//-----
// Euler's method for landfilled dimension at dt step [d(H)/dt]
//-----
void Cell::cal_H_step(void){
H = ((ORG_T+S_INO)*V/r_sld)+V_L+V_G)/S;
}

```

```

#####
#####
// Calculation concentration of gaseous and liquid phases after Equilibrium
// condition. This section is addressed to calculate concentration of component pH
// dependent. The parent concentration already calculate by Euler's method, while
// daughter concentration must be calculate after new pH determined. This include
// Total Ammonia in liquid phase [NH3_T], Ammonia concentration [NH3], Ammonium ion
// concentration [NH4], Ammonia adsorb in solid phase [NH4_abs], Partial pressure NH3
// [P_NH3], Acetic acid [CH3COOH], Acetate ion [CH3COO], and Inorganic carbon in
// liquid [IC]. Whilst concentration Carbonic Acid [H2CO3], Bicarbonate ion [HCO3],
// Carbonate ion [CO3], and Partial pressure CO2 [P_CO2] already calculate in pH
// calculation module. Concentration each component is calculate as follows:
#####
#####
//-----
// Calculation of Inorganic carbon in liquid [IC]
//-----
void Cell::cal_IC(void){
IC = 12*H2CO3_T*1000;
}

//-----
// Calculation of Total Ammonia in liquid phase [NH3_T]
//-----
void Cell::cal_NH3_T(void){
NH3_T = T_NH3/(1.0+CP.Kp_NH3*r_sld*(V_S/V_L)/(1.0+(CP.Kd_NH3/OH_min))
* (CP.Kd_NH3/OH_min));
}

//-----
// Calculation of Ammonia concentration [NH3]
//-----
void Cell::cal_NH3(void){
NH3 = NH3_T/(1.0+(CP.Kd_NH3/OH_min));
}

//-----
// Calculation of Ammonium ion concentration [NH4]
//-----
void Cell::cal_NH4(void){
NH4 = NH3_T/(1.0+(CP.Kd_NH3/OH_min))* (CP.Kd_NH3/OH_min);
}

//-----
// Calculation of Ammonia adsorb in solid phase [NH4_abs]
//-----
void Cell::cal_NH4_Adsorp_inCell(void){
NH4_abs = CP.Kp_NH3*r_sld*(V_S/V_L)*NH4;
}

//-----
// Calculation of [P_NH3]
//-----
void Cell::cal_PNH3(void){
P_NH3 = CP.Henry_NH3*NH3_T/(1.0+(H_plus/CP.Kd_NH3));
}

//-----
// Calculation of Acetic acid [CH3COOH]
//-----
void Cell::cal_CH3COOH(void){
CH3COOH = CH3COOH_T/(1.0+(CP.Kd_CH3COOH/H_plus));
}

//-----
// Calculation of Acetate ion [CH3COO]
//-----
void Cell::cal_CH3COO(void){
CH3COO = CH3COOH_T/(1.0+(CP.Kd_CH3COOH/H_plus))* (CP.Kd_CH3COOH/H_plus);
}

//-----

```

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```

// Calculation of Propionate [CH3CH2COOH]
//-----
void Cell::cal_CH3CH2COOH(void){
CH3CH2COOH = CH3CH2COOH_T/(1.0+(CP.Kd_CH3CH2COOH/H_plus));
}

//-----
// Calculation of Propionate ion [CH3CH2COO]
//-----
void Cell::cal_CH3CH2COO(void){
CH3CH2COO = CH3CH2COOH_T/(1.0+(CP.Kd_CH3CH2COOH/H_plus))*(CP.Kd_CH3CH2COOH/H_plus);
}

//-----
// Calculation of Butyrate [CH3CH2CH2COOH]
//-----
void Cell::cal_CH3CH2CH2COOH(void){
CH3CH2CH2COOH = CH3CH2CH2COOH_T/(1.0+(CP.Kd_CH3CH2CH2COOH/H_plus));
}

//-----
// Calculation of Butyrate ion [CH3CH2CH2COO]
//-----
void Cell::cal_CH3CH2CH2COO(void){
CH3CH2CH2COO = CH3CH2CH2COOH_T/(1.0+(CP.Kd_CH3CH2CH2COOH/H_plus))
                *(CP.Kd_CH3CH2CH2COOH/H_plus);
}

#####
#####
// Calculation of Accumulated amount
#####
#####
//-----
// Calculation of Accumulated amount of wet gas [kmol]
//-----
void Cell::cal_Acu_QGout(void){
Acu_QGout = Acu_QGout+QGout*dt;
}

//-----
// Accumulated amount of CO2 gas [kmol]
//-----
void Cell::cal_Acu_CO2(void){
if(QGout >= 0.0){
    if(P_CO2 > 0.0) Acu_CO2 = Acu_CO2+P_CO2/PT*QGout*dt;
    }
    else{
        Acu_CO2 = Acu_CO2+atm.P_CO2/atm.P*QGout*dt;
    }
}

//-----
// Accumulated amount of CH4 gas [kmol]
//-----
void Cell::cal_Acu_CH4(void){
    if(QGout >= 0.0){
        if(P_CH4 > 0.0) Acu_CH4 = Acu_CH4+P_CH4/PT*QGout*dt;
    }
    else{
        Acu_CH4 = Acu_CH4+atm.P_CH4/atm.P*QGout*dt;
    }
}

//-----
// Accumulated amount of H2 gas [kmol]
//-----
void Cell::cal_Acu_H2(void){
    if(QGout >= 0.0){
        if(P_H2 > 0.0) Acu_H2 = Acu_H2+P_H2/PT*QGout*dt;
    }
}

```

```

    else{
        Acu_H2 = Acu_H2+atm.P_H2/atm.P*QGout*dt;
    }
}

//-----
// Accumulated amount of N2 gas [kmol]
//-----
void Cell::cal_Acu_N2(void){
    if(QGout >= 0.0){
        if(P_N2 > 0.0) Acu_N2 = Acu_N2+P_N2/PT*QGout*dt;
    }
    else{
        Acu_N2 = Acu_N2+atm.P_N2/atm.P*QGout*dt;
    }
}

//-----
// Accumulated amount of NH3 gas [kmol]
//-----
void Cell::cal_Acu_PNH3(void){
    if(QGout >= 0.0){
        if(P_NH3 > 0.0) Acu_PNH3 = Acu_PNH3+P_NH3/PT*QGout *dt;
    }
    else{
        Acu_PNH3 = Acu_PNH3+atm.P_NH3/atm.P*QGout*dt;
    }
}

//-----
// Accumulated amount of O2 gas [kmol]
//-----
void Cell::cal_Acu_O2(void){
    if(QGout >= 0.0){
        if(P_O2 > 0.0) Acu_O2 = Acu_O2+P_O2/PT*QGout*dt;
    }
    else{
        Acu_O2 = Acu_O2+atm.P_O2/atm.P*QGout*dt;
    }
}

//-----
// Calculation of Accumulated amount of leachate [QLout]
//-----
void Cell::cal_Acu_QLout(void){
    Acu_QLout = Acu_QLout+QLout*dt;
}

//-----
// Accumulated amount of CH3COOH-C [kmol-C]
//-----
void Cell::cal_Acu_CH3COOH(void){
    if(CH3COOH_T > 0.0) Acu_CH3COOH = Acu_CH3COOH+xi()*CH3COOH_T*QLout*dt*2;
}

//-----
// Accumulated amount of CH3CH2COOH-C [kmol-C]
//-----
void Cell::cal_Acu_CH3CH2COOH(void){
    if(CH3CH2COOH_T > 0.0) Acu_CH3CH2COOH = Acu_CH3CH2COOH+xi()*
    *CH3CH2COOH_T*QLout*dt*3;
}

//-----
// Accumulated amount of CH3CH2CH2COOH-C [kmol-C]
//-----
void Cell::cal_Acu_CH3CH2CH2COOH(void){
    if(CH3CH2CH2COOH_T > 0.0) Acu_CH3CH2CH2COOH = Acu_CH3CH2CH2COOH+xi()*
    CH3CH2CH2COOH_T * QLout*dt*4;
}

```

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```
//-----
// Accumulated amount of Total Inorganic Carbon [IC] [mg-C]
//-----
void Cell::cal_Acu_IC(void){
    if(IC > 0.0) Acu_IC = Acu_IC+xi()*IC*dt*QLout*1000;
}

//-----
// Accumulated amount of ammonia-nitrogen [kmol-N]
//-----
void Cell::cal_Acu_NH3(void){
    if(NH3_T > 0.0) Acu_NH3 = Acu_NH3+xi()*NH3_T*QLout*dt*2;
}

//-----
// Accumulated amount of nitrate-nitrogen [kmol-N]
//-----
void Cell::cal_Acu_NO3(void){
    if(NO3 > 0.0) Acu_NO3 = Acu_NO3+xi()*NO3*QLout*dt;
}

//-----
// Accumulated amount of Ca [kmol-Ca]
//-----
void Cell::cal_Acu_Caout(void){
    if(Ca_plus > 0.0) Acu_Caout = Acu_Caout+xi()*Ca_plus*QLout*dt;
}

//-----
// Calculation of Chemical Organic Demand in leachate [COD]
//-----
void Cell::cal_COD(void){
    double A, B, newHUMUS;

// A is decomposition rate of total organic carbon [kmol/m3/d]
    A = 0.0;
    if(R_PRO_OP < 0.0) A = A-R_PRO_OP;
    if(R_FAT_OF < 0.0) A = A-R_FAT_OF;
    if(R_GLU_OG < 0.0) A = A-R_GLU_OG;
    if(R_CEL_OS < 0.0) A = A-R_CEL_OS;
    if(R_LIG_OH < 0.0) A = A-R_LIG_OH;
    if(R_PRO_NP < 0.0) A = A-R_PRO_NP;
    if(R_FAT_NF < 0.0) A = A-R_FAT_NF;
    if(R_GLU_NG < 0.0) A = A-R_GLU_NG;
    if(R_CEL_NS < 0.0) A = A-R_CEL_NS;
    if(R_LIG_NH < 0.0) A = A-R_LIG_NH;
    if(R_X_OP < 0.0) A = A-R_X_OP;
    if(R_X_OF < 0.0) A = A-R_X_OF;
    if(R_X_OG < 0.0) A = A-R_X_OG;
    if(R_X_OS < 0.0) A = A-R_X_OS;
    if(R_X_OH < 0.0) A = A-R_X_OH;
    if(R_X_NP < 0.0) A = A-R_X_NP;
    if(R_X_NF < 0.0) A = A-R_X_NF;
    if(R_X_NG < 0.0) A = A-R_X_NG;
    if(R_X_NS < 0.0) A = A-R_X_NS;
    if(R_X_NH < 0.0) A = A-R_X_NH;
    if(R_X_AP < 0.0) A = A-R_X_AP;
    if(R_X_AB < 0.0) A = A-R_X_AB;
    if(R_X_MT < 0.0) A = A-R_X_MT;
    if(R_X_MT2 < 0.0) A = A-R_X_MT2;
    if(R_X_AO < 0.0) A = A-R_X_AO;
    if(R_X_PO < 0.0) A = A-R_X_PO;
    if(R_X_BO < 0.0) A = A-R_X_BO;
    if(R_X_NO < 0.0) A = A-R_X_NO;
    if(R_X_DN < 0.0) A = A-R_X_DN;
    if(R_CH3COOH_AO < 0.0) A = A-R_CH3COOH_AO;

    B = -xi()*QLout*HUMUS;

    newHUMUS = HUMUS+dt*(1.0/V_L)*(V*A*RFC+B);
    HUMUS = newHUMUS;
    COD = 32000*HUMUS+64000*0.05*CH3COOH_T;
}

```

```
}

#####
#####
// The other parameters
#####
#####
void Other_param_cal(Cell& ce){
ce.TOC = 24000*ce.CH3COOH_T;      // Calculation of TOC
ce.BOD = 0.4*(32/12)*ce.TOC;    // Calculation of BOD
ce.TN  = 14000*ce.NH3_T;        // Calculation of T-N
}
```

## Module V: Chemical Reaction

```

#include "Cell.h"
extern double dt;           // Differential calculation time
extern double t;           // Start calculation time
extern double t_end;      // End calculation time
extern double prt_dt;     // Interval printout calculation results
extern Global_const CP;   // Global constants
extern Atmospheric_cond atm; // Atmosphere condition
extern Environment_cond env; // Environment condition

double epsX= 1.0E-10, epsN= 1.0E-3, epsC= 1.0E-2;
double funcRconst_T_wc_PH(RCONST what,Cell& cx);

#####
#####
// Setting constants and reaction rate related to biodegradation process
#####
#####
void Cell::RESET_reaction_Rate(void){
// OP Aerobic decomposition of Protein [kmol/m3-d]
  R_X_OP = 0.0; // OP : Net microbial growth rate
  R_OP_G = 0.0; // : Biomass growth rate
  R_OP_D = 0.0; // : Biomass decay rate
  R_PRO_OP = 0.0; // : Protein substances consumptions rate
  R_O2_OP = 0.0; // : Oxygen generation rate
  R_CO2_OP = 0.0; // : CO2 generation rate
  R_NH3_OP = 0.0; // : Ammonia generation rate
  R_H2O_OP = 0.0; // : Water generation rate
  R_CH3COOH_OP = 0.0; // : Acetic acid generation rate
  R_H2_OP = 0.0; // : Hydrogen generation rate
// OF Aerobic decomposition of Fats [kmol/m3-d]
  R_X_OF = 0.0; // OF : Net microbial growth rate
  R_OF_G = 0.0; // : Biomass growth rate
  R_OF_D = 0.0; // : Biomass decay rate
  R_FAT_OF = 0.0; // : Fats substances consumptions rate
  R_O2_OF = 0.0; // : Oxygen generation rate
  R_CO2_OF = 0.0; // : CO2 generation rate
  R_NH3_OF = 0.0; // : Ammonia generation rate
  R_H2O_OF = 0.0; // : Water generation rate
  R_CH3COOH_OF = 0.0; // : Acetic acid generation rate
  R_H2_OF = 0.0; // : Hydrogen generation rate
// OG Aerobic decomposition of Carbohydrate [kmol/m3-d]
  R_X_OG = 0.0; // OG : Net microbial growth rate
  R_OG_G = 0.0; // : Biomass growth rate
  R_OG_D = 0.0; // : Biomass decay rate
  R_GLU_OG = 0.0; // : Fats substances consumptions rate
  R_O2_OG = 0.0; // : Oxygen generation rate
  R_CO2_OG = 0.0; // : CO2 generation rate
  R_NH3_OG = 0.0; // : Ammonia generation rate
  R_H2O_OG = 0.0; // : Water generation rate
  R_CH3COOH_OG = 0.0; // : Acetic acid generation rate
  R_H2_OG = 0.0; // : Hydrogen generation rate
// OS Aerobic decomposition of Cellulose [kmol/m3-d]
  R_X_OS = 0.0; // OS : Net microbial growth rate
  R_OS_G = 0.0; // : Biomass growth rate
  R_OS_D = 0.0; // : Biomass decay rate
  R_CEL_OS = 0.0; // : Cellulose substances consumptions rate
  R_O2_OS = 0.0; // : Oxygen generation rate
  R_CO2_OS = 0.0; // : CO2 generation rate
  R_NH3_OS = 0.0; // : Ammonia generation rate
  R_H2O_OS = 0.0; // : Water generation rate
  R_CH3COOH_OS = 0.0; // : Acetic acid generation rate
  R_H2_OS = 0.0; // : Hydrogen generation rate
// OH Aerobic decomposition of Lignin [kmol/m3-d]
  R_X_OH = 0.0; // OH : Net microbial growth rate
  R_OH_G = 0.0; // : Biomass growth rate
  R_OH_D = 0.0; // : Biomass decay rate
  R_LIG_OH = 0.0; // : Lignin substances consumptions rate

```

```

R_O2_OH      = 0.0;      //      : Oxygen generation rate
R_CO2_OH     = 0.0;      //      : CO2 generation rate
R_NH3_OH     = 0.0;      //      : Ammonia generation rate
R_H2O_OH     = 0.0;      //      : Water generation rate
R_CH3COOH_OH = 0.0;      //      : Acetic acid generation rate
R_H2_OH      = 0.0;      //      : Hydrogen generation rate
// NP Anaerobic decomposition of Protein [kmol/m3-d]
R_X_NP       = 0.0;      // NP  : Net microbial growth rate
R_NP_G       = 0.0;      //      : Biomass growth rate
R_NP_D       = 0.0;      //      : Biomass decay rate
R_PRO_NP     = 0.0;      //      : Protein organic consumption rate
R_CH3COOH_NP = 0.0;      //      : Acetic acid generation rate
R_CH3CH2COOH_NP = 0.0; //      : Propionic acid generation rate
R_CH3CH2CH2COOH_NP = 0.0; //      : Butyric acid generation rate
R_CO2_NP     = 0.0;      //      : CO2 generation rate
R_H2_NP      = 0.0;      //      : Hydrogen generation rate
R_NH3_NP     = 0.0;      //      : Ammonia generation rate
R_H2O_NP     = 0.0;      //      : Water generation rate
R_O2_NP      = 0.0;      //      : Oxygen generation rate
// NF Anaerobic decomposition of Fats [kmol/m3-d]
R_X_NF       = 0.0;      // NF  : Net microbial growth rate
R_NF_G       = 0.0;      //      : Biomass growth rate
R_NF_D       = 0.0;      //      : Biomass decay rate
R_FAT_NF     = 0.0;      //      : Fats organic consumption rate
R_CH3COOH_NF = 0.0;      //      : Acetic acid generation rate
R_CO2_NF     = 0.0;      //      : CO2 generation rate
R_NH3_NF     = 0.0;      //      : Ammonia generation rate
R_H2O_NF     = 0.0;      //      : Water generation rate
R_H2_NF      = 0.0;      //      : Hydrogen generation rate
R_O2_NF      = 0.0;      //      : Oxygen generation rate
// NG Anaerobic decomposition of Carbohydrate [kmol/m3-d]
R_X_NG       = 0.0;      // NG  : Net microbial growth rate
R_NG_G       = 0.0;      //      : Biomass growth rate
R_NG_D       = 0.0;      //      : Biomass decay rate
R_GLU_NG     = 0.0;      //      : Carbohydrate organic consumption rate
R_CH3COOH_NG = 0.0;      //      : Acetic acid generation rate
R_CO2_NG     = 0.0;      //      : CO2 generation rate
R_NH3_NG     = 0.0;      //      : Ammonia generation rate
R_H2O_NG     = 0.0;      //      : Water generation rate
R_H2_NG      = 0.0;      //      : Hydrogen generation rate
R_O2_NG      = 0.0;      //      : Oxygen generation rate
// NS Anaerobic decomposition of Cellulose [kmol/m3-d]
R_X_NS       = 0.0;      // NS  : Net microbial growth rate
R_NS_G       = 0.0;      //      : Biomass growth rate
R_NS_D       = 0.0;      //      : Biomass decay rate
R_CEL_NS     = 0.0;      //      : Cellulose organic consumption rate
R_CH3COOH_NS = 0.0;      //      : Acetic acid generation rate
R_CO2_NS     = 0.0;      //      : CO2 generation rate
R_NH3_NS     = 0.0;      //      : Ammonia generation rate
R_H2O_NS     = 0.0;      //      : Water generation rate
R_H2_NS      = 0.0;      //      : Hydrogen generation rate
R_O2_NS      = 0.0;      //      : Oxygen generation rate
// NH Anaerobic decomposition of Lignin [kmol/m3-d]
R_X_NH       = 0.0;      // NH  : Net microbial growth rate
R_NH_G       = 0.0;      //      : Biomass growth rate
R_NH_D       = 0.0;      //      : Biomass decay rate
R_LIG_NH     = 0.0;      //      : Lignin organic consumption rate
R_CH3COOH_NH = 0.0;      //      : Acetic acid generation rate
R_CO2_NH     = 0.0;      //      : CO2 generation rate
R_NH3_NH     = 0.0;      //      : Ammonia generation rate
R_H2O_NH     = 0.0;      //      : Water generation rate
R_H2_NH      = 0.0;      //      : Hydrogen generation rate
R_O2_NH      = 0.0;      //      : Oxygen generation rate
// AP Acetogenesis of Propionic acid [kmol/m3-d]
R_X_AP       = 0.0;      // AP  : Net microbial growth rate
R_AP_G       = 0.0;      //      : Biomass growth rate
R_AP_D       = 0.0;      //      : Biomass decay rate
R_CH3CH2COOH_AP = 0.0; //      : Propionic acids consumption rate
R_H2O_AP     = 0.0;      //      : Water generation rate
R_NH3_AP     = 0.0;      //      : Ammonia generation rate
R_CH3COOH_AP = 0.0;      //      : Acetic acid generation rate
R_CO2_AP     = 0.0;      //      : CO2 generation rate

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R_H2_AP      = 0.0;      //      : Hydrogen generation rate
R_O2_AP      = 0.0;      //      : Oxygen generation rate
// AB Acetogenesis of Butyric acid [kmol/m3-d]
R_X_AB       = 0.0;      // AB   : Net microbial growth rate
R_AB_G       = 0.0;      //      : Biomass growth rate
R_AB_D       = 0.0;      //      : Biomass decay rate
R_CH3CH2CH2COOH_AB= 0.0; //      : Butyric acids consumption rate
R_H2O_AB     = 0.0;      //      : Water generation rate
R_NH3_AB     = 0.0;      //      : Ammonia generation rate
R_CH3COOH_AB = 0.0;      //      : Acetic acid generation rate
R_CO2_AB     = 0.0;      //      : CO2 generation rate
R_H2_AB      = 0.0;      //      : Hydrogen generation rate
R_O2_AB      = 0.0;      //      : Oxygen generation rate
// MT Methane formation from Acetic acid [kmol/m3-d]
R_X_MT       = 0.0;      // MT   : Net microbial growth rate
R_MT_G       = 0.0;      //      : Biomass growth rate
R_MT_D       = 0.0;      //      : Biomass decay rate
R_CH3COOH_MT = 0.0;      //      : Acetic acid generation rate
R_CH4_MT     = 0.0;      //      : Methane generation rate
R_CO2_MT     = 0.0;      //      : CO2 generation rate
R_NH3_MT     = 0.0;      //      : Ammonia generation rate
R_H2O_MT     = 0.0;      //      : Water generation rate
R_H2_MT      = 0.0;      //      : Hydrogen generation rate
R_O2_MT      = 0.0;      //      : Oxygen generation rate
// MT2 Methane formation from CO2+H2 [kmol/m3-d]
R_X_MT2      = 0.0;      // MT2  : Net microbial growth rate
R_MT2_G      = 0.0;      //      : Biomass growth rate
R_MT2_D      = 0.0;      //      : Biomass decay rate
R_CH3COOH_MT2 = 0.0;    //      : Acetic acid generation rate
R_CH4_MT2    = 0.0;      //      : Methane generation rate
R_CO2_MT2    = 0.0;      //      : CO2 generation rate
R_NH3_MT2    = 0.0;      //      : Ammonia generation rate
R_H2O_MT2    = 0.0;      //      : Water generation rate
R_H2_MT2     = 0.0;      //      : Hydrogen generation rate
R_O2_MT2     = 0.0;      //      : Oxygen generation rate
// AO Aerobic oxidation of Acetic acid [kmol/m3-d]
R_X_AO       = 0.0;      // AO   : Net microbial growth rate
R_AO_G       = 0.0;      //      : Biomass growth rate
R_AO_D       = 0.0;      //      : Biomass decay rate
R_CH3COOH_AO = 0.0;      //      : Acetic acid consumption rate
R_O2_AO      = 0.0;      //      : Oxygen consumption rate
R_NH3_AO     = 0.0;      //      : Ammonia consumption rate
R_CO2_AO     = 0.0;      //      : CO2 generate rate
R_H2O_AO     = 0.0;      //      : Water generation rate
R_H2_AO      = 0.0;      //      : Hydrogen generation rate
// PO Aerobic oxidation of Propionic acid
R_X_PO       = 0.0;      // PO   : Net microbial growth rate
R_PO_G       = 0.0;      //      : Biomass growth rate
R_PO_D       = 0.0;      //      : Biomass decay rate
R_CH3CH2COOH_PO = 0.0; //      : Propionic acid consumption rate
R_O2_PO      = 0.0;      //      : Oxygen consumption rate
R_NH3_PO     = 0.0;      //      : Ammonia consumption rate
R_CH3COOH_PO = 0.0;      //      : Acetic acid generate rate
R_CO2_PO     = 0.0;      //      : CO2 generate rate
R_H2O_PO     = 0.0;      //      : Water generation rate
R_H2_PO      = 0.0;      //      : Water generation rate
// BO Aerobic oxidation of Butyric acid
R_X_BO       = 0.0;      // BO   : Net microbial growth rate
R_BO_G       = 0.0;      //      : Biomass growth rate
R_BO_D       = 0.0;      //      : Biomass decay rate
R_CH3CH2CH2COOH_BO= 0.0; //      : Butyric acid consumption rate
R_O2_BO      = 0.0;      //      : Oxygen consumption rate
R_NH3_BO     = 0.0;      //      : Ammonia consumption rate
R_CH3COOH_BO = 0.0;      //      : Acetic acid generate rate
R_CO2_BO     = 0.0;      //      : CO2 generate rate
R_H2O_BO     = 0.0;      //      : Water generation rate
R_H2_BO      = 0.0;      //      : Water generation rate
// NO Aerobic nitrification of Ammonia [kmol/m3-d]
R_X_NO       = 0.0;      // NO   : Net microbial growth rate
R_NO_G       = 0.0;      //      : Biomass growth rate
R_NO_D       = 0.0;      //      : Biomass decay rate
R_NH3_NO     = 0.0;      //      : Ammonia consumption rate

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R_O2_NO      = 0.0;      //      : Oxygen consumption rate
R_CH3COOH_NO = 0.0;      //      : Acetic acid consumption rate
R_NO3_NO     = 0.0;      //      : Nitrate generate rate
R_CO2_NO     = 0.0;      //      : CO2 generate rate
R_H2O_NO     = 0.0;      //      : Water generation rate
R_H2_NO      = 0.0;      //      : Hydrogen consumption rate
// DN Anaerobic denitrification of Nitrate [kmol/m3-d]
R_X_DN       = 0.0;      // DN  : Net microbial growth rate
R_DN_G       = 0.0;      //      : Biomass growth rate
R_DN_D       = 0.0;      //      : Biomass decay rate
R_NO3_DN     = 0.0;      //      : Nitric acid generation rate
R_CH3COOH_DN = 0.0;      //      : Acetic acid generation rate
R_N2_DN      = 0.0;      //      : Nitrogen formation rate
R_CO2_DN     = 0.0;      //      : CO2 generation rate
R_H2O_DN     = 0.0;      //      : Water generation rate
R_H2_DN      = 0.0;      //      : Hydrogen consumption rate
R_NH3_DN     = 0.0;      //      : Ammonia consumption rate
R_O2_DN      = 0.0;      //      : Oxygen generation rate
}

#####
#####
// Correction constants and reaction rate by taken into account temperature, moisture
// contents, and pH
#####
#####
double funcRconst_T_wc_PH(RCONST what, Cell& cx) {
double f, f1, f2, f3;
double cT1, cT2, Tsd1, Tsd2, cT_set1, cT_set2, cT_set3;
double cpH, vpH, pHopt, cpH_set1, cpH_set2, cpH_set3;
double cWC, vWC, WCOpt;
// f      : over all correction factor
// f      = f1*f2*f3
// f1     : temperature correction factor
// f2     : moisture content correction factor
// f3     : pH correction factor

double a1, a2, a3;
// Parameter for Temperature correction factor
// a1     : lower limit of Temperature for microbial activity
// a2     : optimum Temperature for microbial activity
// a3     : upper limit of Temperature for microbial activity

double b1, b2;
// Parameters for pH correction factor
// b1     : lower limit of pH for microbial activity
// b2     : upper limit of pH for microbial activity

double c1, c2, c3;
// Parameters for water content correction factor
// c1     : lower limit of moisture content for microbial activity
// c2     : upper limit of moisture content for microbial activity
// c3     : correction factor at upper limit of moisture content

switch(what) {
case mOP:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 11.8;           Tsd2     = 4.0;
cpH      = 3.759942411947;   vpH      = 1.50;           pHopt    = 7.5;
cWC      = 0.313328534329;   vWC      = 0.125;        WCOpt    = 0.4;
a1       = 273.15;         a2       = 328.15;         a3       = 353.15;
b1       = 0.0;           b2       = 14.0;
c1       = 0.0;           c2       = 0.80;           c3       = 0.0;
cT_set1  = 2.68520E-1;     cT_set2  = 4.01288E-1;     cT_set3  = 5.57458E-1;
cpH_set1 = 6.06531E-1;     cpH_set2 = 8.00737E-1;     cpH_set3 = 9.45959E-1;
break;
case mOF:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 11.8;           Tsd2     = 4.0;
cpH      = 3.759942411947;   vpH      = 1.50;           pHopt    = 7.5;
cWC      = 0.313328534329;   vWC      = 0.125;        WCOpt    = 0.4;

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a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.80;      c3      = 0.0;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1; cpH_set2 = 8.00737E-1; cpH_set3 = 9.45959E-1;
break;
case MOG:
cT1     = 7.380432187427; cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947; vpH     = 1.50;      pHopt   = 7.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.80;      c3      = 0.0;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1; cpH_set2 = 8.00737E-1; cpH_set3 = 9.45959E-1;
break;
case MOS:
cT1     = 7.380432187427; cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947; vpH     = 1.50;      pHopt   = 7.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.80;      c3      = 0.0;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1; cpH_set2 = 8.00737E-1; cpH_set3 = 9.45959E-1;
break;
case MOH:
cT1     = 7.380432187427; cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947; vpH     = 1.50;      pHopt   = 7.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.80;      c3      = 0.0;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1; cpH_set2 = 8.00737E-1; cpH_set3 = 9.45959E-1;
break;
case mNP:
cT1     = 7.380432187427; cT2     = 2.79259596281003;
Tsd1    = 18.5;         Tsd2    = 7.0;
cpH     = 3.634610998215; vpH     = 1.45;      pHopt   = 6.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.40;      c3      = 1.00;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 9.42280E-1; cpH_set2 = 1.00;      cpH_set3 = 9.42280E-1;
break;
case mNF:
cT1     = 7.380432187427; cT2     =
Tsd1    = 18.5;         Tsd2    = 7.0;
cpH     = 3.634610998215; vpH     = 1.45;      pHopt   = 6.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.40;      c3      = 1.00;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 9.42280E-1; cpH_set2 = 1.00;      cpH_set3 = 9.42280E-1;
break;
case mNG:
cT1     = 7.380432187427; cT2     = 2.79259596281003;
Tsd1    = 18.5;         Tsd2    = 7.0;
cpH     = 3.634610998215; vpH     = 1.45;      pHopt   = 6.5;
cWC     = 0.313328534329; vWC     = 0.125;    WCopt  = 0.4;
a1      = 273.15;      a2      = 328.15;      a3      = 353.15;
b1      = 0.0;        b2      = 14.0;
c1      = 0.0;        c2      = 0.40;      c3      = 1.00;
cT_set1 = 2.68520E-1; cT_set2 = 4.01288E-1; cT_set3 = 5.57458E-1;
cpH_set1 = 9.42280E-1; cpH_set2 = 1.00;      cpH_set3 = 9.42280E-1;
break;

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case mNS:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 18.5;             Tsd2     = 7.0;
cpH      = 3.634610998215;   vpH      = 1.45;             pHopt    = 6.5;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 328.15;          a3       = 353.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 2.68520E-1;       cT_set2  = 4.01288E-1;     cT_set3  = 5.57458E-1;
cpH_set1 = 9.42280E-1;       cpH_set2 = 1.00;           cpH_set3 = 9.42280E-1;
break;
case mNH:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 18.5;             Tsd2     = 7.0;
cpH      = 3.634610998215;   vpH      = 1.45;             pHopt    = 6.5;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 328.15;          a3       = 353.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 2.68520E-1;       cT_set2  = 4.01288E-1;     cT_set3  = 5.57458E-1;
cpH_set1 = 9.42280E-1;       cpH_set2 = 1.00;           cpH_set3 = 9.42280E-1;
break;
case mAP:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 18.5;             Tsd2     = 7.0;
cpH      = 3.634610998215;   vpH      = 1.45;             pHopt    = 6.5;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 328.15;          a3       = 353.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 2.68520E-1;       cT_set2  = 4.01288E-1;     cT_set3  = 5.57458E-1;
cpH_set1 = 9.42280E-1;       cpH_set2 = 1.00;           cpH_set3 = 9.42280E-1;
break;
case mAB:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 18.5;             Tsd2     = 7.0;
cpH      = 3.634610998215;   vpH      = 1.45;             pHopt    = 6.5;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 328.15;          a3       = 353.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 2.68520E-1;       cT_set2  = 4.01288E-1;     cT_set3  = 5.57458E-1;
cpH_set1 = 9.42280E-1;       cpH_set2 = 1.00;           cpH_set3 = 9.42280E-1;
break;
case mMT:
cT1      = 4.707518908737;   cT2      = 1.595769121606;
Tsd1     = 11.8;             Tsd2     = 4.0;
cpH      = 2.130634033436;   vpH      = 0.85;             pHopt    = 7.0;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 308.15;          a3       = 323.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 6.98310E-1;       cT_set2  = 9.14139E-1;     cT_set3  = 1.00;
cpH_set1 = 5.00553E-01;     cpH_set2 = 8.41129E-1;     cpH_set3 = 1.00;
break;
case mMT2:
cT1      = 4.707518908737;   cT2      = 1.595769121606;
Tsd1     = 11.8;             Tsd2     = 4.0;
cpH      = 2.130634033436;   vpH      = 0.85;             pHopt    = 7.0;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 308.15;          a3       = 323.15;
b1       = 0.0;             b2       = 14.0;
c1       = 0.0;             c2       = 0.40;           c3       = 1.00;
cT_set1  = 6.98310E-1;       cT_set2  = 9.14139E-1;     cT_set3  = 1.00;
cpH_set1 = 5.00553E-01;     cpH_set2 = 8.41129E-1;     cpH_set3 = 1.00;
break;
case kAO:
cT1      = 7.380432187427;   cT2      = 2.79259596281003;
Tsd1     = 11.8;             Tsd2     = 4.0;
cpH      = 3.759942411947;   vpH      = 1.50;             pHopt    = 7.5;
cWC      = 0.313328534329;   vWC      = 0.125;           WCOpt   = 0.4;
a1       = 273.15;          a2       = 328.15;          a3       = 353.15;

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b1      = 0.0;          b2      = 14.0;          c3      = 0.0;
c1      = 0.0;          c2      = 0.80;          cT_set3 = 5.57458E-1;
cT_set1 = 2.68520E-1;  cT_set2 = 4.01288E-1;  cpH_set3 = 9.45959E-1;
cpH_set1 = 6.06531E-1; cpH_set2 = 8.00737E-1;
break;
case kPO:
cT1     = 7.380432187427;  cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947;  vpH     = 1.50;          pHopt   = 7.5;
cWC     = 0.313328534329;  vWC     = 0.125;        WCopt   = 0.4;
a1      = 273.15;        a2      = 328.15;        a3      = 353.15;
b1      = 0.0;          b2      = 14.0;
c1      = 0.0;          c2      = 0.80;          c3      = 0.0;
cT_set1 = 2.68520E-1;  cT_set2 = 4.01288E-1;  cT_set3 = 5.57458E-1;
cpH_set1 = 8.00737E-1;  cpH_set2 = 9.45959E-1;  cpH_set3 = 1.00;
break;
case kBO:
cT1     = 7.380432187427;  cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947;  vpH     = 1.50;          pHopt   = 7.5;
cWC     = 0.313328534329;  vWC     = 0.125;        WCopt   = 0.4;
a1      = 273.15;        a2      = 328.15;        a3      = 353.15;
b1      = 0.0;          b2      = 14.0;
c1      = 0.0;          c2      = 0.80;          c3      = 0.0;
cT_set1 = 2.68520E-1;  cT_set2 = 4.01288E-1;  cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1;  cpH_set2 = 8.00737E-1;  cpH_set3 = 9.45959E-1;
break;
case kNO:
cT1     = 7.380432187427;  cT2     = 2.79259596281003;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 3.759942411947;  vpH     = 1.50;          pHopt   = 7.5;
cWC     = 0.313328534329;  vWC     = 0.125;        WCopt   = 0.4;
a1      = 273.15;        a2      = 328.15;        a3      = 353.15;
b1      = 0.0;          b2      = 14.0;
c1      = 0.0;          c2      = 0.80;          c3      = 0.0;
cT_set1 = 2.68520E-1;  cT_set2 = 4.01288E-1;  cT_set3 = 5.57458E-1;
cpH_set1 = 6.06531E-1;  cpH_set2 = 8.00737E-1;  cpH_set3 = 9.45959E-1;
break;
case kDN:
cT1     = 4.707518908737;  cT2     = 1.595769121606;
Tsd1    = 11.8;          Tsd2    = 4.0;
cpH     = 2.130634033436;  vpH     = 0.85;          pHopt   = 7.0;
cWC     = 0.313328534329;  vWC     = 0.125;        WCopt   = 0.4;
a1      = 273.15;        a2      = 308.15;        a3      = 323.15;
b1      = 0.0;          b2      = 14.0;
c1      = 0.0;          c2      = 0.40;          c3      = 1.00;
cT_set1 = 6.98310E-1;  cT_set2 = 9.14139E-1;  cT_set3 = 1.00;
cpH_set1 = 5.00553E-1;  cpH_set2 = 8.41129E-1;  cpH_set3 = 1.00;
break;
}

//-----
// Temperature correction factor
//-----
if(cx.Temp < a1)          f1 = 0.0;
if(cx.Temp >= a1 && cx.Temp <= a2) f1 = cT1*(1.0/Tsd1*sqrt (2*PI))*exp (-0.5*pow
((cx.Temp-a2)/Tsd1),2));
if(cx.Temp >= a2 && cx.Temp <= a3) f1 = cT2*(1.0/Tsd2*sqrt (2*PI))*exp (-0.5*pow
((cx.Temp-a2)/Tsd2),2));
if(cx.Temp > a3)          f1 = 0.0;

//-----
// pH correction factor
//-----
if(cx.pH < b1)            f2 = 0.0;
if(cx.pH >= b1 && cx.pH <= b2) f2 = cpH*(1.0/vpH*sqrt (2*PI))*exp (-0.5*pow
((cx.pH-pHopt)/vpH),2));
if(cx.pH > b2)            f2 = 0.0;

```

```

//-----
// Water content correction factor
//-----
if(cx.wc < c1)          f3 = 0.0;
if(cx.wc >= c1 && cx.wc <= c2)  f3 = cWC*(1.0/vWC*sqrt(2*PI))*exp(-0.5*pow
((cx.wc-WCOpt)/vWC),2));
if(cx.wc > c2)          f3 = c3;

f = f1*f2*f3;

return f;
}

#####
#####
// Calculation of reaction rate determined by the amount of Oxygen (P_O2)
#####
#####
void Cell_reaction_rate(Cell& ce){
double fc;
// -----
// Reset of reaction rate
// -----
ce.RESET_reaction_Rate();

// When partial pressure of oxygen is more than (PO2_1) organic matter will degraded
// by aerobic way and no denitrification occur.
if(ce.P_O2 > ce.jdgP_O2_1){
// 1 ) Aerobic decomposition of Protein (OP)
fc=funcRconst_T_wc_PH(mOP,ce);    ce.AerobicDecompositionProtein(fc);
// 6') Aerobic decomposition of NP biomass
fc=funcRconst_T_wc_PH(mNP,ce);    ce.NP_AerobicDecompositionBiomass(fc);
// 2 ) Aerobic decomposition of Fats (OF)
fc=funcRconst_T_wc_PH(mOF,ce);    ce.AerobicDecompositionFats(fc);
// 7') Aerobic decomposition of NF biomass
fc=funcRconst_T_wc_PH(mNF,ce);    ce.NF_AerobicDecompositionBiomass(fc);
// 3 ) Aerobic decomposition of Carbohydrate (OG)
fc=funcRconst_T_wc_PH(mOG,ce);    ce.AerobicDecompositionCarbohydrate(fc);
// 8') Aerobic decomposition of NG biomass
fc=funcRconst_T_wc_PH(mNG,ce);    ce.NG_AerobicDecompositionBiomass(fc);
// 4 ) Aerobic decomposition of Cellulose (OS)
fc=funcRconst_T_wc_PH(mOS,ce);    ce.AerobicDecompositionCellulose(fc);
// 9') Aerobic decomposition of NS biomass
fc=funcRconst_T_wc_PH(mNS,ce);    ce.NS_AerobicDecompositionBiomass(fc);
// 5 ) Aerobic decomposition of Lignin (OH)
fc=funcRconst_T_wc_PH(mOH,ce);    ce.AerobicDecompositionLignin(fc);
// 10') Aerobic decomposition of NH biomass
fc=funcRconst_T_wc_PH(mNH,ce);    ce.NH_AerobicDecompositionBiomass(fc);
// 11') Aerobic decomposition of AP biomass
fc=funcRconst_T_wc_PH(mAP,ce);    ce.AP_AerobicDecompositionBiomass(fc);
// 12') Aerobic decomposition of AB biomass
fc=funcRconst_T_wc_PH(mAB,ce);    ce.AB_AerobicDecompositionBiomass(fc);
// 13") Aerobic decomposition of MT biomass
fc=funcRconst_T_wc_PH(mMT,ce);    ce.MT_AerobicDecompositionBiomass(fc);
// 14") Aerobic decomposition of MT2 biomass
fc=funcRconst_T_wc_PH(mMT2,ce);    ce.MT2_AerobicDecompositionBiomass(fc);
// 15 ) Aerobic oxidation of Acetic acid (AO)
fc=funcRconst_T_wc_PH(kAO,ce);    ce.AerobicOxidationAceticAcid(fc);
// 16 ) Aerobic oxidation of Propionic acid (PO)
fc=funcRconst_T_wc_PH(kPO,ce);    ce.AerobicOxidationPropionicAcid(fc);
// 17 ) Aerobic oxidation of Butyric acid (BO)
fc=funcRconst_T_wc_PH(kBO,ce);    ce.AerobicOxidationButyricAcid(fc);
// 18 ) Aerobic nitrification of Ammonia (NO)
fc=funcRconst_T_wc_PH(kNO,ce);    ce.AerobicNitrificationAmmonia(fc);
// 19') Aerobic decomposition of DN biomass
fc=funcRconst_T_wc_PH(kDN,ce);    ce.DN_AerobicDecompositionBiomass(fc);
}
}

```

```

// When partial pressure of oxygen is more than (PO2_2) and less than (PO2_1) organic
// matter will be degraded by aerobic way and denitrification occur.
if(ce.P_O2 < ce.jdgP_O2_1 && ce.P_O2 > ce.jdgP_O2_2){
  // 1 ) Aerobic decomposition of Protein (OP)
  fc=funcRconst_T_wc_PH(mOP,ce);      ce.AerobicDecompositionProtein(fc);
  // 6') Aerobic decomposition of NP biomass
  fc=funcRconst_T_wc_PH(mNP,ce);      ce.NP_AerobicDecompositionBiomass(fc);
  // 2 ) Aerobic decomposition of Fats (OF)
  fc=funcRconst_T_wc_PH(mOF,ce);      ce.AerobicDecompositionFats(fc);
  // 7') Aerobic decomposition of NF biomass
  fc=funcRconst_T_wc_PH(mNF,ce);      ce.NF_AerobicDecompositionBiomass(fc);
  // 3 ) Aerobic decomposition of Carbohydrate (OG)
  fc=funcRconst_T_wc_PH(mOG,ce);      ce.AerobicDecompositionCarbohydrate(fc);
  // 8') Aerobic decomposition of NG biomass
  fc=funcRconst_T_wc_PH(mNG,ce);      ce.NG_AerobicDecompositionBiomass(fc);
  // 4 ) Aerobic decomposition of Cellulose (OS)
  fc=funcRconst_T_wc_PH(mOS,ce);      ce.AerobicDecompositionCellulose(fc);
  // 9') Aerobic decomposition of NS biomass
  fc=funcRconst_T_wc_PH(mNS,ce);      ce.NS_AerobicDecompositionBiomass(fc);
  // 5 ) Aerobic decomposition of Lignin (OH)
  fc=funcRconst_T_wc_PH(mOH,ce);      ce.AerobicDecompositionLignin(fc);
  // 10') Aerobic decomposition of NH biomass
  fc=funcRconst_T_wc_PH(mNH,ce);      ce.NH_AerobicDecompositionBiomass(fc);
  // 11') Aerobic decomposition of AP biomass
  fc=funcRconst_T_wc_PH(mAP,ce);      ce.AP_AerobicDecompositionBiomass(fc);
  // 12') Aerobic decomposition of AB biomass
  fc=funcRconst_T_wc_PH(mAB,ce);      ce.AB_AerobicDecompositionBiomass(fc);
  // 13") Aerobic decomposition of MT biomass
  fc=funcRconst_T_wc_PH(mMT,ce);      ce.MT_AerobicDecompositionBiomass(fc);
  // 14") Aerobic decomposition of MT2 biomass
  fc=funcRconst_T_wc_PH(mMT2,ce);      ce.MT2_AerobicDecompositionBiomass(fc);
  // 15 ) Aerobic oxidation of Acetic acid (AO)
  fc=funcRconst_T_wc_PH(kAO,ce);      ce.AerobicOxidationAceticAcid(fc);
  // 16 ) Aerobic oxidation of Propionic acid (PO)
  fc=funcRconst_T_wc_PH(kPO,ce);      ce.AerobicOxidationPropionicAcid(fc);
  // 17 ) Aerobic oxidation of Butyric acid (BO)
  fc=funcRconst_T_wc_PH(kBO,ce);      ce.AerobicOxidationButyricAcid(fc);
  // 18 ) Aerobic nitrification of Ammonia (NO)
  fc=funcRconst_T_wc_PH(kNO,ce);      ce.AerobicNitrificationAmmonia(fc);
  // 19 ) Anaerobic denitrification of Nitrate (DN)
  fc=funcRconst_T_wc_PH(kDN,ce);      ce.AnaerobicDenitrificationNitrate(fc);
}

// When partial pressure of oxygen is more than PO2_3 and less than PO2_2 organic
// matter will
// degraded by anaerobic way and Denitrification occurs. No Nitrification and VFA
// oxidation
// taking place.
if(ce.P_O2 < ce.jdgP_O2_2 && ce.P_O2 > ce.jdgP_O2_3){
  // 6 ) Anaerobic fermentation of Protein (NP)
  fc=funcRconst_T_wc_PH(mNP,ce);      ce.AnaerobicFermentationProtein(fc);
  // 1') Anaerobic fermentation of OP biomass
  fc=funcRconst_T_wc_PH(mOP,ce);      ce.OP_AnaerobicFermentationBiomass(fc);
  // 7 ) Anaerobic fermentation of Fats (NF)
  fc=funcRconst_T_wc_PH(mNF,ce);      ce.AnaerobicFermentationFats(fc);
  // 2') Anaerobic fermentation of OF biomass
  fc=funcRconst_T_wc_PH(mOF,ce);      ce.OF_AnaerobicFermentationBiomass(fc);
  // 8 ) Anaerobic fermentation of Carbohydrate (NG)
  fc=funcRconst_T_wc_PH(mNG,ce);      ce.AnaerobicFermentationCarbohydrate(fc);
  // 3') Anaerobic fermentation of OG biomass
  fc=funcRconst_T_wc_PH(mOG,ce);      ce.OG_AnaerobicFermentationBiomass(fc);
  // 9 ) Anaerobic fermentation of Cellulose (NS)
  fc=funcRconst_T_wc_PH(mNS,ce);      ce.AnaerobicFermentationCellulose(fc);
  // 4') Anaerobic fermentation of OS biomass
  fc=funcRconst_T_wc_PH(mOS,ce);      ce.OS_AnaerobicFermentationBiomass(fc);
  // 10 ) Anaerobic fermentation of Lignin (NH)
  fc=funcRconst_T_wc_PH(mNH,ce);      ce.AnaerobicFermentationLignin(fc);
  // 5') Anaerobic fermentation of OH biomass
  fc=funcRconst_T_wc_PH(mOH,ce);      ce.OH_AnaerobicFermentationBiomass(fc);
  // 11 ) Acetogenesis of Propionate (AP)
  fc=funcRconst_T_wc_PH(mAP,ce);      ce.AcetogenesisPropionicAcid(fc);
  // 12 ) Acetogenesis of Butyrate (AB)

```

```

fc=funcRconst_T_wc_PH(mAB,ce);      ce.AcetogenesisButyricAcid(fc);
// 13') Anaerobic fermentation of MT biomass
fc=funcRconst_T_wc_PH(mMT,ce);      ce.MT_AnaerobicFermentationBiomass(fc);
// 14') Anaerobic fermentation of MT2 biomass
fc=funcRconst_T_wc_PH(mMT2,ce);     ce.MT2_AnaerobicFermentationBiomass(fc);
// 15') Anaerobic fermentation of AO biomass
fc=funcRconst_T_wc_PH(kAO,ce);      ce.AO_AnaerobicFermentationBiomass(fc);
// 16') Anaerobic fermentation of PO biomass
fc=funcRconst_T_wc_PH(kPO,ce);      ce.PO_AnaerobicFermentationBiomass(fc);
// 17') Anaerobic fermentation of BO biomass
fc=funcRconst_T_wc_PH(kBO,ce);      ce.BO_AnaerobicFermentationBiomass(fc);
// 18') Anaerobic fermentation of NO biomass
fc=funcRconst_T_wc_PH(kNO,ce);      ce.NO_AnaerobicFermentationBiomass(fc);
// 19 ) Anaerobic denitrification of Nitrate (DN)
fc=funcRconst_T_wc_PH(kDN,ce);      ce.AnaerobicDenitrificationNitrate(fc);
}

// When partial pressure of oxygen is less than (PO2_3) organic matter will degraded
// by Anaerobic
// way Methane fermentation is begun. No Nitrification and VFA oxidation taking
// place.
if(ce.P_O2 < ce.jdgP_O2_3){
// 6 ) Anaerobic fermentation of Protein (NF)
fc=funcRconst_T_wc_PH(mNP,ce);      ce.AnaerobicFermentationProtein(fc);
// 1') Anaerobic fermentation of OP biomass
fc=funcRconst_T_wc_PH(mOP,ce);      ce.OP_AnaerobicFermentationBiomass(fc);
// 7 ) Anaerobic fermentation of Fats (NF)
fc=funcRconst_T_wc_PH(mNF,ce);      ce.AnaerobicFermentationFats(fc);
// 2') Anaerobic fermentation of OF biomass
fc=funcRconst_T_wc_PH(mOF,ce);      ce.OF_AnaerobicFermentationBiomass(fc);
// 8 ) Anaerobic fermentation of Carbohydrate (NG)
fc=funcRconst_T_wc_PH(mNG,ce);      ce.AnaerobicFermentationCarbohydrate(fc);
// 3') Anaerobic fermentation of OG biomass
fc=funcRconst_T_wc_PH(mOG,ce);      ce.OG_AnaerobicFermentationBiomass(fc);
// 9 ) Anaerobic fermentation of Cellulose (NS)
fc=funcRconst_T_wc_PH(mNS,ce);      ce.AnaerobicFermentationCellulose(fc);
// 4') Anaerobic fermentation of OS biomass
fc=funcRconst_T_wc_PH(mOS,ce);      ce.OS_AnaerobicFermentationBiomass(fc);
// 10 ) Anaerobic fermentation of Lignin (NH)
fc=funcRconst_T_wc_PH(mNH,ce);      ce.AnaerobicFermentationLignin(fc);
// 5') Anaerobic fermentation of OH biomass
fc=funcRconst_T_wc_PH(mOH,ce);      ce.OH_AnaerobicFermentationBiomass(fc);
// 11 ) Acetogenesis of Propionate (AP)
fc=funcRconst_T_wc_PH(mAP,ce);      ce.AcetogenesisPropionicAcid(fc);
// 12 ) Acetogenesis of Butyrate (AB)
fc=funcRconst_T_wc_PH(mAB,ce);      ce.AcetogenesisButyricAcid(fc);
// 13 ) Methane fermentation from acetic acid (MT)
fc=funcRconst_T_wc_PH(mMT,ce);      ce.MethaneFormationAceticAcid(fc);
// 14 ) Methane fermentation from H2 and CO2 (MT2)
fc=funcRconst_T_wc_PH(mMT2,ce);     ce.MethaneFormationCO2andH2(fc);
// 15') Anaerobic fermentation of AO biomass
fc=funcRconst_T_wc_PH(kAO,ce);      ce.AO_AnaerobicFermentationBiomass(fc);
// 16') Anaerobic fermentation of PO biomass
fc=funcRconst_T_wc_PH(kPO,ce);      ce.PO_AnaerobicFermentationBiomass(fc);
// 17') Anaerobic fermentation of BO biomass
fc=funcRconst_T_wc_PH(kBO,ce);      ce.BO_AnaerobicFermentationBiomass(fc);
// 18') Anaerobic fermentation of NO biomass
fc=funcRconst_T_wc_PH(kNO,ce);      ce.NO_AnaerobicFermentationBiomass(fc);
// 19 ) Anaerobic denitrification of Nitrate (DN)
fc=funcRconst_T_wc_PH(kDN,ce);      ce.AnaerobicDenitrificationNitrate(fc);
}
}

#####
#####
// Chemical reaction equations
#####
// -----
// 1 ) Aerobic decomposition of Protein (OP)
// -----

```

## Edi Munawar

```

void Cell::AerobicDecompositionProtein(double fx){
// If there is protein (S_PRO) available, the bacteria will growing up follow below
// equation. If there is no protein any more, decomposition of protein not occurs and
// the bacteria also not growing up.
if(S_PRO > 0.0)
    R_OP_G = fx*mu_OP*(X_OP/MX)*(S_PRO/(K_OP_S+S_PRO))*(P_O2/(K_OP_O+P_O2));
else
    R_OP_G = 0.0;

R_OP_D = K_OP_D*((X_OP-X_OPini)/MX);
else
R_OP_D      = 0.0;
R_PRO_OP    = -R_OP_G/Y_OP;
R_O2_OP     = -0.25*(4*Pro_a+Pro_b-2*Pro_c-3*Pro_n-Y_OP*(4*Bio_x+Bio_u-2*Bio_v-
3*Bio_w))*R_OP_G/Y_OP-0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_OP_D;
R_X_OP      = R_OP_G-R_OP_D;
R_CO2_OP    = (Pro_a-Bio_x*Y_OP)*R_OP_G/Y_OP+Bio_x*R_OP_D;
R_H2O_OP    = 0.5*(Pro_b-3*Pro_n-Y_OP*(Bio_u-3*Bio_w))*R_OP_G/Y_OP
+0.5*(Bio_u-3*Bio_w)*R_OP_D;
R_NH3_OP    = (Pro_n-Bio_w*Y_OP)*R_OP_G/Y_OP+Bio_w*R_OP_D;
R_CH3COOH_OP = 0.0;
R_H2_OP     = 0.0;
}

// -----
// 1') Anaerobic fermentation of OP biomass
// -----
void Cell::OP_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_OP_G  = 0.0;

// As long as X_OP does not increase more than the initial value, biomass decay will
// not occur.
if((X_OP-X_OPini) > 0.0)
    R_OP_D = K_NP_D*((X_OP-X_OPini)/MX);
else
    R_OP_D = 0.0;

R_X_OP      = -R_OP_D;
R_H2O_OP    = -(2*Bio_x-Bio_v-2*R2)*R_OP_D;
R_CH3COOH_OP = R2*R_OP_D;
R_CO2_OP    = (Bio_x-2*R2)*R_OP_D;
R_H2_OP     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_OP_D;
R_NH3_OP    = Bio_w*R_OP_D;
R_O2_OP     = 0.0;
R_PRO_OP    = 0.0;
}

// -----
// 2 ) Aerobic decomposition of Fats (OF)
// -----
void Cell::AerobicDecompositionFats(double fx){
// If both fats (S_FAT) and nitrogen source (NH3_T) are available, the bacteria will
// growing up follow below equation. If either fats or nitrogen source not available
// any more, decomposition of fats not occurs and the bacteria also not growing up.
if(S_FAT > 0.0 && NH3_T > 0.0)
    R_OF_G = fx*mu_OF*(X_OF/MX)*(S_FAT/(K_OF_S+S_FAT))*(P_O2/(K_OS_O+P_O2));
else
    R_OF_G = 0.0;

// As long as X_OF does not increase more than the initial value, biomass decay will
// not occur.
if((X_OF-X_OFini) > 0.0)
    R_OF_D = K_OF_D*((X_OF-X_OFini)/MX);
else
    R_OF_D = 0.0;

R_FAT_OF    = -R_OF_G/Y_OF;
R_O2_OF     = -0.25*(4*Fat_a+Fat_b-2*Fat_c-Y_OF*(4*Bio_x+Bio_u-2*Bio_v-3

```

```

        * Bio_w))*R_OF_G/Y_OF
        -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_OF_D;
R_NH3_OF =-Bio_w*Y_OF*R_OF_G/Y_OF+Bio_w*R_OF_D;
R_X_OF   = R_OF_G-R_OF_D;
R_CO2_OF = (Fat_a-Bio_x*Y_OF)*R_OF_G/Y_OF+Bio_x*R_OF_D;
R_H2O_OF = 0.5*(Fat_b-Y_OF*(Bio_u-3*Bio_w))*R_OF_G/Y_OF
          + 0.5*(Bio_u-3*Bio_w)*R_OS_D;
R_CH3COOH_OF = 0.0;
R_H2_OF     = 0.0;
}

// -----
// 2') Anaerobic fermentation of OF biomass
// -----
void Cell::OF_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_OF_G  = 0.0;

// As long as X_OF does not increase more than the initial value, biomass decay will
// not occur.
if((X_OF-X_OFini) > 0.0)
    R_OF_D = K_NF_D*((X_OF-X_OFini)/MX);
else
    R_OF_D = 0.0;

R_X_OF   =-R_OF_D;
R_H2O_OF =-(2*Bio_x-Bio_v-2*R2)*R_OF_D;
R_CH3COOH_OF = R2*R_OF_D;
R_CO2_OF = (Bio_x-2*R2)*R_OF_D;
R_H2_OF  = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_OF_D;
R_NH3_OF = Bio_w*R_OF_D;
R_O2_OF  = 0.0;
R_FAT_OF = 0.0;
}

// -----
// 3 ) Aerobic decomposition of Carbohydrate (OG)
// -----
void Cell::AerobicDecompositionCarbohydrate(double fx){
// If both carbohydrate (S_GLU) and nitrogen source are available, the bacteria will
// growing up follow below equation. If either carbohydrate or nitrogen sources not
// available any more, decomposition of carbohydrate not occurs and the bacteria also
// not growing up.
if(S_GLU > 0.0 && NH3_T > 0.0)
    R_OG_G = fx*mu_OG*(X_OG/MX)*(S_GLU/(K_OG_S*X_OG+S_GLU))
            *(P_O2/(K_OG_O+P_O2));
else
    R_OG_G = 0.0;

// As long as X_OG does not increase more than the initial value, biomass decay will
// not occur.
if((X_OG-X_OGini) > 0.0)
    R_OG_D = K_OG_D*((X_OG-X_OGini)/MX);
else
    R_OG_D = 0.0;

R_GLU_OG =-R_OG_G/Y_OG;
R_O2_OG  =-0.25*(24*Glu_n-Y_OG*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_OG_G/Y_OG
          -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_OG_D;
R_NH3_OG =-(Bio_w*Y_OG)*R_OG_G/Y_OG+Bio_w*R_OG_D;
R_X_OG   = R_OG_G-R_OG_D;
R_CO2_OG = (6*Glu_n-Bio_x*Y_OG)*R_OG_G/Y_OG+Bio_x*R_OG_D;
R_H2O_OG = 0.5*(10*Glu_n-Y_OG*(Bio_u-3*Bio_w))*R_OG_G/Y_OG
          +0.5*(Bio_u-3*Bio_w)*R_OG_D;
R_CH3COOH_OG = 0.0;
R_H2_OG     = 0.0;
}

// -----
// 3') Anaerobic fermentation of OG biomass

```

## Edi Munawar

```

// -----
void Cell::OG_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_OG_G  = 0.0;

// As long as X_OG does not increase more than the initial value, biomass decay will
// not occur.
if((X_OG-X_OGini) > 0.0)
    R_OG_D = K_NG_D*((X_OG-X_OGini)/MX);
else
    R_OG_D = 0.0;

R_X_OG      ==-R_OG_D;
R_H2O_OG    ==-(2*Bio_x-Bio_v-2*R2)*R_OG_D;
R_CH3COOH_OG = R2*R_OG_D;
R_CO2_OG    = (Bio_x-2*R2)*R_OG_D;
R_H2_OG     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_OG_D;
R_NH3_OG    = Bio_w*R_OG_D;
R_O2_OG     = 0.0;
R_GLU_OG    = 0.0;
}

// -----
// 4 ) Aerobic decomposition of Cellulose (OS)
// -----
void Cell::AerobicDecompositionCellulose(double fx){
// If both cellulose (S_CEL) and nitrogen source are available, the bacteria will
// growing up follow below equation. If either cellulose or nitrogen source not
// available any more, decomposition of cellulose not occurs and the bacteria also
// not growing up.
if(S_CEL > 0.0 && NH3_T > 0.0)
    R_OS_G = fx*mu_OS*(X_OS/MX)*(S_CEL/(K_OS_S+S_CEL))*(P_O2/(K_OS_O+P_O2));
else
    R_OS_G = 0.0;

// As long as X_OS does not increase more than the initial value, biomass decay will
// not occur.
if((X_OS-X_OSini) > 0.0)
    R_OS_D = K_OS_D*((X_OS-X_OSini)/MX);
else
    R_OS_D = 0.0;

R_CEL_OS      ==-R_OS_G/Y_OS;
R_O2_OS       ==-0.25*(24*Cel_n-Y_OS*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_OS_G/Y_OS
-0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_OS_D;
R_NH3_OS      ==-(Bio_w*Y_OS)*R_OS_G/Y_OS+Bio_w*R_OS_D;
R_X_OS        = R_OS_G-R_OS_D;
R_CO2_OS      = (6*Cel_n-Bio_x*Y_OS)*R_OS_G/Y_OS+Bio_x*R_OS_D;
R_H2O_OS      = 0.5*(10*Cel_n-Y_OS*(Bio_u-3*Bio_w))*R_OS_G/Y_OS
+0.5*(Bio_u-3*Bio_w)*R_OS_D;
R_CH3COOH_OS  = 0.0;
R_H2_OS       = 0.0;
}

// -----
// 4') Anaerobic fermentation of OS biomass
// -----
void Cell::OS_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_OS_G  = 0.0;

// As long as X_OS does not increase more than the initial value, biomass decay will
// not occur.
if((X_OS-X_OSini) > 0.0)
    R_OS_D = K_NS_D*((X_OS-X_OSini)/MX);
else
    R_OS_D = 0.0;

```

```

R_X_OS      = -R_OS_D;
R_H2O_OS    = -(2*Bio_x-Bio_v-2*R2)*R_OS_D;
R_CH3COOH_OS = R2*R_OS_D;
R_CO2_OS    = (Bio_x-2*R2)*R_OS_D;
R_H2_OS     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_OS_D;
R_NH3_OS    = Bio_w*R_OS_D;
R_O2_OS     = 0.0;
R_CEL_OS    = 0.0;
}

// -----
// 5 ) Aerobic decomposition of Lignin (OH)
// -----
void Cell::AerobicDecompositionLignin(double fx){
// If both Lignin (S_LIG) and nitrogen source are available, the bacteria will
// growing up follow below equation. If either Lignin or nitrogen source not
// available any more, decomposition of Lignin not occurs and the bacteria also not
// growing up.
if(S_LIG > 0.0 && NH3_T > 0.0)
    R_OH_G = fx*mu_OH*(X_OH/MX)*(S_LIG/(K_OH_S+S_LIG))*(P_O2/(K_OS_O+P_O2));
else
    R_OH_G = 0.0;

// As long as X_OH does not increase more than the initial value, biomass decay will
// not occur.
if((X_OH-X_OHini) > 0.0)
    R_OH_D = K_OH_D*(X_OH-X_OHini)/MX;
else
    R_OH_D = 0.0;

R_LIG_OH    = -R_OH_G/Y_OH;
R_O2_OH     = -0.25*(4*Lig_a+Lig_b-2*Lig_c-Y_OH*(4*Bio_x+Bio_u-2*Bio_v-3
    * Bio_w))*R_OH_G/Y_OH
    -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_OH_D;
R_NH3_OH    = -Bio_w*Y_OH*R_OH_G/Y_OH+Bio_w*R_OH_D;
R_X_OH      = R_OH_G-R_OH_D;
R_CO2_OH    = (Lig_a-Bio_x*Y_OH)*R_OH_G/Y_OH+Bio_x*R_OH_D;
R_H2O_OH    = 0.5*(Lig_b-Y_OH*(Bio_u-3*Bio_w))*R_OH_G/Y_OH
    +0.5*(Bio_u-3*Bio_w)*R_OS_D;
R_CH3COOH_OH = 0.0;
R_H2_OH     = 0.0;
}

// -----
// 5') Anaerobic fermentation of OH biomass
// -----
void Cell::OH_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_OH_G  = 0.0;

// As long as X_OH does not increase more than the initial value, biomass decay will
// not occur.
if((X_OH-X_OHini) > 0.0)
    R_OH_D = K_NH_D*(X_OH-X_OHini)/MX;
else
    R_OH_D = 0.0;

R_X_OH      = -R_OH_D;
R_H2O_OH    = -(2*Bio_x-Bio_v-2*R2)*R_OH_D;
R_CH3COOH_OH = R2*R_OH_D;
R_CO2_OH    = (Bio_x-2*R2)*R_OH_D;
R_H2_OH     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_OH_D;
R_NH3_OH    = Bio_w*R_OH_D;
R_O2_OH     = 0.0;
R_LIG_OH    = 0.0;
}

// -----
// 6 ) Anaerobic fermentation of Protein (NP)
// -----

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void Cell::AnaerobicFermentationProtein(double fx){
double R1,R2;

R1      = R_NP;
R2      = R_NX;

// If there is protein (S_PRO) available, the bacteria will growing up follow below
// equation. If there is no protein any more, decomposition of protein not occurs and
// the bacteria also not growing up.
if(S_PRO > 0.0)
    R_NP_G = fx*mu_NP*(X_NP/MX)*(S_PRO/(K_NP_S+S_PRO));
else
    R_NP_G = 0.0;

// As long as X_NP does not increase more than the initial value, biomass decay will
// not occur.
if((X_NP-X_NPini) > 0.0)
    R_NP_D = K_NP_D*((X_NP-X_NPini)/MX);
else
    R_NP_D = 0.0;

R_PRO_NP      =-R_NP_G/Y_NP;
R_H2O_NP      =-(2*Pro_a-Pro_c-11.4533*R1-Y_NP*(2*Bio_x-Bio_v))*R_NP_G/Y_NP
              -(2*Bio_x-Bio_v-2*R2)*R_NP_D;
R_X_NP        = R_NP_G-R_NP_D;
R_CH3COOH_NP  = R1*R_NP_G/Y_NP+R2*R_NP_D;
R_CH3CH2COOH_NP= 0.9333*R1*R_NP_G/Y_NP;
R_CH3CH2CH2COOH_NP = 0.9533*R1*R_NP_G/Y_NP;
R_CO2_NP      = (Pro_a-8.6133*R1-Bio_x*Y_NP)*R_NP_G/Y_NP
              +(Bio_x-2*R2)*R_NP_D;
R_H2_NP       = 0.5*(4*Pro_a+Pro_b-2*Pro_c-3*Pro_n-40.1333*R1-Y_NP
              *(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_NP_G/Y_NP
              +0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NP_D;
R_NH3_NP      = (Pro_n-Bio_w*Y_NP)*R_NP_G/Y_NP+Bio_w*R_NP_D;
R_O2_NP       = 0.0;
}

// -----
// 6') Aerobic decomposition of NP biomass
// -----
void Cell::NP_AerobicDecompositionBiomass(double fx){

R_NP_G = 0.0;

// As long as X_NP does not increase more than the initial value, biomass decay will
// not occur.
if((X_NP-X_NPini) > 0.0)
    R_NP_D = K_OP_D*((X_NP-X_NPini)/MX);
else
    R_NP_D = 0.0;

R_X_NP      =-R_NP_D;
R_O2_NP     =-0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NP_D;
R_CO2_NP    = Bio_x*R_NP_D;
R_H2O_NP    = 0.5*(Bio_u-3*Bio_w)*R_NP_D;
R_NH3_NP    = Bio_w*R_NP_D;
R_CH3COOH_NP = 0.0;
R_H2_NP     = 0.0;
R_PRO_NP    = 0.0;
}

// -----
// 7 ) Anaerobic fermentation of Fats (NF)
// -----
void Cell::AnaerobicFermentationFats(double fx){
double R1,R2;

R1      = R_NF;
R2      = R_NX;

// If either fats (S_FAT) or nitrogen source (NH3_T) are available, the bacteria will
// growing up follow below equation. If either fats or nitrogen sources not available

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// any more, decomposition of fats not occurs and the bacteria also not growing up.
if(S_FAT > 0.0 && NH3_T > 0.0)
    R_NF_G = fx*mu_NF*(X_NF/MX)*(S_FAT/(K_NF_S+S_FAT));
else
    R_NF_G = 0.0;

// As long as X_NF does not increase more than the initial value, biomass decay will
// not occur.
if((X_NF-X_NFini) > 0.0)
    R_NF_D = K_NF_D*((X_NF-X_NFini)/MX);
else
    R_NF_D = 0.0;

R_FAT_NF      = -R_NF_G/Y_NF;
R_H2O_NF      = -(2*Fat_a-Fat_c-2*R1-Y_NF*(2*Bio_x-Bio_v))*R_NF_G/Y_NF
               - (2*Bio_x-Bio_v-2*R2)*R_NF_D;
R_NH3_NF      = -Bio_w*Y_NF*R_NF_G/Y_NF+Bio_w*R_NF_D;
R_X_NF        = R_NF_G-R_NF_D;
R_CH3COOH_NF  = R1*R_NF_G/Y_NF+R2*R_NF_D;
R_CO2_NF      = (Fat_a-Bio_x*Y_NF-2*R1)*R_NF_G/Y_NF
               + (Bio_x-2*R2)*R_NF_D;
R_H2_NF       = 0.5*(4*Fat_a+Fat_b-2*Fat_c-8*R1-Y_NF*(4*Bio_x+Bio_u-2
               * Bio_v+3*Bio_w))*R_NF_G/Y_NF
               +0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NF_D;
R_O2_NF       = 0.0;
}

// -----
// 7) Aerobic decomposition of NF biomass
// -----
void Cell::NF_AerobicDecompositionBiomass(double fx){

    R_NF_G = 0.0;

// As long as X_NF does not increase more than the initial value, biomass decay will
// not occur.
if((X_NF-X_NFini) > 0.0)
    R_NF_D = K_OF_D*((X_NF-X_NFini)/MX);
else
    R_NF_D = 0.0;

R_X_NF        = -R_NF_D;
R_O2_NF       = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NF_D;
R_CO2_NF      = Bio_x*R_NF_D;
R_H2O_NF      = 0.5*(Bio_u-3*Bio_w)*R_NF_D;
R_NH3_NF      = Bio_w*R_NF_D;
R_CH3COOH_NF  = 0.0;
R_H2_NF       = 0.0;
R_FAT_NF      = 0.0;
}

// -----
// 8 ) Anaerobic fermentation of Carbohydrate (NG)
// -----
void Cell::AnaerobicFermentationCarbohydrate(double fx){
double R1,R2;

R1            = R_NG;
R2            = R_NX;

// If both carbohydrate (S_GLU) or nitrogen source (NH3_T) are available, the
// bacteria will growing up follow below equation. If either carbohydrate or nitrogen
// sources not available any more, decomposition of carbohydrate not occurs and the
// bacteria also not growing up.
if(S_GLU > 0.0 && NH3_T > 0.0)
    R_NG_G = fx*mu_NG*(X_NG/MX)*(S_GLU/(K_NG_S+S_GLU));
else
    R_NG_G = 0.0;

// As long as X_NG does not increase more than the initial value, biomass decay will
// not occur.
if((X_NG-X_NGini) > 0.0)

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        R_NG_D = K_NG_D*((X_NG-X_NGini)/MX);
    else
        R_NG_D = 0.0;

    R_GLU_NG    = -R_NG_G/Y_NG;
    R_H2O_NG    = -(7*Glu_n-2*R1-Y_NG*(2*Bio_x-Bio_v))*R_NG_G/Y_NG
                - (2*Bio_x-Bio_v-2*R2)*R_NG_D;
    R_NH3_NG    = -Bio_w*Y_NG*R_NG_G/Y_NG+Bio_w*R_NG_D;
    R_X_NG      = R_NG_G-R_NG_D;
    R_CH3COOH_NG = R1*R_NG_G/Y_NG+R2*R_NG_D;
    R_CO2_NG    = (6*Glu_n-2*R1-Bio_x*Y_NG)*R_NG_G/Y_NG
                + (Bio_x-2*R2)*R_NG_D;
    R_H2_NG     = 0.5*(24*Glu_n-8*R1-Y_NG*(4*Bio_x+Bio_u-2*Bio_v-3
                * Bio_w))*R_NG_G/Y_NG
                +0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NG_D;
    R_O2_NG     = 0.0;
}

// -----
// 8') Aerobic decomposition of NG biomass
// -----
void Cell::NG_AerobicDecompositionBiomass(double fx){
    R_NG_G = 0.0;

// As long as X_NG does not increase more than the initial value, biomass decay will
// not occur.
    if((X_NG-X_NGini) < 0.0)
        R_NG_D = K_OG_D*((X_NG-X_NGini)/MX);
    else
        R_NG_D = 0.0;

    R_X_NG      = -R_NG_D;
    R_O2_NG     = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NG_D;
    R_CO2_NG    = Bio_x*R_NG_D;
    R_H2O_NG    = 0.5*(Bio_u-3*Bio_w)*R_NG_D;
    R_NH3_NG    = Bio_w*R_NG_D;
    R_CH3COOH_NG = 0.0;
    R_H2_NG     = 0.0;
    R_GLU_NG    = 0.0;
}

// -----
// 9 ) Anaerobic fermentation of Cellulose (NS)
// -----
void Cell::AnaerobicFermentationCellulose(double fx){
    double R1,R2;

    R1      = R_NS;
    R2      = R_NX;

// If both cellulose (S_CEL) or nitrogen source (NH3_T) are available, the bacteria
// will growing up follow below equation. If either cellulose or nitrogen sources not
// available any more, decomposition of cellulose not occurs and the bacteria also
// not
// growing up.
    if(S_CEL > 0.0 && NH3_T > 0.0)
        R_NS_G = fx*mu_NS*(X_NS/MX)*(S_CEL/(K_NS_S+S_CEL));
    else
        R_NS_G = 0.0;

// As long as X_NS does not increase more than the initial value, biomass decay will
// not occur.
    if((X_NS-X_NSini) > 0.0)
        R_NS_D = K_NS_D*((X_NS-X_NSini)/MX);
    else
        R_NS_D = 0.0;

    R_CEL_NS    = -R_NS_G/Y_NS;
    R_H2O_NS    = -(7*Cel_n-2*R1-Y_NS*(2*Bio_x-Bio_v))*R_NS_G/Y_NS
                - (2*Bio_x-Bio_v-2*R2)*R_NS_D;
    R_NH3_NS    = -Bio_w*Y_NS*R_NS_G/Y_NS+Bio_w*R_NS_D;
    R_X_NS     = R_NS_G-R_NS_D;

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R_CH3COOH_NS = R1*R_NS_G/Y_NS+R2*R_NS_D;
R_CO2_NS     = (6*Cel_n-2*R1-Bio_x*Y_NS)*R_NS_G/Y_NS
              +(Bio_x-2*R2)*R_NS_D;
R_H2_NS      = 0.5*(24*Cel_n-8*R1-Y_NS*(4*Bio_x+Bio_u-2*Bio_v-3
              *Bio_w))*R_NS_G/Y_NS
              +0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NS_D;
R_O2_NS      = 0.0;
}

// -----
// 9) Aerobic decomposition of NS biomass
// -----
void Cell::NS_AerobicDecompositionBiomass(double fx){
R_NS_G = 0.0;

// As long as X_NS does not increase more than the initial value, biomass decay will
// not occur.
if((X_NS-X_NSini) < 0.0)
    R_NS_D = K_OS_D*(X_NS-X_NSini)/MX;
else
    R_NS_D = 0.0;

R_X_NS      = -R_NS_D;
R_O2_NS     = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NS_D;
R_CO2_NS    = Bio_x*R_NS_D;
R_H2O_NS    = 0.5*(Bio_u-3*Bio_w)*R_NS_D;
R_NH3_NS    = Bio_w*R_NS_D;
R_CH3COOH_NS = 0.0;
R_H2_NS     = 0.0;
R_CEL_NS    = 0.0;
}

// -----
// 10 ) Anaerobic fermentation of Lignin (NH)
// -----
void Cell::AnaerobicFermentationLignin(double fx){
double R1,R2;

R1      = R_NH;
R2      = R_NX;

// If both Lignin (S_LIG) or nitrogen source (NH3_T) are available, the bacteria
// will growing up follow below equation. If either Lignin or nitrogen sources not
// available any more, decomposition of lignin not occurs and the bacteria also not
// growing up.
if(S_LIG > 0.0 && NH3_T > 0.0)
    R_NH_G = fx*mu_NH*(X_NH/MX)*(S_LIG/(K_NH_S+S_LIG));
else
    R_NH_G = 0.0;

// As long as X_NH does not increase more than the initial value, biomass decay will
// not occur.
if((X_NH-X_NHini) > 0.0)
    R_NH_D = K_NH_D*(X_NH-X_NHini)/MX;
else
    R_NH_D = 0.0;

R_LIG_NH    = -R_NH_G/Y_NH;
R_H2O_NH    = -(2*Lig_a-Lig_c-2*R1-Y_NH*(2*Bio_x-Bio_v))*R_NH_G/Y_NH
              -(2*Bio_x-Bio_v-2*R2)*R_NH_D;
R_NH3_NH    = -Bio_w*Y_NH*R_NH_G/Y_NH+Bio_w*R_NH_D;
R_X_NH      = R_NH_G-R_NH_D;
R_CH3COOH_NH = R1*R_NH_G/Y_NH+R2*R_NH_D;
R_CO2_NH    = (Lig_a-Bio_x*Y_NH-2*R1)*R_NH_G/Y_NH
              +(Bio_x-2*R2)*R_NH_D;
R_H2_NH     = 0.5*(4*Lig_a+Lig_b-2*Lig_c-8*R1-Y_NH*(4*Bio_x+Bio_u-2
              *Bio_v+3*Bio_w))*R_NH_G/Y_NH
              +0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NH_D;
R_O2_NH     = 0.0;
}

// -----

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// 10') Aerobic decomposition of NH biomass
// -----
void Cell::NH_AerobicDecompositionBiomass(double fx){

    R_NH_G = 0.0;

// As long as X_NH does not increase more than the initial value, biomass decay will
// not occur.
    if((X_NH-X_NHini) > 0.0)
        R_NH_D = K_OH_D*((X_NH-X_NHini)/MX);
    else
        R_NH_D = 0.0;

    R_X_NH      =-R_NH_D;
    R_O2_NH     =-0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NH_D;
    R_CO2_NH    = Bio_x*R_NH_D;
    R_H2O_NH    = 0.5*(Bio_u-3*Bio_w)*R_NH_D;
    R_NH3_NH    = Bio_w*R_NH_D;
    R_CH3COOH_NH = 0.0;
    R_H2_NH     = 0.0;
    R_LIG_NH    = 0.0;
}

// -----
// 11 ) Acetogenesis of Propionate (AP)
// -----
void Cell::AcetogenesisPropionicAcid(double fx){
    double R1,R2;

    R1      = R_AP;
    R2      = R_NX;

// If both propionic acids (CH3CH2COOH_T) and nitrogen source (NH3_T) are available,
// the bacteria will growing up follow below equation. If either propionic acids
// or nitrogen sources not available any more, decomposition of fats not occurs and
// the bacteria also not growing up.
    if(CH3CH2COOH_T > 0.0 && NH3_T > 0.0)
        R_AP_G = fx*mu_AP*(X_AP/MX)*(CH3CH2COOH_T/(K_AP_S+CH3CH2COOH_T));
    else
        R_AP_G = 0.0;

// As long as X_AP does not increase more than the initial value, biomass decay will
// not occur.
    if((X_AP-X_APini) > 0.0)
        R_AP_D = K_AP_D*((X_AP-X_APini)/MX);
    else
        R_AP_D = 0.0;

    R_CH3CH2COOH_AP=-R_AP_G/Y_AP;
    R_H2O_AP      =-(4-2*R1-Y_AP*(2*Bio_x-Bio_v))*R_AP_G/Y_AP
                  -(2*Bio_x-Bio_v-2*R2)*R_AP_D;
    R_NH3_AP     =-Bio_w*Y_AP*R_AP_G/Y_AP+Bio_w*R_AP_D;
    R_X_AP       = R_AP_G-R_AP_D;
    R_CH3COOH_AP = R1*R_AP_G/Y_AP+R2*R_AP_D;
    R_CO2_AP     = (3-Bio_x*Y_AP-2*R1)*R_AP_G/Y_AP
                  +(Bio_x-2*R2)*R_AP_D;
    R_H2_AP      = 0.5*(14-8*R1-Y_AP*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_AP_G/Y_AP
                  + 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_AP_D;
    R_O2_AP      = 0.0;
}

// -----
// 11') Aerobic decomposition of AP biomass
// -----
void Cell::AP_AerobicDecompositionBiomass(double fx){

    R_AP_G = 0.0;

// As long as X_AP does not increase more than the initial value, biomass decay will
// not occur.
    if((X_AP-X_APini) > 0.0)
        R_AP_D = K_AP_D*((X_AP-X_APini)/MX);

```

```

else
    R_AP_D = 0.0;

    R_X_AP      = -R_AP_D;
    R_O2_AP     = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_AP_D;
    R_CO2_AP    = Bio_x*R_AP_D;
    R_H2O_AP    = 0.5*(Bio_u-3*Bio_w)*R_AP_D;
    R_NH3_AP    = Bio_w*R_AP_D;
    R_CH3COOH_AP = 0.0;
    R_H2_AP     = 0.0;
    R_CH3CH2COOH_AP = 0.0;
}

// -----
// 12 ) Acetogenesis of Butyrate (AB)
// -----
void Cell::AcetogenesisButyricAcid(double fx){
    double R1,R2;

    R1      = R_AB;
    R2      = R_NX;

// If both Butyric acids (CH3CH2CH2COOH_T) and nitrogen source (NH3_T) are
// available, the bacteria will growing up follow below equation. If either
// Butyric acids or nitrogen sources not available any more, Acetogenesis of Butyrate
// not occurs and the bacteria also not growing up.
    if(CH3CH2CH2COOH_T > 0.0 && NH3_T > 0.0)
        R_AB_G = fx*mu_AB*(X_AB/MX)*(CH3CH2CH2COOH_T/(K_AB_S+CH3CH2CH2COOH_T));
    else
        R_AB_G = 0.0;

// As long as X_AB does not increase more than the initial value, biomass decay will
// not occur.
    if((X_AB-X_ABini) > 0.0)
        R_AB_D = K_AB_D*((X_AB-X_ABini)/MX);
    else
        R_AB_D = 0.0;

    R_CH3CH2CH2COOH_AB = -R_AB_G/Y_AB;
    R_H2O_AB            = -(6-2*R1-Y_AB*(2*Bio_x-Bio_v))*R_AB_G/Y_AB
                        - (2*Bio_x-Bio_v-2*R2)*R_AB_D;
    R_NH3_AB            = -Bio_w*Y_AB*R_AB_G/Y_AB+Bio_w*R_AB_D;
    R_X_AB              = R_AB_G-R_AB_D;
    R_CH3COOH_AB        = R1*R_AB_G/Y_AB+R2*R_AB_D;
    R_CO2_AB            = (4-Bio_x*Y_AB-2*R1)*R_AB_G/Y_AB
                        + (Bio_x-2*R2)*R_AB_D;
    R_H2_AB             = 0.5*(18-8*R1-Y_AB*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_AB_G/Y_AB
                        + 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_AB_D;
    R_O2_AB             = 0.0;
}

// -----
// 12') Aerobic decomposition of AB biomass
// -----
void Cell::AB_AerobicDecompositionBiomass(double fx){

    R_AB_G = 0.0;

// As long as X_AB does not increase more than the initial value, biomass decay will
// not occur.
    if((X_AB-X_ABini) > 0.0)
        R_AB_D = K_AB_D*((X_AB-X_ABini)/MX);
    else
        R_AB_D = 0.0;

    R_X_AB      = -R_AB_D;
    R_O2_AB     = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_AB_D;
    R_CO2_AB    = Bio_x*R_AB_D;
    R_H2O_AB    = 0.5*(Bio_u-3*Bio_w)*R_AB_D;
    R_NH3_AB    = Bio_w*R_AB_D;
    R_CH3COOH_AB = 0.0;
    R_H2_AB     = 0.0;
}

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R_CH3CH2CH2COOH_AB = 0.0;
}

// -----
// 13 ) Methane fermentation from acetic acid (MT)
// -----
void Cell::MethaneFormationAceticAcid(double fx){
double R2;

R2      = R_NX;

// If both acetic acids (CH3COOH_T) and nitrogen source (NH3_T) are available, the
// bacteria will growing up follow below equation. If either acetic acids or
// nitrogen sources not available any more, methane formation of acetic acids not
// occurs and the bacteria also not growing up.
if(CH3COOH_T > 0.0 && NH3_T > 0.0)
    R_MT_G = fx*mu_MT*(X_MT/MX)*CH3COOH_T/(K_MT_S+CH3COOH_T);
else
    R_MT_G = 0.0;

// As long as X_MT does not increase more than the initial value, biomass decay will
// not occur.
if((X_MT-X_MTini) > 0.0)
    R_MT_D = K_MT_D*((X_MT-X_MTini)/MX);
else
    R_MT_D = 0.0;

R_CH3COOH_MT ==-R_MT_G/Y_MT+R2*R_MT_D;
R_NH3_MT      ==-Bio_w*Y_MT*R_MT_G/Y_MT+Bio_w*R_MT_D;
R_X_MT        = R_MT_G-R_MT_D;
R_CH4_MT      = 0.125*(8-Y_MT*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_MT_G/Y_MT;
R_CO2_MT      = 0.125*(8-Y_MT*(4*Bio_x-Bio_u+2*Bio_v+3*Bio_w))*R_MT_G/Y_MT
+(Bio_x-2*R2)*R_MT_D;
R_H2O_MT      = 0.125*(Y_MT*(8*Bio_x-2*Bio_u-4*Bio_v+6*Bio_w))*R_MT_G/Y_MT
-(2*Bio_x-Bio_v-2*R2)*R_MT_D;
R_H2_MT       = 0.0;
R_O2_MT       = 0.0;
}

// -----
// 13') Anaerobic fermentation of MT biomass
// -----
void Cell::MT_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_MT_G  = 0.0;

// If X_MT does not increase more than the initial value, biomass decay will not
// occur.
if((X_MT-X_MTini) > 0.0)
    R_MT_D = K_MT_D*((X_MT-X_MTini)/MX);
else
    R_MT_D = 0.0;

R_X_MT      ==-R_MT_D;
R_H2O_MT    ==-(2*Bio_x-Bio_v-2*R2)*R_MT_D;
R_CH3COOH_MT = R2*R_MT_D;
R_CO2_MT    = (Bio_x-2*R2)*R_MT_D;
R_H2_MT     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_MT_D;
R_NH3_MT    = Bio_w*R_MT_D;
R_O2_MT     = 0.0;
R_CH4_MT    = 0.0;
}

// -----
// 13") Aerobic decomposition of MT biomass
// -----
void Cell::MT_AerobicDecompositionBiomass(double fx){

```

```

R_MT_G = 0.0;

// As long as X_MT does not increase more than the initial value, biomass decay will
// not occur.
if((X_MT-X_MTini) > 0.0)
    R_MT_D = K_MT_D*((X_MT-X_MTini)/MX);
else
    R_MT_D = 0.0;

R_X_MT      = -R_MT_D;
R_O2_MT     = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_MT_D;
R_CO2_MT    = Bio_x*R_MT_D;
R_H2O_MT    = 0.5*(Bio_u-3*Bio_w)*R_MT_D;
R_NH3_MT    = Bio_w*R_MT_D;
R_CH3COOH_MT = 0.0;
R_H2_MT     = 0.0;
R_CH4_MT    = 0.0;
}

// -----
// 14 ) Methane fermentation from H2 and CO2 (MT2)
// -----
void Cell::MethaneFormationCO2andH2(double fx){
double R2;

R2          = R_NX;

// If all hydrogen (P_H2), nitrogen (NH3_T) and carbon sources (CH3COOH_T) are
// available, the methane formation will occurs follow below equation. If either
// hydrogen, nitrogen or carbon sources not available any more, methane formation
// of hydrogen not occurs and the bacteria also not growing up.
if(P_H2 > 0.0 && NH3_T > 0.0)
    R_MT2_G = fx*mu_MT2*(X_MT2/MX)*(P_H2/PT/(K_MT2_S+P_H2/PT));
else
    R_MT2_G = 0.0;

// As long as X_MT2 does not increase more than the initial value, biomass decay will
// not occur.
if((X_MT2-X_MT2ini) > 0.0)
    R_MT2_D = K_MT2_D*((X_MT2-X_MT2ini)/MX);
else
    R_MT2_D = 0.0;

R_CO2_MT2   = -R_MT2_G/Y_MT2+(Bio_x-2*R2)*R_MT2_D;
R_H2_MT2    = -0.5*(8-Y_MT2*(4*Bio_x-Bio_u+2*Bio_v+3*Bio_w))*R_MT2_G/Y_MT2
              + 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_MT2_D;
R_NH3_MT2   = -Bio_w*Y_MT2*R_MT2_G/Y_MT2+Bio_w*R_MT2_D;
R_X_MT2     = R_MT2_G-R_MT2_D;
R_CH4_MT2   = (1-Bio_x*Y_MT2)*R_MT2_G/Y_MT2;
R_H2O_MT2   = (2-Bio_v*Y_MT2)*R_MT2_G/Y_MT2
              - (2*Bio_x-Bio_v-2*R2)*R_MT2_D;
R_CH3COOH_MT2 = R2*R_MT2_D;
R_O2_MT2    = 0.0;
}

// -----
// 14') Anaerobic fermentation of MT2 biomass
// -----
void Cell::MT2_AnaerobicFermentationBiomass(double fx){
double R2;

R2          = R_NX;
R_MT2_G     = 0.0;

// As long as X_MT2 does increase more than the initial value, biomass decay will not
// occur.
if((X_MT2-X_MT2ini) > 0.0)
    R_MT2_D = K_MT2_D*((X_MT2-X_MT2ini)/MX);
else
    R_MT2_D = 0.0;

R_X_MT2     = -R_MT2_D;

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R_H2O_MT2      =-(2*Bio_x-Bio_v-2*R2)*R_MT2_D;
R_CH3COOH_MT2 = R2*R_MT2_D;
R_CO2_MT2      = (Bio_x-2*R2)*R_MT2_D;
R_H2_MT2       = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_MT2_D;
R_NH3_MT2      = Bio_w*R_MT2_D;
R_O2_MT2       = 0.0;
R_CH4_MT2      = 0.0;
}

// -----
// 14") Aerobic decomposition of MT2 biomass
// -----
void Cell::MT2_AerobicDecompositionBiomass(double fx){

R_MT2_G = 0.0;

// As long as X_MT2 does increase more than the initial value, biomass decay will not
// occur.
if((X_MT2-X_MT2ini) > 0.0)
    R_MT2_D = K_MT2_D*((X_MT2-X_MT2ini)/MX);
else
    R_MT2_D = 0.0;

R_X_MT2      =-R_MT2_D;
R_O2_MT2     =-0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_MT2_D;
R_CO2_MT2    = Bio_x*R_MT2_D;
R_H2O_MT2    = 0.5*(Bio_u-3*Bio_w)*R_MT2_D;
R_NH3_MT2    = Bio_w*R_MT2_D;
R_CH3COOH_MT2 = 0.0;
R_H2_MT2     = 0.0;
R_CH4_MT2    = 0.0;
}

// -----
// 15 ) Aerobic oxidation of Acetic acid (AO)
// -----
void Cell::AerobicOxidationAceticAcid(double fx){
double R2;

R2      = R_NX;

// If both acetic acids (CH3COOH_T) and nitrogen source (NH3_T) are available, the
// bacteria will growing up follow below equation. If either acetic acids or
// nitrogen sources not available any more, oxidation of acetic acids not occurs and
// the bacteria also not growing up.
if(CH3COOH_T > 0.0 && NH3_T > 0.0)
    R_AO_G = fx*mu_AO*(X_AO/MX)*(CH3COOH_T/(K_AO_S+CH3COOH_T))
            *(P_O2/(K_AO_O+P_O2));
else
    R_AO_G = 0.0;

// As long as X_AO does not increase more than the initial value, biomass decay will
// not occur
if((X_AO-X_AOini) > 0.0)
    R_AO_D = K_AO_D*((X_AO-X_AOini)/MX);
else
    R_AO_D = 0.0;

R_CH3COOH_AO =-R_AO_G/Y_AO+R2*R_AO_D;
R_O2_AO      =-0.25*(8-Y_AO*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_AO_G/Y_AO
- 0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_AO_D;
R_NH3_AO     =-Bio_w*Y_AO*R_AO_G/Y_AO+Bio_w*R_AO_D;
R_X_AO       = R_AO_G-R_AO_D;
R_CO2_AO     = (2-Bio_x*Y_AO)*R_AO_G/Y_AO+Bio_x*R_AO_D;
R_H2O_AO     = 0.5*(4-Y_AO*(Bio_u-3*Bio_w))*R_AO_G/Y_AO
+ 0.5*(Bio_u-3*Bio_w)*R_AO_D;
R_H2_AO      = 0.0;
}

```

```

// -----
// 15') Anaerobic fermentation of AO biomass
// -----
void Cell::AO_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_AO_G  = 0.0;

// As long as X_AO does increase more than the initial value, biomass decay will not
// occur.
if((X_AO-X_AOini) > 0.0)
    R_AO_D = K_AO_D*(X_AO-X_AOini)/MX);
else
    R_AO_D = 0.0;

R_X_AO      =-R_AO_D;
R_H2O_AO    =-(2*Bio_x-Bio_v-2*R2)*R_AO_D;
R_CH3COOH_AO = R2*R_AO_D;
R_CO2_AO    = (Bio_x-2*R2)*R_AO_D;
R_H2_AO     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_AO_D;
R_NH3_AO    = Bio_w*R_AO_D;
R_O2_AO     = 0.0;
}

// -----
// 16 ) Aerobic oxidation of Propionic acid (PO)
// -----
void Cell::AerobicOxidationPropionicAcid(double fx){
double R2;

R2      = R_NX;

// If both propionic acids (CH3CH2COOH_T) and nitrogen source (NH3_T) are available,
// the bacteria will growing up follow below equation. If either propionic acids
// or nitrogen sources not available any more, oxidation of propionic acids not
// occurs and the bacteria also not growing up.
if(CH3CH2COOH_T > 0.0 && NH3_T > 0.0)
    R_PO_G = fx*mu_PO*(X_PO/MX)*(CH3CH2COOH_T/(K_PO_S+CH3CH2COOH_T))
            *(P_O2/(K_PO_O+P_O2));
else
    R_PO_G = 0.0;

// As long as X_PO does not increase more than the initial value, biomass decay will
// not occur.
if((X_PO-X_POini) > 0.0)
    R_PO_D = K_PO_D*(X_PO-X_POini)/MX);
else
    R_PO_D = 0.0;

R_CH3CH2COOH_PO=-R_PO_G/Y_PO+R2*R_PO_D;
R_O2_PO         =-0.25*(14-Y_PO*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_PO_G/Y_PO
                -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_PO_D;
R_NH3_PO        =-Bio_w*Y_PO*R_PO_G/Y_PO+Bio_w*R_PO_D;
R_X_PO          = R_PO_G-R_PO_D;
R_CO2_PO        = (3-Bio_x*Y_PO)*R_PO_G/Y_PO+Bio_x*R_PO_D;
R_H2O_PO        = 0.5*(6-Y_PO*(Bio_u-3*Bio_w))*R_PO_G/Y_PO
                +0.5*(Bio_u-3*Bio_w)*R_PO_D;
R_CH3COOH_PO    = 0.0;
R_H2_PO         = 0.0;
}

// -----
// 16') Anaerobic fermentation of PO biomass
// -----
void Cell::PO_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_PO_G  = 0.0;

// As long as X_PO does increase more than the initial value, biomass decay will not

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// occur.
if((X_PO-X_POini) > 0.0)
  R_PO_D = K_PO_D*((X_PO-X_POini)/MX);
else
  R_PO_D = 0.0;

R_X_PO      = -R_PO_D;
R_H2O_PO    = -(2*Bio_x-Bio_v-2*R2)*R_PO_D;
R_CH3COOH_PO = R2*R_PO_D;
R_CO2_PO    = (Bio_x-2*R2)*R_PO_D;
R_H2_PO     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_PO_D;
R_NH3_PO    = Bio_w*R_PO_D;
R_O2_PO     = 0.0;
R_CH3CH2COOH_PO = 0.0;
}
// -----
// 17 ) Aerobic oxidation of Butyric acid (BO)
// -----
void Cell::AerobicOxidationButyricAcid(double fx){
double R2;

R2      = R_NX;

// If both butyric acids (CH3CH2CH2COOH_T) and nitrogen source (NH3_T) are
// available, the bacteria will growing up follow below equation. If either
// butyric acids or nitrogen sources not available any more, oxidation of butyric
// acids not occurs and the bacteria also not growing up.
if(CH3CH2CH2COOH_T > 0.0 && NH3_T > 0.0)
  R_BO_G = fx*mu_BO*(X_BO/MX)*(CH3CH2CH2COOH_T/(K_BO_S+CH3CH2CH2COOH_T))
          *(P_O2/(K_BO_O+P_O2));
else
  R_BO_G = 0.0;

// As long as X_BO does not increase more than the initial value, biomass decay will
// not occur.
if((X_BO-X_BOini) > 0.0)
  R_BO_D = K_BO_D*((X_BO-X_BOini)/MX);
else
  R_BO_D = 0.0;

R_CH3CH2CH2COOH_BO = -R_BO_G/Y_BO+R2*R_BO_D;
R_O2_BO            = -0.25*(20-Y_BO*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w))*R_BO_G/Y_BO
                    -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_BO_D;
R_NH3_BO           = -Bio_w*Y_BO*R_BO_G/Y_BO+Bio_w*R_BO_D;
R_X_BO             = R_BO_G-R_BO_D;
R_CO2_BO           = (4-Bio_x*Y_BO)*R_BO_G/Y_BO+Bio_x*R_BO_D;
R_H2O_BO           = 0.5*(8-Y_BO*(Bio_u-3*Bio_w))*R_BO_G/Y_BO
                    +0.5*(Bio_u-3*Bio_w)*R_BO_D;
R_CH3COOH_BO      = 0.0;
R_H2_BO            = 0.0;
}

// -----
// 17') Anaerobic fermentation of BO biomass
// -----
void Cell::BO_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_BO_G  = 0.0;

// As long as X_BO does increase more than the initial value, biomass decay will not
// occur.
if((X_BO-X_BOini) > 0.0)
  R_BO_D = K_BO_D*((X_BO-X_BOini)/MX);
else
  R_BO_D = 0.0;

R_X_BO      = -R_BO_D;
R_H2O_BO    = -(2*Bio_x-Bio_v-2*R2)*R_BO_D;
R_CH3COOH_BO = R2*R_BO_D;
R_CO2_BO    = (Bio_x-2*R2)*R_BO_D;

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R_H2_BO      = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_BO_D;
R_NH3_BO     = Bio_w*R_BO_D;
R_O2_BO      = 0.0;
R_CH3CH2CH2COOH_BO = 0.0;
}

// -----
// 18 ) Aerobic nitrification of Ammonia (NO)
// -----
void Cell::AerobicNitrificationAmmonia(double fx){
double R2;

R2      = R_NX;

// If both ammonia (NH3_T) and carbon source (CH3COOH_T) are available, the bacteria
// will growing up follow below equation. If either ammonia or carbon sources not
// available any more, nitrification of ammonia not occurs and the bacteria also not
// growing up.
if(NH3_T > 0.0 && CH3COOH_T > 0.0)
    R_NO_G = fx*mu_NO*(X_NO/MX)*(T_NH3/(K_NO_S+T_NH3))*(P_O2/(K_NO_O+P_O2));
else
    R_NO_G = 0.0;

// As long as X_NO does not increase more than the initial value, biomass decay will
// not occur.
if((X_NO-X_NOini) > 0.0)
    R_NO_D = K_NO_D*(X_NO-X_NOini)/MX;
else
    R_NO_D = 0.0;

R_NH3_NO      = -R_NO_G/Y_NO+Bio_w*R_NO_D;
R_CH3COOH_NO  = -0.5*(Bio_x*Y_NO)*R_NO_G/Y_NO;
R_O2_NO       = -0.25*(9-Y_NO*(Bio_u-2*Bio_v+6*Bio_w))*R_NO_G/Y_NO
               -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_NO_D;
R_X_NO        = R_NO_G-R_NO_D;
R_NO3_NO      = (1-Bio_w*Y_NO)*R_NO_G/Y_NO;
R_H2O_NO      = 0.5*(3+Y_NO*(2*Bio_x-Bio_u))*R_NO_G/Y_NO
               +0.5*(Bio_u-3*Bio_w)*R_NO_D;
R_CO2_NO      = 0.0;
R_H2_NO       = 0.0;
}

// -----
// 18') Anaerobic fermentation of NO biomass
// -----
void Cell::NO_AnaerobicFermentationBiomass(double fx){
double R2;

R2      = R_NX;
R_NO_G  = 0.0;

// As long as X_NO does increase more than the initial value, biomass decay will not
// occur.
if((X_NO-X_NOini) > 0.0)
    R_NO_D = K_NO_D*(X_NO-X_NOini)/MX;
else
    R_NO_D = 0.0;

R_X_NO      = -R_NO_D;
R_H2O_NO    = -(2*Bio_x-Bio_v-2*R2)*R_NO_D;
R_CH3COOH_NO = R2*R_NO_D;
R_CO2_NO    = (Bio_x-2*R2)*R_NO_D;
R_H2_NO     = 0.5*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w-8*R2)*R_NO_D;
R_NH3_NO    = Bio_w*R_NO_D;
R_O2_NO     = 0.0;
R_NO3_NO    = 0.0;
}

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// -----
// 19 ) Anaerobic denitrification of Nitrate (DN)
// -----
void Cell::AnaerobicDenitrificationNitrate(double fx){
    double R2;

    R2      = R_NX;

    // If both nitrate (NO3) and carbon source (CH3COOH_T) are available, the bacteria
    // will growing up follow below equation. If either nitrate or carbon sources not
    // available any more, denitrification of nitrate not occurs and the bacteria also
    // not growing up.
    if(NO3 > 0.0 && CH3COOH_T > 0.0)
        R_DN_G = fx*mu_DN*(X_DN/MX)*(NO3/(K_DN_S+NO3));
    else
        R_DN_G = 0.0;

    // As long as X_DN does not increase more than the initial value, biomass decay will
    // not occur.
    if((X_DN-X_DNini) > 0.0)
        R_DN_D = K_DN_D*((X_DN-X_DNini)/MX);
    else
        R_DN_D = 0.0;

    R_NO3_DN      = -R_DN_G/Y_DN;
    R_CH3COOH_DN  = -0.25*(3+Y_NO*(2*Bio_x+0.5*Bio_u-Bio_v))*R_DN_G/Y_DN+R2*R_DN_D;
    R_X_DN         = R_DN_G-R_DN_D;
    R_N2_DN        = 0.5*(1- Bio_w*Y_NO)*R_DN_G/Y_DN;
    R_CO2_DN       = 0.25*(6+Y_DN*(Bio_u-2*Bio_v))*R_DN_G/Y_DN
    + (Bio_x-2*R2)*R_MT_D;
    R_H2O_DN       = 0.25*(6+Y_DN*(4*Bio_x-Bio_u-2*Bio_v))*R_DN_G/Y_DN
    - (2*Bio_x-Bio_v-2*R2)*R_DN_D;
    R_NH3_DN       = Bio_w*R_DN_D;
    R_H2_DN        = 0.0;
    R_O2_DN        = 0.0;
}

// -----
// 19') Aerobic decomposition of DN biomass
// -----
void Cell::DN_AerobicDecompositionBiomass(double fx){

    R_DN_G = 0.0;

    // As long as X_DN does not increase more than the initial value, biomass decay will
    // not occur.
    if((X_DN-X_DNini) > 0.0)
        R_DN_D = K_DN_D*((X_DN-X_DNini)/MX);
    else
        R_DN_D = 0.0;

    R_X_DN         = -R_DN_D;
    R_O2_DN        = -0.25*(4*Bio_x+Bio_u-2*Bio_v-3*Bio_w)*R_DN_D;
    R_CO2_DN       = Bio_x*R_DN_D;
    R_H2O_DN       = 0.5*(Bio_u-3*Bio_w)*R_DN_D;
    R_NH3_DN       = Bio_w*R_DN_D;
    R_CH3COOH_DN  = 0.0;
    R_H2_DN        = 0.0;
    R_NO3_DN       = 0.0;
}

```

## Module VI: Heat Transfer

```

#include "Cell.h"
extern double t; // Start calculation time
extern double dt; // Differential calculation time
extern Atmospheric_cond atm; // Atmosphere condition
extern Heat_param HP; // Heat transfer parameters
extern Environment_cond env; // Environment condition
extern Circumference_media LayM[7];

#####
// Heat transfer by conduction
#####
// -----
// Since the Cell consist of 6 sides (up, down, right, left, front, and rear), the
// heat transfer occurs throughout all sides. The calculation order of heat transfer
// is follows; Firstly determine the characteristics of up, down, right, left, front,
// and rear sides such as temperature, resistance coefficient. Then, calculate the
// flux heat transfer qe[1]:up, qe[2]:bottom, qe[3]:left, qe[4]:right, qe[5]:front,
// qe[6]:rear. Conditions (such as media types and temperature)in the vicinity of
// Cell are given by a file
// -----
// -----
// Flux heat transfer by conduction
// -----
int Heat_flux_cal(Cell& ce){
    int i;
    int t_day;
    double _Temp;
    double Resist;
    t_day = (int)t;

    for(i=1;i<=6;i++){
        if(LayM[i].media!=none){
            ce.qe[i] = 0.0;
        }
        else{
            switch(LayM[i].media){
                case air:
                    _Temp = env.Tair[t_day];
                    Resist = 1.0/HP.Ua;
                    break;
                case waste:
                    _Temp = LayM[i].temp;
                    Resist = LayM[i].H * 0.5/HP.K_waste(LayM[i].wc);
                    break;
                case cover:
                    _Temp = env.Tair[t_day];
                    Resist = (LayM[i].H * 0.7/HP.K_cover) + (LayM[i].H * 0.3/HP.K_grav);
                    break;
                case soil:
                    _Temp = LayM[i].temp;
                    Resist = LayM[i].H/HP.K_soil;
                    break;
                case grav:
                    _Temp = LayM[i].temp;
                    Resist = (LayM[i].H * 0.02/HP.K_grav) + (LayM[i].H * 0.98/HP.K_soil);
                    break;
            }
            if(i==1){
                ce.qe[i] = (_Temp-ce.Temp)/(Resist);
            }
            if(i==2){
                ce.qe[i] = (_Temp-ce.Temp)/(Resist);
            }
            if(i==3 || i==4){
                ce.qe[i] = (_Temp-ce.Temp)/(Resist);
            }
        }
    }
}

```

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```

    }
    if(i==5 || i==6){
        ce.qe[i] = (_Temp-ce.Temp)/(Resist);
    }
}
else ce.qe[i]= 0.0;
}
return 0;
}

//#####
//#####
// Calculating temperature after dt
//#####
//#####
// -----
// The order of calculation is as follows;
// Firstly calculate from the bottom of Cell (The top upper Cell on the spot) to the
// first Cell Then calculate a gravel Cell at the bottom of the first Cell
// -----

int Temp_step_cal(Cell& ce){
double A,B,C;
double NewTemp;
double Heat_O2_OP, // 1 )Aerobic decomposition of Protein (OP)
Heat_CH3COOH_OP, // 1' )Anaerobic fermentation of OP biomass
Heat_O2_OF, // 2 )Aerobic decomposition of Fats (OF)
Heat_CH3COOH_OF, // 2' )Anaerobic fermentation of OF biomass
Heat_O2_OG, // 3 )Aerobic decomposition of Glucose (OG)
Heat_CH3COOH_OG, // 3' )Anaerobic fermentation of OG biomass
Heat_O2_OS, // 4 )Aerobic decomposition of Cellulose (OS)
Heat_CH3COOH_OS, // 4' )Anaerobic decomposition of OS biomass
Heat_O2_OH, // 5 )Aerobic decomposition of Lignin (OH)
Heat_CH3COOH_OH, // 5' )Anaerobic decomposition of OH biomass
Heat_CH3COOH_NP, // 6 )Anaerobic decomposition of Protein (NP)
Heat_CH3CH2C0OH_NP, // 6' )Anaerobic decomposition of Protein (NP)
Heat_CH3CH2CH2COOH_NP, // 6" )Anaerobic decomposition of Protein (NP)
Heat_O2_NP, // 6'" )Anaerobic decomposition of NP biomass
Heat_CH3COOH_NF, // 7 )Anaerobic fermentation of Fats (NF)
Heat_O2_NF, // 7' )Aerobic decomposition of NF biomass
Heat_CH3COOH_NG, // 8 )Anaerobic fermentation of Glucose (NG)
Heat_O2_NG, // 8' )Aerobic decomposition of NG biomass
Heat_CH3COOH_NS, // 9 )Anaerobic fermentation of Cellulose (NS)
Heat_O2_NS, // 9' )Aerobic decomposition of NS biomass
Heat_CH3COOH_NH, //10 )Anaerobic fermentation of Lignin (NH)
Heat_O2_NH, //10' )Aerobic decomposition of NH biomass
Heat_CH3COOH_AP, //11 )Acetogenesis of Propionate (AP)
Heat_O2_AP, //11' )Aerobic decomposition of AP biomass
Heat_CH3COOH_AB, //12 )Acetogenesis of Butyrate (AB)
Heat_O2_AB, //12' )Aerobic decomposition of AB biomass
Heat_CH4_MT, //13 )Methane formation from Acetic acid (MT)
Heat_CH3COOH_MT, //13' )Anaerobic fermentation of MT biomass
Heat_O2_MT, //13" )Aerobic decomposition of MT biomass
Heat_CH4_MT2, //14 )Methane formation from CO2 and H2 (MT2)
Heat_CH3COOH_MT2, //14' )Anaerobic fermentation of MT2 biomass
Heat_O2_MT2, //14" )Aerobic decomposition of MT2 biomass
Heat_O2_AO, //15 )Aerobic oxidation of Acetic acid (AO)
Heat_CH3COOH_AO, //15' )Anaerobic fermentation of AO biomass
Heat_O2_PO, //16 )Aerobic oxidation of Propionic acid (PO)
Heat_CH3COOH_PO, //16' )Anaerobic fermentation of PO biomass
Heat_O2_BO, //17 )Aerobic oxidation of Butyric acid (BO)
Heat_CH3COOH_BO, //17' )Anaerobic fermentation of BO biomass
Heat_NH3_NO, //18 )Aerobic nitrification of Ammonia (NO)
Heat_CH3COOH_NO, //18' )Anaerobic fermentation of NO biomass
Heat_NO3_DN, //19 )Aerobic denitrification of Nitrate (DN)
Heat_CH3COOH_DN; //19' )Anaerobic decomposition of DN biomass

```

```

#####
#####
// Calculation heat balance
#####
// -----
// Heat generate by of reaction
// -----
Heat_O2_OP           = ce.dH_O2_OP           * (-1) * ce.R_O2_OP ;
Heat_CH3COOH_OP      = ce.dH_CH3COOH_OP      * ce.R_CH3COOH_OP;
Heat_O2_OF           = ce.dH_O2_OF           * (-1) * ce.R_O2_OF ;
Heat_CH3COOH_OF      = ce.dH_CH3COOH_OF      * ce.R_CH3COOH_OF;
Heat_O2_OG           = ce.dH_O2_OG           * (-1) * ce.R_O2_OG ;
Heat_CH3COOH_OG      = ce.dH_CH3COOH_OG      * ce.R_CH3COOH_OG;
Heat_O2_OS           = ce.dH_O2_OS           * (-1) * ce.R_O2_OS ;
Heat_CH3COOH_OS      = ce.dH_CH3COOH_OS      * ce.R_CH3COOH_OS;
Heat_O2_OH           = ce.dH_O2_OH           * (-1) * ce.R_O2_OH;
Heat_CH3COOH_OH      = ce.dH_CH3COOH_OH      * ce.R_CH3COOH_OH;
Heat_CH3COOH_NP      = ce.dH_CH3COOH_NP      * ce.R_CH3COOH_NP;
Heat_CH3CH2COOH_NP  = ce.dH_CH3CH2COOH_NP    * ce.R_CH3CH2COOH_NP;
Heat_CH3CH2CH2COOH_NP = ce.dH_CH3CH2CH2COOH_NP * ce.R_CH3CH2CH2COOH_NP;
Heat_O2_NP           = ce.dH_O2_NP           * (-1) * ce.R_O2_NP;
Heat_CH3COOH_NF      = ce.dH_CH3COOH_NF      * ce.R_CH3COOH_NF;
Heat_O2_NF           = ce.dH_O2_NF           * (-1) * ce.R_O2_NF;
Heat_CH3COOH_NG      = ce.dH_CH3COOH_NG      * ce.R_CH3COOH_NG;
Heat_O2_NG           = ce.dH_O2_NG           * (-1) * ce.R_O2_NG;
Heat_CH3COOH_NS      = ce.dH_CH3COOH_NS      * ce.R_CH3COOH_NS;
Heat_O2_NS           = ce.dH_O2_NS           * (-1) * ce.R_O2_NS;
Heat_CH3COOH_NH      = ce.dH_CH3COOH_NH      * ce.R_CH3COOH_NH;
Heat_O2_NH           = ce.dH_O2_NH           * (-1) * ce.R_O2_NH;
Heat_CH3COOH_AP      = ce.dH_CH3COOH_AP      * ce.R_CH3COOH_AP;
Heat_O2_AP           = ce.dH_O2_AP           * (-1) * ce.R_O2_AP;
Heat_CH3COOH_AB      = ce.dH_CH3COOH_AB      * ce.R_CH3COOH_AB;
Heat_O2_AB           = ce.dH_O2_AB           * (-1) * ce.R_O2_AB;
Heat_CH4_MT          = ce.dH_CH4_MT          * ce.R_CH4_MT;
Heat_CH3COOH_MT      = ce.dH_CH3COOH_MT      * ce.R_CH3COOH_MT;
Heat_O2_MT           = ce.dH_O2_MT           * (-1) * ce.R_O2_MT;
Heat_CH4_MT2         = ce.dH_CH4_MT2         * ce.R_CH4_MT2;
Heat_CH3COOH_MT2     = ce.dH_CH3COOH_MT2     * ce.R_CH3COOH_MT2;
Heat_O2_MT2         = ce.dH_O2_MT2         * (-1) * ce.R_O2_MT2;
Heat_O2_AO           = ce.dH_O2_AO           * (-1) * ce.R_O2_AO;
Heat_CH3COOH_AO      = ce.dH_CH3COOH_AO      * ce.R_CH3COOH_AO;
Heat_O2_PO           = ce.dH_O2_PO           * (-1) * ce.R_O2_PO;
Heat_CH3COOH_PO      = ce.dH_CH3COOH_PO      * ce.R_CH3COOH_PO;
Heat_O2_BO           = ce.dH_O2_BO           * (-1) * ce.R_O2_BO;
Heat_CH3COOH_BO      = ce.dH_CH3COOH_BO      * ce.R_CH3COOH_BO;
Heat_NH3_NO          = ce.dH_NH3_NO          * (-1) * ce.R_NH3_NO;
Heat_CH3COOH_NO      = ce.dH_CH3COOH_NO      * ce.R_CH3COOH_NO;
Heat_CH3COOH_DN      = ce.dH_CH3COOH_DN      * ce.R_CH3COOH_DN;
Heat_NO3_DN          = ce.dH_NO3_DN          * (-1) * ce.R_NO3_DN;

// -----
// Heat transfer by conduction in the vicinity of Cell
// -----
A = ce.W * ce.L * (ce.qe[1] + ce.qe[2])
  + ce.H * ce.L * (ce.qe[3] + ce.qe[4])
  + ce.H * ce.W * (ce.qe[5] + ce.qe[6]);

// -----
// Heat-in and out of Cell by input and output water
// -----
if (LayM[1].media==none) {
  upTemp = ce.Temp;
}
else upTemp=LayM[1].temp;
if (LayM[2].media==none) {
  lowTemp = ce.Temp;
}
else lowTemp=LayM[2].temp;
B = HP.cp_water * HP.re_water * ((upTemp + ce.Temp) * ce.QLin
  - (ce.Temp + lowTemp) * ce.QLout)/2.0;

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// -----
// Heat-production by reactions in Cell
// -----
C = (Heat_O2_OP   + Heat_CH3COOH_OP
     + Heat_O2_OF   + Heat_CH3COOH_OF
     + Heat_O2_OG   + Heat_CH3COOH_OG
     + Heat_O2_OS   + Heat_CH3COOH_OS
     + Heat_O2_OH   + Heat_CH3COOH_OH
     + Heat_O2_NP   + Heat_CH3COOH_NP + Heat_CH3CH2COOH_NP + Heat_CH3CH2CH2COOH_NP
     + Heat_O2_NF   + Heat_CH3COOH_NF
     + Heat_O2_NG   + Heat_CH3COOH_NG
     + Heat_O2_NS   + Heat_CH3COOH_NS
     + Heat_O2_NH   + Heat_CH3COOH_NH
     + Heat_O2_AP   + Heat_CH3COOH_AP
     + Heat_O2_AB   + Heat_CH3COOH_AB
     + Heat_O2_MT   + Heat_CH3COOH_MT + Heat_CH4_MT
     + Heat_O2_MT2  + Heat_CH3COOH_MT2 + Heat_CH4_MT2
     + Heat_O2_AO   + Heat_CH3COOH_AO
     + Heat_O2_PO   + Heat_CH3COOH_PO
     + Heat_O2_BO   + Heat_CH3COOH_BO
     + Heat_NH3_NO  + Heat_CH3COOH_NO
     + Heat_NO3_DN  + Heat_CH3COOH_DN)
  * ce.V;

// -----
// Update the temperature of Cell
// -----
ce.oldTemp = ce.Temp;
NewTemp    = ce.Temp + (A + B + C)/(ce.V * HP.cp_waste(ce.wc)
                          * HP.re_waste(ce.wc)) * dt;
ce.Temp    = NewTemp;

return 0;
}

```

## Module VII: pH Calculation

```

#include "Cell.h"
extern double dt; // Differential calculation time
extern double t; // Start calculation time
extern double t_end; // End calculation time
extern double prt_dt; // Interval printout calculation results
extern Global_const CP; // Global constants
extern Atmospheric_cond atm; // Atmosphere condition
extern Environment_cond env; // Environment condition

static const double TOLERANCE = 1E-4;
static const int BISECTION_TRIAL_MAX = 1000;
static const double LOWER_END = 1.0E-14;
static const double UPPER_END = 1.0E-0;

double bisection_custom(Cell *);
double det_CO3, det_Ca, det_CaCO3;

// -----
// pH Calculation Function
// -----
void Cell::pH_calculation() {

// -----
// bisection
// -----
H_plus = bisection_custom(this);
pH = -log10(H_plus);
OH_min = pow(10.0, pH-14);

// -----
// Calculated temporary parameter
// -----
CO3 = det_CO3;
Ca_plus = det_Ca;
CaCO3 = det_CaCO3;

// -----
// Carbonate
// -----
HCO3 = CO3 * (H_plus/CP.Kd_HCO3);
H2CO3 = CO3 * sqrt(H_plus)/(CP.Kd_H2CO3 * CP.Kd_HCO3);
H2CO3_T = CO3 * (1.0 + (H_plus/CP.Kd_HCO3) + (sqrt(H_plus)/(CP.Kd_H2CO3
* CP.Kd_HCO3)));
P_CO2 = CP.Henry_CO2 * H2CO3;
}

double Cell::Ion_Balance(double seekH_plus){
double tmp_OH_min, tmp_Ca_plus;
double tmp_CO3, tmp_CaCO3;

// -----
// OH- concentration from self-ionization
// -----
// OH- is calculated from self-ionization by using Kw = 1E-14 as below:
tmp_OH_min = 1E-14/seekH_plus; // (0)

// -----
// CO32- concentration
// -----
tmp_CO3 = TIC/(1.0 + (sqrt(seekH_plus)/(CP.Kd_H2CO3 * CP.Kd_HCO3))
+ (seekH_plus/CP.Kd_HCO3)); // (1)

// -----
// Ca2+ concentration
// -----
tmp_Ca_plus = CP.Ksp_CaCO3/tmp_CO3; // (2)

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// -----
// CaCO3 concentration
// -----
tmp_CaCO3 = (TCa - tmp_Ca_plus) * (V_L/V_S)/r_sld; // (3)

// CO32-: (1); Ca2+: (2); CaCO3: (3)

// -----
// pH constituent in absences CaCO3
// -----
// If CaCO3 inside landfill not available any more, CaCO3 concentration must be set
// zero.
if(tmp_CaCO3 <= 0.0){
    tmp_CaCO3 = 0.0; // (4)

// -----
// Ca2+ concentration in absences Ca(OH)2 and CaCO3
// -----
// If CaCO3 in landfill not available, Ca2+ concentration must be equal with TCa.
// Ca2+ concentration is determined as below:
tmp_Ca_plus = TCa; // (5)
}

// CO32-: (1); Ca2+: (5); CaCO3: (4)

det_CO3 = tmp_CO3;
det_Ca = tmp_Ca_plus;
det_CaCO3 = tmp_CaCO3;

// -----
// The followings are the calculation of other ions
// -----
// -----
// HCO3- concentration
// -----
// HCO3- concentration is determined based on CO32- concentration and 2nd
// dissociation constant as below:
double tmp_HCO3 = tmp_CO3 * (seekH_plus/CP.Kd_HCO3);

// -----
// CH3COO- concentration
// -----
// CH3COO- concentration is determined based CH3COOH dissociation as below:
double tmp_CH3COO; {
tmp_CH3COO = CH3COOH_T/(1.0 + (CP.Kd_CH3COOH/seekH_plus))
    * (CP.Kd_CH3COOH/seekH_plus);
}

// -----
// CH3CH2COO- concentration
// -----
// CH3CH2COO- concentration is determined based CH3CH2COOH dissociation as below:
double tmp_CH3CH2COO; {
tmp_CH3CH2COO = CH3CH2COOH_T/(1.0 + (CP.Kd_CH3CH2COOH/seekH_plus))
    * (CP.Kd_CH3CH2COOH/seekH_plus);
}

// -----
// CH3CH2CH2COO- concentration
// -----
// CH3CH2CH2COO- concentration is determined based CH3CH2CH2COOH dissociation as
// below:
double tmp_CH3CH2CH2COO; {
tmp_CH3CH2CH2COO = CH3CH2CH2COOH_T/(1.0 + (CP.Kd_CH3CH2CH2COOH/seekH_plus))
    * (CP.Kd_CH3CH2CH2COOH/seekH_plus);
}

```

```

// -----
// NH4+ concentration
// -----
// NH4+ concentration is determined based dissolved Ammonia [NH4OH] dissociation as
// below:
double tmp_NH4; {
double tmp_NH3_T;
tmp_NH3_T = T_NH3/(1.0 + CP.Kp_NH3 * r_sld * (V_S/V_L)/(1.0
+ (CP.Kd_NH3/tmp_OH_min) * (CP.Kd_NH3/tmp_OH_min));
tmp_NH4 = tmp_NH3_T/(1.0 + (CP.Kd_NH3/tmp_OH_min)) * (CP.Kd_NH3/tmp_OH_min);
}

// -----
// Ion balance
// -----
// Ion balance is calculation based on differences between anion and cation as below:
double balance; {
double anion, cation;

anion = (tmp_CH3COO + tmp_CH3CH2COO + tmp_CH3CH2CH2COO + tmp_HCO3
+ 2 * tmp_CO3 + tmp_OH_min + NO3 + Cl_min);
cation = (tmp_NH4 + seekH_plus + 2 * tmp_Ca_plus + Na_plus);
balance = (anion - cation);
}
return balance;
}

double bisection_custom(Cell* pc) {
double a, b, c;
double fa,fb,fc;

a = LOWER_END;
b = UPPER_END;

fa = (pc -> Ion_Balance)(a); // if (fa == 0) return a;
fb = (pc -> Ion_Balance)(b); // if (fb == 0) return b;

for (int i = 0; i< BISECTION_TRIAL_MAX; i++) {

c = pow(10, (-((-log10(a))+(-log10(b)))/2));

fc = (pc -> Ion_Balance)(c);
if (fc == 0.0) return c;
if (fc * fa > 0.0){
a = c;
fa = fc;
}
else{
b = c;
fb = fc;
}
}
return c;
}
}

```

## Appendix B

### Input Data

-----  
 CLACULATION CONDITION SETTING  
 -----

Calculation time step (max)	(dt)	[day]	0.0001
Total calculation time	(t_end)	[day]	750
Printout interval	(prt_dt)	[day]	1

-----  
 CONSTANT PARAMETER SETTING  
 -----

Gas constant	(R)	[m3*Pa/kmol-K]	8314
Henry's law constant for CO2	(Henry_CO2)	[Pa*m3/kmol]	3.02E+06
Henry's law constant for NH3	(Henry_NH3)	[Pa*m3/kmol]	5635
First acid dissociation constant	(Kd_HCO3)	[kmol/m3]	4.79E-11
Second acid dissociation constant	(Kd_H2CO3)	[kmol/m3]	4.30E-07
Equilibrium constant of NH3	(Kd_NH3)	[kmol/m3]	3.16E-11
Equilibrium constant of acetic acid	(Kd_CH3COOH)	[kmol/m3]	1.74E-05
Equilibrium constant of acetic acid	(Kd_CH3COOH)	[kmol/m3]	1.34E-05
Equilibrium constant of acetic acid	(Kd_CH3COOH)	[kmol/m3]	1.52E-05
Calcium carbonate solubility constant	(Ksp_CaCO3)	[kmol/m3]	4.80E-08
Ammonia adsorption distribution coefficient	(Kp_NH3)	[m3/kg-solid]	0.01
Diffusion coefficient of i gas component	(Dif)	[m2/d]	0.0001
Chemical formula of Protein (CaHbOcNn)			
a [-]	b [-]	c [-]	n [-]
46	77	17	12
MW [kg/kmol]			
1070.06			
Chemical formula of Fats (CaHbOc)			
a [-]	b [-]	c [-]	MW [kg/kmol]
55	104	6	861.53
Chemical formula of Carbohydrate (12a+b+14c)n			
a [-]	b [-]	c [-]	n [-]
6	10	5	1
MW [kg/kmol]			
162.11			
Chemical formula of Cellulose (12a+b+14c)n			
a [-]	b [-]	c [-]	n [-]
6	10	5	3
MW [kg/kmol]			
486.33			
Chemical formula of Lignin (CaHbOc)			
a [-]	b [-]	c [-]	MW [kg/kmol]
10	12	3	180.19
Chemical formula of bacteria (CxHuOvNw)			
x [-]	u [-]	v [-]	w [-]
5	7	2	1
MW [kg/kmol]			
113.1			

-----  
 Constants related to reaction rate  
 -----

++++Aerobic Decomposition of Protein OP++++			
Yield coefficient	(Y_OP)	[-]	0.1
Maximum specific growth rate constant	(mu_OP)	[1/d]	5
Substrate saturation constant	(K_OP_S)	[-]	0.015
Saturation constant for partial pressure of O2	(K_OP_O)	[Pa]	2026
Decay rate coefficient	(K_OP_D)	[1/d]	0.25
++++Aerobic Decomposition of Fats OF++++			
Yield coefficient	(Y_OF)	[-]	0.1
Maximum specific growth rate constant	(mu_OF)	[1/d]	5
Substrate saturation constant	(K_OF_S)	[-]	0.015
Saturation constant for partial pressure of O2	(K_OF_O)	[Pa]	2026
Decay rate coefficient	(K_OF_D)	[1/d]	0.25
++++Aerobic Decomposition of Glucose OG++++			
Yield coefficient	(Y_OG)	[-]	0.1
Maximum specific growth rate constant	(mu_OG)	[1/d]	5
Contois constant	(K_OG_S)	[-]	100
Saturation constant for partial pressure of O2	(K_OG_O)	[Pa]	2026
Decay rate coefficient	(K_OG_D)	[1/d]	0.25

++++Aerobic Decomposition of Cellulose OS++++			
Yield coefficient	(Y_OS)	[-]	0.1
Maximum specific growth rate constant	(mu_OS)	[1/d]	1
Substrate saturation constant	(K_OS_S)	[-]	0.15
Saturation constant for partial pressure of O2	(K_OS_O)	[Pa]	2026
Decay rate coefficient	(K_OS_D)	[1/d]	0.05
++++Aerobic Decomposition of Lignin OH++++			
Yield coefficient	(Y_OH)	[-]	0.1
Maximum specific growth rate constant	(mu_OH)	[1/d]	1
Substrate saturation constant	(K_OH_S)	[-]	0.15
Saturation constant for partial pressure of O2	(K_OH_O)	[Pa]	2026
Decay rate coefficient	(K_OH_D)	[1/d]	0.05
++++Ratio CO2 and CH3COOH production rate++++			
Acetic acid production of fermentation Protein	(R_NP)	[-]	3.65
Acetic acid production of fermentation Fats	(R_NF)	[-]	20.1
Acetic acid production of fermentation Glucose	(R_NG)	[-]	2.025
Acetic acid production of fermentation Cellulose	(R_NS)	[-]	8.625
Acetic acid production of fermentation Lignin	(R_NH)	[-]	4.625
Acetic acid production of acetogenesis Propionate	(R_AP)	[-]	1.125
Acetic acid production of acetogenesis Butyrate	(R_AB)	[-]	1.625
Acetic acid production of decayed micro-organism	(R_NX)	[-]	2.5
++++Anaerobic Fermentation of Protein NP++++			
Yield coefficient	(Y_NP)	[-]	0.2
Maximum specific growth rate constant	(mu_NP)	[1/d]	0.001
Substrate saturation constant	(K_NP_S)	[kg/m3]	25
Decay rate coefficient	(K_NP_D)	[1/d]	5.00E-05
++++Anaerobic Fermentation of Fats NF++++			
Yield coefficient	(Y_NF)	[-]	0.2
Maximum specific growth rate constant	(mu_NF)	[1/d]	0.002
Substrate saturation constant	(K_NF_S)	[kg/m3]	25
Decay rate coefficient	(K_NF_D)	[1/d]	0.0001
++++Anaerobic Fermentation of Glucose NG++++			
Yield coefficient	(Y_NG)	[-]	0.05
Maximum specific growth rate constant	(mu_NG)	[1/d]	0.002
Substrate saturation constant	(K_NG_S)	[kg/m3]	25
Decay rate coefficient	(K_NG_D)	[1/d]	0.0001
++++Anaerobic Fermentation of Cellulose NS++++			
Yield coefficient	(Y_NS)	[-]	0.15
Maximum specific growth rate constant	(mu_NS)	[1/d]	0
Substrate saturation constant	(K_NS_S)	[kg/m3]	250
Decay rate coefficient	(K_NS_D)	[1/d]	0
++++Anaerobic Fermentation of Lignin NH++++			
Yield coefficient	(Y_NH)	[-]	0.15
Maximum specific growth rate constant	(mu_NH)	[1/d]	0
Substrate saturation constant	(K_NH_S)	[kg/m3]	500
Decay rate coefficient	(K_NH_D)	[1/d]	0
++++Acetogenesis of Propionate AP++++			
Yield coefficient	(Y_AP)	[-]	0.05
Maximum specific growth rate constant	(mu_AP)	[1/d]	0.1
Substrate saturation constant	(K_AP_S)	[kg/m3]	10
Decay rate coefficient	(K_AP_D)	[1/d]	0.005
++++Acetogenesis of Butyrate AB++++			
Yield coefficient	(Y_AB)	[-]	0.05
Maximum specific growth rate constant	(mu_AB)	[1/d]	0.1
Substrate saturation constant	(K_AB_S)	[kg/m3]	10
Decay rate coefficient	(K_AB_D)	[1/d]	0.005
++++Methane fermentation from Acetic acid MT++++			
Maximum specific growth rate constant	(mu_MT)	[1/d]	0.009
Yield coefficient	(Y_MT)	[-]	0.005
Saturation constant for CH3COOH	(K_MT_S)	[kmol/m3]	30
Decay rate coefficient of methane bacteria	(K_MT_D)	[1/d]	0.00045
++++Methane formation from CO2 and H2 MT2++++			
Maximum specific growth rate constant	(mu_MT2)	[1/d]	0.75
Yield coefficient	(Y_MT2)	[-]	0.005
Saturation constant for methane formation CO2&H2	(K_MT2_S)	[kmol/m3]	15
Decay rate coefficient of methane bacteria	(K_MT2_D)	[1/d]	0.0375
++++Acetic acid aerobic oxidation AO++++			
Yield coefficient	(Y_AO)	[-]	0.2
Maximum specific growth rate constant	(mu_AO)	[1/d]	1
Substrate saturation constant	(K_AO_S)	[-]	0.02
Saturation constant for partial pressure of O2	(K_AO_O)	[Pa]	2026
Decay rate coefficient	(K_AO_D)	[1/d]	0.05

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++++Propionic acid aerobic oxidation PO++++			
Yield coefficient	(Y_PO)	[-]	0.2
Maximum specific growth rate constant	(mu_PO)	[1/d]	1
Substrate saturation constant	(K_PO_S)	[-]	0.02
Saturation constant for partial pressure of O2	(K_PO_O)	[Pa]	2026
Decay rate coefficient	(K_PO_D)	[1/d]	0.05
++++Butyric acid aerobic oxidation BO++++			
Yield coefficient	(Y_BO)	[-]	0.2
Maximum specific growth rate constant	(mu_BO)	[1/d]	1
Substrate saturation constant	(K_BO_S)	[-]	0.02
Saturation constant for partial pressure of O2	(K_BO_O)	[Pa]	2026
Decay rate coefficient	(K_BO_D)	[1/d]	0.05
++++Nitrification of ammonia NO++++			
Yield coefficient	(Y_NO)	[-]	0.2
Maximum specific growth rate constant	(mu_NO)	[1/d]	1
Substrate saturation constant	(K_NO_S)	[-]	0.02
Saturation constant for partial pressure of O2	(K_NO_O)	[Pa]	2026
Decay rate coefficient	(K_NO_D)	[1/d]	0.05
++++Denitrification of Nitrate DN++++			
Yield coefficient	(Y_DN)	[-]	0.05
Maximum specific growth rate constant	(mu_DN)	[1/d]	0.001
Substrate saturation constant	(K_DN_S)	[kmol/m3]	0.3
Decay rate coefficient	(K_DN_D)	[1/d]	5.00E-05
++++Critical amount of acetic acid Tcri++++			
Critical amount of acetic acid	(CH3COOH_Tcri)	[kmol/m3]	0.002
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Initial Density of Landfilled Waste			
-----			
Dry density	(r_dry)	[kg/m3]	453.44
Wet density	(r_wet)	[kg/m3]	863.44
True density	(r_slD)	[kg/m3]	1040
#####			
## Dimension and Initial Landfill Properties ##			
#####			
-----			
1. Dimension of Landfill Cell			
-----			
Height of Cell	(H)	[m]	2
Diameter of Cell	(D)	[m]	0.7
Surface area of Cell	(S)	[m2]	0.396
Volume of Cell	(V)	[m3]	0.792
-----			
2. Volume of Each Phase			
-----			
Water volume within Cell	(V_L)	[m3]	0.325
Gas volume within Cell	(V_G)	[m3]	0.122
Solid volume within Cell	(V_S)	[m3]	0.345
Field capacity of Cell	(wcp)	[-]	0.35
-----			
3. Initial Amount of Landfill Phase			
-----			
The amount of input water in Cell	(QLin)	[mm/d]	505.15
The amount of output gas from	(QGout)	[kmol]	0
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4. The Other Parameters			
-----			
Temperature within Cell	(Temp)	[K]	303.15
Atmospheric pressure	(P)	[MPa]	0.1013
#####			
## Initial Concentration in Cell ##			
#####			
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1. Fraction of Solid Organic Matter			
-----			
Protein fraction	(S_PRO)	[kg/m3]	9.069
Fats fraction	(S_FAT)	[kg/m3]	4.534
Glucose fraction	(S_GLU)	[kg/m3]	36.27

Cellulose fraction	(S_CEL)	[kg/m3]	90.69
Lignin fraction	(S_LIG)	[kg/m3]	31.74
Inorganic fraction	(S_INO)	[kg/m3]	281.133

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 2. Partial Pressure of Gas [Pa]  
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Partial pressure of CO2	(P_CO2)	[Pa]	38.8282
Partial pressure of Ammonia	(P_NH3)	[Pa]	0
Partial pressure of O2	(P_O2)	[Pa]	20384.8
Partial pressure of N2	(P_N2)	[Pa]	76646.8
Partial pressure of H2	(P_H2)	[Pa]	0
Partial pressure of Methane gas	(P_CH4)	[Pa]	0

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 3. Concentrations in Liquid Phase  
 -----

Total of acetic acid	(CH3COOH_T)	[kmol/m3]	0.15
Acetic acid	(CH3COOH)	[kmol/m3]	0.008161
Acetate ion	(CH3COO)	[kmol/m3]	0.141839
Total of Propionic acid	(CH3CH2COOH_T)	[kmol/m3]	0
Propionic acid	(CH3CH2COOH)	[kmol/m3]	0
Propionic ion	(CH3CH2COO)	[kmol/m3]	0
Total of Butyric acid	(CH3(CH2)2COOH_T)	[kmol/m3]	0
Butyric acid	(CH3(CH2)2COOH)	[kmol/m3]	0
Butyric ion	(CH3CH2CH2COO)	[kmol/m3]	0
COD	(COD)	[mg/L]	0
Total of NH3 in cell	(T_NH3)	[kmol/m3]	0
Ammonia	(NH3)	[kmol/m3]	0
Ammonium ion	(NH4)	[kmol/m3]	0
Total of ammonia	(NH3_T)	[kmol/m3]	0
Total inorganic carbon in Cell	(TIC)	[kmol/m3]	1.84E-05
Nitrate	(NO3)	[kmol/m3]	0
Hydrogen ion	(H_plus)	[kmol/m3]	1.00E-06
CaCO3	(CaCO3)	[kmol/m3]	0.0004
Carbonic acid	(H2CO3)	[kmol/m3]	1.29E-05
Bicarbonate ion	(HCO3)	[kmol/m3]	5.53E-06
Carbonate ion	(CO3)	[kmol/m3]	2.65E-10
Total of Carbonate in liquid phase	(H2CO3_T)	[kmol/m3]	1.84E-05
Inorganic carbon	(IC)	[mg/L]	0.220918

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 4. Accumulated Amount  
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Accumulated amount of CH3COOH	(Acu_CH3COOH)	[kmol]	0
Accumulated amount of CH3CH2COOH	(Acu_CH3CH2COOH)	[kmol]	0
Accumulated amount of CH3(CH2)2COOH	(Acu_CH3(CH2)2COOH)	[kmol]	0
Accumulated amount of IC	(Acu_IC)	[mg-C]	0
Accumulated amount of NH4	(Acu_NH3)	[kmol]	0
Accumulated amount of NO3	(Acu_NO3)	[kmol]	0
Accumulated amount of gas	(Acu_QGout)	[kmol]	0
Accumulated amount of CO2 gas	(Acu_CO2)	[kmol]	0
Accumulated amount of CH4	(Acu_CH4)	[kmol]	0
Accumulated amount of H2	(Acu_H2)	[kmol]	0
Accumulated amount of N2	(Acu_N2)	[kmol]	0
Accumulated amount of NH3	(Acu_PNH3)	[kmol]	0
Accumulated amount of O2	(Acu_O2)	[kmol]	0

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 5. Initial pH of Landfilled Waste  
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Initial pH	(pH)	[-]	6
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 6. Initial Amount of Bacteria in landfill waste [kg/m3-compartment]  
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Aerobic decomposition bacteria of Protein	(X_OP)	0.15
Aerobic decomposition bacteria of Fats	(X_OF)	0.15
Aerobic decomposition bacteria of Glucose	(X_OG)	0.15
Aerobic decomposition bacteria of Cellulose	(X_OS)	0.15
Aerobic decomposition bacteria of Lignin	(X_OH)	0.15
Anaerobic fermentation bacteria of Protein	(X_NP)	0.15

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Anaerobic fermentation bacteria of Fats	(X_NF)	0.15
Anaerobic fermentation bacteria of Glucose	(X_NG)	0.15
Anaerobic fermentation bacteria of Cellulose	(X_NS)	0.15
Anaerobic fermentation bacteria of Lignin	(X_NH)	0.15
Acetogenesis bacteria of Propionate	(X_AP)	0.15
Acetogenesis bacteria of Butyrate	(X_AB)	0.15
Methane formation bacteria from Acetic acid	(X_MT)	0.15
Methane formation bacteria from CO <sub>2</sub> +H <sub>2</sub>	(X_MT2)	0.15
Acetic acid oxidation bacteria	(X_AO)	0.15
Propionic acid oxidation bacteria	(X_PO)	0.15
Butyric acid oxidation bacteria	(X_BO)	0.15
Nitrification Ammonia bacteria	(X_NO)	0.15
Denitrification Nitrate bacteria	(X_DN)	0.15

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## Appendix C

### Curriculum Vitae



#### A. Personal Data

Full name : Edi Munawar  
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#### B. Educational Background

2008 – 2014 : Doctoral Program at Institute for Water Quality, Resource and Waste Management, Vienna University of Technology, Vienna – Austria.  
Oct. – Dec. 2011 : Visiting researcher at Division of Environmental Engineering Graduate School of Engineering, Hokkaido University, Sapporo – Japan.  
Oct. – Dec. 2006 : Visiting researcher at Institute for Water Quality, Resource and Waste Management, Vienna University of Technology, Vienna – Austria.  
Feb. – Mar. 2005 : Visiting researcher at Ecological Engineering Department, Toyohashi University of Technology, Toyohashi – Japan.  
2002 – 2004 : Master Program at Ecological Engineering Department, Toyohashi University of Technology, Toyohashi – Japan.  
1989 – 2006 : Undergraduate studies at Chemical Engineering Department, Syiah Kuala University, Banda Aceh – Indonesia.

#### C. Working Experience

March 2014 : Project Assistant of Christian Doppler Labor für Anthropogene Ressourcen am Institut für Wassergüte, Ressourcenmanagement und Abfallwirtschaft eingerichtet, Technische Universität Wien, Wien – Österreich.  
Jul – Sep. 2013 : Project Assistant of Christian Doppler Labor für Anthropogene Ressourcen am Institut für Wassergüte, Ressourcenmanagement und Abfallwirtschaft

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- eingerichtet, Technische Universität Wien, Wien – Österreich.  
 March – Nov. 2009 : Project Assistant of Specific Targeted Research Project of the 6th European Union Framework Programme (The FORWAST Project), Vienna University of Technology, Vienna – Austria.  
 Aug. – Dec. 2007 : Waste Management Consultant of United Nation Development Programme (UNDP), Banda Aceh–Indonesia.  
 Jun. – Jul. 2007 : Composting Expert of Federation of Canadian Municipalities (FCM) – Canada Aceh Local Government Assistance Program (CALGAP), Banda Aceh – Indonesia  
 2006 – 2007 : Tender Committee Chairman of Task Force for Higher Education of NAD – Nias Rehabilitation and Reconstruction Agency (BRR NAD–Nias), Banda Aceh – Indonesia.  
 2005 – 2007 : Department Coordinator of Technological and Professional Skills Development Sector Project (TPSDP) under ADB Loan No. 1792 – INO, Syiah Kuala University, Banda Aceh – Indonesia  
 2004 – 2008 : Head of Instrumentation and Analysis at Department of Chemical Engineering, Syiah Kuala University, Banda Aceh – Indonesia.  
 2001 – 2002 : Assistant Equipment Engineer at Pacific Consultant International (PCI) in association with Nissoken Architect & Engineers and PT. Cakra Manggilingan Jaya, Banda Aceh – Indonesia.  
 2000 – 2008 : Lecturer and researcher at Department of Chemical Engineering, Syiah Kuala University, Banda Aceh – Indonesia  
 1998 – 1999 : Teaching staff members at Department of Chemical Engineering, Syiah Kuala University, Banda Aceh – Indonesia  
 1996 – 1998 : Head of laboratory of PT. Nilam Sari Palm Oil Mill.

#### **D. Publication**

1. Edi Munawar and Johann Fellner (2013), Landfilling in Tropical Climates – Measures for Better Design and Operation, ISWA World Congress 2013, October 7–11<sup>th</sup>, 2013, Vienna – Austria.
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3. Edi Munawar, Anna Kubin and Johann Fellner (2012), Landfills in Tropical Climates – Knowledgebase for an Environmentally Friendly Operation, ISWA World Solid Waste Congress, September 17 – 19th, 2012, Florence – Italy.

4. Edi Munawar, Johann Fellner and Paul Hans Brunner (2011), Modeling to Determine Fate Organic Matter and Extending Maintenance Period due to “Do Nothing” after Capping MSW Landfill: Case Study Breitenau Landfill, Austria, 4<sup>th</sup> International Workshop Hydro–physic–mechanics of Landfills (HPM4), April 27 – 28<sup>th</sup>, 2011, Santander – Spain.
5. Jakob Lederer, Edi Munawar, Carolina Massmann, Johann Fellner, Martin Obermoser, Gloria Pessina, Paul H. Brunner, Heinz Buschmann, Bernd Brandt, Stefan Neumayer, Hans Daxbeck (2010). Description of the environmental pressures for each relevant combination of material and recycling/treatment technology (Project FORWAST). Vienna University of Technology, Institute for Water Quality, Resource and Waste Management & Resource Management Agentur (RMA), Vienna.
6. Edi Munawar, Michio Ubaura, Naohiro Goto and Koichi Fujie (2004), Greenhouse Gases (GHGs) and Other Gas Pollutant Emissions of Indonesian Urea Fertilizer Manufacture, Proceeding Japan Environmental Scientific Meeting 2004, September 30<sup>th</sup> – October 1<sup>st</sup>, 2004, Nishinomiya City, Kobe – Japan.
7. Edi Munawar, Michio Ubaura, Naohiro Goto and Koichi Fujie (2004), Estimation CO<sub>2</sub>, Non–CO<sub>2</sub> GHGs and Other Gas pollutant Emissions of Indonesia’s Urea Fertilizer Factories, Proceeding 13<sup>th</sup> US EPA International Emission Inventory Conference, June 8–10, 2004, Clear Water FL – USA

