

Urban digital Twin - Waste Management

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WASTE MANAGEMENT SIMULATION  
THEORETICAL BASE AND PROGRAM MANUAL



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## Abstract

This report presents a comprehensive waste management simulation program designed to model various waste management scenarios, providing valuable insights for policymakers and decision-makers. The simulation focuses on Municipal Solid Waste (MSW) and Separately Collected Waste (SCW), examining multiple processing techniques such as composting, anaerobic digestion, incineration, landfill, and gasification.

The used methodology follows the guidelines set by the Intergovernmental Panel on Climate Change (IPCC), the simulation categorizes outputs into energy recovery, greenhouse gas emissions, and material recovery. The program relies on default values but allows for adjustments to enhance accuracy based on local data, following a tiered approach to data input quality. This report not only elucidates the theoretical underpinnings of the simulation models but also provides a user manual to facilitate proper usage and customization of the program.

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## 1 Introduction

Waste management has become increasingly important in recent decades due to the rising volume of waste generated by humanity. Additionally, there's overwhelming evidence indicating that improper waste management negatively impacts the environment and human health. Given that waste production is unavoidable, it's crucial to implement effective waste management plans that balance sustainability with minimal inconvenience to the public.

Considering this, a simulation program has been developed to model various waste management scenarios. These simulations aim to provide policymakers and decision-makers with valuable insights, facilitating informed comparisons and decisions regarding suitable waste management plans.

This report aims to explain the theory behind the program and provide instructions for its proper use. It's worth noting that, apart from the program itself, two additional Excel files—`Inventory_data` and `Assumptions.data`—are required for the simulation to function correctly. This dependency is temporary, as the program will eventually be integrated into an Urban Digital Twin, which will likely change the format of the input files to a more dynamic nature. However, at the time of writing this report, the Digital Twin is not ready for that implementation, so the current waste management simulation program operates independently.

The program can be easily accessed through the following GitHub repository:

<https://github.com/FranciscoGouveia47/IN—waste-management.git>

## 2 Theoretical base

The program's theoretical models draw upon the established Guidelines by the IPCC [1]. These models aim to yield results, whenever feasible, categorized into three main areas: **Energy recovered, Greenhouse gas emissions, and Material recovery**. It's important to mention that, according to IPCC guidelines, certain percentages of these values or impacts may be allocated to different sectors. For instance, emissions resulting from burning  $CH_4$  captured from anaerobic digestion are attributed not to the Waste sector, but rather to the Energy Sector.

The program comes preloaded with default values and assumptions. However, it's crucial to recognize that the accuracy of any simulation model hinges on the quality of its data input. Therefore, it's highly recommended to thoroughly assess whether the default values need adjustment to better suit the specific simulation requirements.

In the realm of data acquisition, the IPCC has delineated three tiers for simulations based on the data input. Tier 1 entails using default data for simulation. Tier 2 utilizes national-level data, leveraging nationwide averages to approximate assumption values. Tier 3, on the other hand,

employs local data, with each waste stream relying on locally tested parameters for simulation. As mentioned earlier, while this program primarily utilizes default values, users have the flexibility to adjust parameters to elevate the simulation to a higher tier.

Category of specific data acquisition is outside the scope of this report but is recommended to follow the IPCC guidelines for data acquisition if a higher degree of the simulation is required.

Given this context, it is assumed that the reader has a basic understanding of thermodynamics and chemistry. Therefore, fundamental definitions and concepts will not be covered in this section.

## 2.1 MSW - Municipal Solid Waste

“Municipal solid waste” (MSW) commonly denotes waste collected by municipalities or local authorities. However, this definition can vary across countries. Generally, MSW encompasses household waste, garden and park waste, as well as commercial and institutional waste. In the context of this program, MSW was divided in the following categories:

- Paper/Cardboard
- Textiles
- Food Waste
- Wood
- Garden and Park waste
- Rubber and Leather
- Plastics
- Metal
- Glass

Users have the freedom to introduce extra categories, but it’s advisable to back up the program before doing so. In Section 3, instructions on adding extra categories to the code will be provided.

MSW streams can be handled in various ways, but certain conditions are commonly shared among most scenarios. For instance, estimating emissions during waste transportation from pickup sites to treatment facilities can be challenging but can be approximated using ratios based on the amount and type of waste being transported [2]. Table 2 in the Appendix provides these values for different potential outcomes of the waste stream.

In MSW management, a prevalent approach involves routing the waste stream through a Mechanical Biological Treatment (MBT) facility. These facilities integrate mechanical processes such as shredding and screening with biological processes like composting or anaerobic digestion to reclaim valuable materials and generate energy or compost. Section 3 will delve into simulating these facilities, detailing how to model them based on the distribution of mass percentages allocated to each waste processing technique.

### 2.1.1 MBT - Composting

The first of MSW processing techniques to be tackled is Composting. Composting, also known as Aerobic Digestion, is a natural process involving the decomposition of organic matter by microorganisms such as bacteria, fungi, and other small organisms. Its primary outputs include  $CO_2$

resulting from the digestion process and compost, which serves as a valuable soil amendment and fertilizer.

It's important to note a significant aspect of organic matter decomposition, which becomes even more apparent in the Anaerobic Digestion section is that the ratio between the production of  $CO_2$  and  $CH_4$  is governed by the presence of oxygen. This means that for Composting, which has access to virtually limitless oxygen, emissions of  $CH_4$  tend to be less than 1 percent. The production of  $N_2O$  is also in the same order magnitude and is dependent on the nitrogen content of the material [3]. These factors are the primary reason gas recovery isn't utilized for composting systems.

That being said, the initial step in simulating organic matter decomposition is to estimate the amount of Degradable Organic Carbon ( $DOC$ ) for each waste category present. Equation (1) is employed for this purpose.

$$DOC_m = \sum_i (DOC_i \bullet W_i) \quad (1)$$

Here,  $DOC_m$  represents the total mass of degradable organic carbon in the waste being simulated,  $DOC_i$  stands for the fraction of degradable organic carbon in waste type  $i$ , and  $W_i$  denotes the mass of each category present. The  $DOC$  values for each category of MSW are available in the Table 3 of the Appendix.

Depending on the prevailing conditions, not all  $DOC$  will be consumed during the composting process. The actual amount of decomposable  $DOC$  ( $DDOC$ ) must be estimated based on the specific emissions of interest being calculated. For instance, within the same batch, the  $DDOC$  value for  $CH_4$  might differ from that associated with  $CO_2$ . As previously noted, for composting,  $CH_4$  emissions are below 1 percent, this means that it is only makes sense to estimate the  $DDOC$  value concerning  $CO_2$  emissions (see equation (2)).

$$DDOC_{CO_2} = DOC_m \bullet CF \simeq DOC_m \bullet (1 - MCF) \quad (2)$$

Where  $DDOC_{CO_2}$  is the total mass of decomposable  $DOC$ , and  $CF$  is a correction factor intended to adjust the  $DOC_m$  value. For composting, the  $CF$  can be approximated using the Methane Correction Factor ( $MCF$ ). This factor represents the degree of anaerobic conditions in a system, which, for composting, can typically be approximated to zero. However, there are situations where the  $MCF$  can differ from zero, such as when a large quantity of waste results in sections being under anaerobic conditions [4].

Having correctly estimated the  $DDOC_{CO_2}$ , it is straightforward to calculate the mass of  $CO_2$  being

emitted. Assuming that for composting, the efficiency of conversion of  $DDOC_{CO_2}$  to  $CO_2$  is nearly perfect, the calculation becomes a simple product between the value calculated in equation (2) and 44/12 (the mass ratio of  $CO_2$  to C).

Regarding the mass of compost being produced, it is very difficult to accurately estimate this value because the definition of compost can apply to a broad spectrum of substances varying in composition and water content. Additionally, compost production is a non-homogeneous, transient process, making it hard to simulate with the available data. To properly estimate the compost mass being produced, a more complex simulation model for composting would need to be employed. However, it is possible to provide a rough estimate based on the mass loss related to the  $DDOC_{CO_2}$ :

$$W_{compost} = \sum_i (W_i - DDOC_i) \quad (3)$$

Where  $W_{compost}$  is the compost mass in wet basis,  $W_i$  is the total waste mass before the composting operation (by category) and  $DDOC_i$  is the mass loss caused by the decomposition of the Carbon in the waste.

### 2.1.2 MBT - Anaerobic Digestion

Anaerobic Digestion (AD) is a process akin to composting, involving the decomposition of organic matter by microorganisms. The primary difference, as indicated by its name, is that this process occurs under anaerobic conditions. Anaerobic digestion refines the composting concept by maintaining temperature, moisture content, and pH near their optimal values, adding complexity to the process and influencing its outputs [3].

The main products of AD are digestate and biogas. While digestate originates similarly to compost, it significantly differs in composition, processing methods, and applications. Regarding biogas production, a high-quality AD facility primarily produces methane ( $CH_4$ ), which is often captured for later use. Emissions of  $CH_4$  from such facilities, due to unintentional leakages during process disturbances or other unexpected events, generally range from 0 to 10 percent of the produced methane [3].

To accurately estimate the relevant quantities in this operation, the initial step is similar to the composting method: estimating the Degradable Organic Carbon (DOC) content of the waste stream using equation (1). Given that this process occurs in the absence of oxygen, theoretically, no  $CO_2$  should be produced. With the calculated  $DOC$  value, it is then possible to estimate the quantity of Degradable DOC (DDOC) necessary for methane production using equation (4).

$$DDOC_{CH_4} = DOC_m \bullet DOC_f \bullet MCF \quad (4)$$

Where  $DDOC_{CH_4}$  represents the mass of decomposable DOC that can convert to methane,  $DOC_m$  denotes the total mass of degradable organic carbon in the waste stream,  $DOC_f$  is the fraction of DOC that can decompose under AD conditions, and  $MCF$  (Methane Correction Factor) characterizes the anaerobic nature of the operational environment.

The next step is to calculate the mass of carbon that converts into methane using equation (5).

$$L_0 = DDOC \bullet F \bullet 16/12 \quad (5)$$

Here,  $L_0$  represents the methane generation potential,  $DDOC$  is the decomposable DOC calculated previously,  $F$  is the fraction of methane in the generated landfill gas (this parameter represents the efficiency of the conversion process), and  $\frac{16}{12}$  is the molecular weight ratio between methane and carbon.

As mentioned earlier, AD facilities employ gas capturing technologies to recover methane for later use. The actual emissions from the AD process can be approximated using equation (6).

$$\text{CH}_4 \text{ Emissions} = (L_0 - R) \bullet (1 - OX) \quad (6)$$

In this equation,  $L_0$  is the methane generation potential calculated in equation (5),  $R$  is the mass of methane recovered from the system, which varies depending on the system, and  $OX$  is the oxidation factor, reflecting the amount of methane oxidized through interactions with the waste and/or foreign materials.

### 2.1.3 Incineration

Waste incineration refers to the combustion of solid and liquid waste in controlled incineration facilities. Modern refuse combustors feature tall stacks and specially designed combustion chambers, which ensure high combustion temperatures, extended residence times, and efficient waste agitation while introducing air for more complete combustion.

According to IPCC guidelines, emissions from waste incineration without energy recovery are reported in the Waste Sector. In contrast, emissions from incineration with energy recovery are reported in the Energy Sector, with both sectors distinguishing between fossil and biogenic  $CO_2$  emissions.

As previously mentioned, one of the objectives of this program is to estimate greenhouse gas emissions. This means that the formation of other air pollutants, such as sulfur oxides ( $SO_x$ ) and non-methane volatile organic compounds (NMVOCs), will not be addressed. Accurately estimating these pollutants would necessitate a complex combustion model tailored to each incineration facility.

Starting with the  $CO_2$  emissions, the first step is to estimate the fraction of fossil carbon in the waste. This is because, similar to biomass-based fuels, biogenic carbon emissions are assumed to be part of a closed cycle in which the emitted carbon is captured by flora that eventually will become new fuel later on. Table 3 of the Appendix has the amount of fossil carbon present in each waste category.

Once the amount of fossil carbon is determined, it is just a matter of applying an oxidation factor and a mass conversion factor from  $C$  to  $CO_2$  to estimate the emissions. Equation (7) illustrates this process.

$$CO_2 \text{ Emissions} = MSW \cdot \sum_j (WF_j \bullet dm_j \bullet CF_j \bullet FCF_j \bullet OF_j) \bullet 44/12 \quad (7)$$

In this context, MSW represents the total amount of municipal solid waste, measured in wet weight, that is incinerated. The term  $WF_j$  denotes the weight fraction of each category  $j$ . The variable  $dm_j$  indicates the dry matter content within component  $j$  of the incinerated MSW. The term  $CF_j$  represents the fraction of carbon in the dry matter of component  $j$ , while  $FCF_j$  specifies the fraction of fossil carbon within the total carbon of category  $j$ . The oxidation factor is denoted as  $OF_j$ , and the factor 44/12 serves as the mass adjustment factor from  $C$  to  $CO_2$ .

Moving on to  $CH_4$  and  $N_2O$  emissions, these gases are produced in significantly smaller quantities compared to  $CO_2$ . In the context of combustion,  $CH_4$  emissions typically result from incomplete combustion, with factors such as temperature, residence time, and air ratio being the main determinants of methane production. Conversely,  $N_2O$  emissions mainly arise from low combustion temperatures (between 500 and 950°C). These prerequisites, coupled with the operational conditions of a typical waste incinerator, mean that both  $CH_4$  and  $N_2O$  emissions are expected to be several orders of magnitude smaller than those of  $CO_2$  [5][6].

Nevertheless, the IPCC provides a methodology for estimating emissions from certain gases. This approach is simpler than the method used for calculating  $CO_2$  emissions, involving a straightforward multiplication of the mass of waste incinerated by a correction factor that aligns the total mass of waste with the emissions of interest. The equation is defined as:

$$X \text{ Emissions} = \sum_i (IW_i \bullet EF_i)_X \quad (8)$$

Where  $X$  represents either  $CH_4$  or  $N_2O$ , depending on the gas being calculated. Here,  $IW_i$  is the mass of type  $i$  solid waste incinerated, and  $EF_i$  is the correction factor, largely dependent on the type of incinerator used. Correction factors are detailed in Tables 11 and 12 in the Appendix.

For energy recovery, the program calculates the heating values of the incinerated waste and applies

a system-wide efficiency factor. Table 1 lists the calorific values of the most common municipal solid waste (MSW) components.

**Table 1:** *Typical Heating Value of MSW Components*

Component	Energy, Btu/lb	
	Range	Typical
Food wastes	1500–3000	2000
Paper	5000–8000	7200
Cardboard	6000–7500	7000
Plastics	12000–16000	14000
Textiles	6500–8000	7500
Rubber	9000–12000	10000
Leather	6500–8500	7500
Garden trimmings	1500–3000	2800
Wood	7500–8500	8000
Glass	50–100	60
Tin cans	100–500	300
Nonferrous metals	—	—
Ferrous metals	100–500	300
Dirt, ashes, brick, etc.	—	—
Municipal solid wastes	4000–6500	4500

*Source:* Brunner and Schwarz (1983) [7].

With the heating values of the waste stream known, calculating the energy recovered becomes straightforward. Energy recovery systems associated with waste incineration typically employ the Rankine cycle to extract power from the combustion chamber and achieve an efficiency of around 21% [6]. Using equation (9), it is possible to calculate the energy recovered from the waste stream.

$$E_{recovered} = \sum_i (IW_i \bullet CV_i) \bullet \eta_{system} \quad (9)$$

where  $E_{recovered}$  is the energy recovered from the waste stream,  $IW_i$  is the mass of a specific waste category incinerated,  $CV_i$  is the calorific value of that waste category, and  $\eta_{system}$  is the overall efficiency of the energy recovery system.

#### 2.1.4 Landfill

Landfills are designated sites for the disposal of solid waste, typically by burial. Traditionally, managing these sites involved daily waste deposits covered with soil, allowing rain to cleanse leachate

through the ground. However, with advancements in landfill technology, systems have been implemented to collect and treat leachate, significantly reducing environmental impacts [8].

The program simulates the landfill scenario in two ways: steady-state analysis and transient analysis (First Order Decay model). Both methods are useful for different applications. Steady-state analysis is more useful for evaluating the total impact of a specific batch of waste sent to the landfill. The First Order Decay (FOD) model is more useful for simulating the landfill as a dynamic system, where waste may already be present before the batch of interest is deposited, and additional waste may be added during the decay process over the years.

### **Steady-state analysis**

The steady-state analysis partially follows the same logic and calculations as the composting and anaerobic digestion (AD) sections. It starts by estimating the DOC content of each category in the waste stream using equation (1), and then uses correction factors to calculate the DDOC for each quantity of interest (equations (2) and (4)). However, unlike composting and AD, where there is typically a single dominant pollutant, the landfill scenario presents a more balanced situation. Depending on the conditions, different gases might dominate in terms of their greenhouse effects.

Like the AD systems, some landfills have methane recovery systems. Additionally, it is sometimes common practice to flare the landfill gas at some facilities. Flaring is an operation where the landfill gas is ignited to reduce its environmental impact by converting  $CH_4$  to  $CO_2$  (since  $CH_4 = 25 CO_2 eq.$ ), and to reduce the risk of gas pockets forming, which might pose an explosion risk. This is described by the equation:

$$CH_4 \text{ Emissions} = (L_0 - R - F) \bullet (1 - OX) \quad (10)$$

where  $L_0$  is the methane generation potential,  $R$  is the mass of methane recovered,  $F$  is the mass of methane being flared, and  $OX$  is the oxidation factor. The mass of flared methane is given by:

$$F = L_0 \bullet F_{fraction} \bullet \eta_{flaring} \quad (11)$$

where  $F_{fraction}$  is the fraction of the produced methane that is flared and  $\eta_{flaring}$  is the efficiency of the flaring process.

### **First Order Decay (FOD) model**

The issue with the Steady-state approach lies in its neglect of the dynamic nature of a landfill. Properly simulating a landfill requires understanding that waste does not decompose instantly, and the rate at which it decomposes depends on the existing materials onsite.

Before delving into the model itself, it's important to note that there are two main approaches for this type of simulation. One approach treats the waste stream as a whole, considering it in bulk and deriving general parameters for simulation. The other approach categorizes the waste stream into categories (similar to previous waste treatment options), defining parameters and simulating each category individually. Both approaches are valid choices as they are approximations, each with its own limitations. The bulk approach generalizes the system but sacrifices accuracy by doing so, while the category-specific approach fails to account for interactions between different categories. According to the IPCC, there is no conclusive data proving that one approach is superior to the other [4].

The First Order Decay (FOD) model provides a way to characterize the evolution of the mass of DDOC over time. It is given by the following differential equation:

$$\frac{\partial(DDOC)}{\partial t} + \frac{\ln(2)}{t_{1/2}} \bullet DDOC = 0 \quad (12)$$

where DDOC is the mass of degradable dissolved organic carbon and  $t_{1/2}$  is the half-life of the material being degraded.

Another important factor to consider is that the decay of waste does not start immediately after it is deposited in the landfill. In reality, there is a period of up to a couple of months where there is little to no noticeable decay [4]. With this in mind, it is possible to simplify the previous equation:

$$DDOC(t) = DDOC_0 \bullet e^{-k(t+t_{delay})}, k = \frac{\ln(2)}{t_{1/2}} \quad (13)$$

The new terms  $DDOC_0$  and  $t_{delay}$  represent the mass of DDOC at  $t = 0$  and the delay period before decay actually begins, respectively.

Having now described the evolution of the mass of DDOC with time, it is simply a matter of using equations (5), (10), and (11) to estimate the evolution of emissions.

### 2.1.5 Gasification

Gasification is a process that converts organic or fossil-based carbonaceous materials into carbon monoxide, hydrogen, carbon dioxide, and other gaseous species. This operation is typically conducted at temperatures above 700°C without reaching combustion. This means that environmental conditions, such as air supply, need to be carefully monitored to maintain efficient processing. The primary output, often referred to as syngas, varies significantly in composition depending on the waste stream used for production. For instance, the presence of moisture in the waste stream is closely linked to the proportion of  $H_2$  in the syngas produced [9].

To properly simulate the composition of the syngas produced based on the CHON (carbon, hydrogen, oxygen, nitrogen) composition of the waste stream would require a complex thermodynamic

model. However, given that such a high degree of accuracy is not necessary, the program instead uses results from existing literature to approximate or predict the composition of the produced syngas. These values can be found in table 15 of the Appendix.

## 2.2 SCW - Separately Collected Waste

Separately Collected Waste (SCW) refers to waste that is sorted at the source. SCW enhances the quality and quantity of recyclable materials by reducing contamination, thus increasing the efficiency of processes such as recycling. Increasing the proportion of SCW supports the circular economy by giving new value to materials that would otherwise be lost.

This sector of waste management has significant growth potential and investment opportunities. For example, in Portugal, there is a push to generate more value from separately collected biowaste. However, the quality of biofuels produced is compromised due to inadequate large-scale separation at the source by consumers [10].

Just like for the case of MSW, some default categories were assumed to represent SCW, but the user can add more if they wish to do so:

- |   |  |   |
|---|--|---|
| <ul style="list-style-type: none"> <li>• Ferrous metal</li> <li>• Non-ferrous metal</li> <li>• PET</li> </ul> | <ul style="list-style-type: none"> <li>• HDPE</li> <li>• Glass</li> <li>• Paper/Cardboard</li> </ul> | <ul style="list-style-type: none"> <li>• Biowaste (Food waste)</li> <li>• Biowaste (Wood)</li> <li>• Biowaste (Garden waste)</li> </ul> |
|---|--|---|

When it comes to handling this waste stream, the methods implemented are recycling, composting, anaerobic digestion (AD), and gasification. The last three are primarily used for managing biowaste. Similar to the municipal solid waste (MSW) stream, emission factors will be applied to account for the collection and transport of the SCW stream.

### 2.2.1 Recycling

At its most basic form, recycling involves transforming waste back into its raw materials. This process has gained increased relevance in recent years as rising consumerism necessitates a shift to a circular economy. It is important to note that recycling still requires energy, so options such as product reconditioning should be applied if possible. Nevertheless, recycling is still a much preferable option to disposing of material in a landfill.

Since there are many recycling techniques that may not be universally shared, the code utilizes factors for each category to estimate the quantities of interest.

$$X = W_i \bullet F_{Xi} \quad (14)$$

where  $X$  is the quantity of interest being estimated (e.g., Emissions, Material recovery, Energy),  $W_i$  is the mass of the category being analyzed, and  $F_{Xi}$  is the factor for each category in reference to the quantity of interest  $X$ .

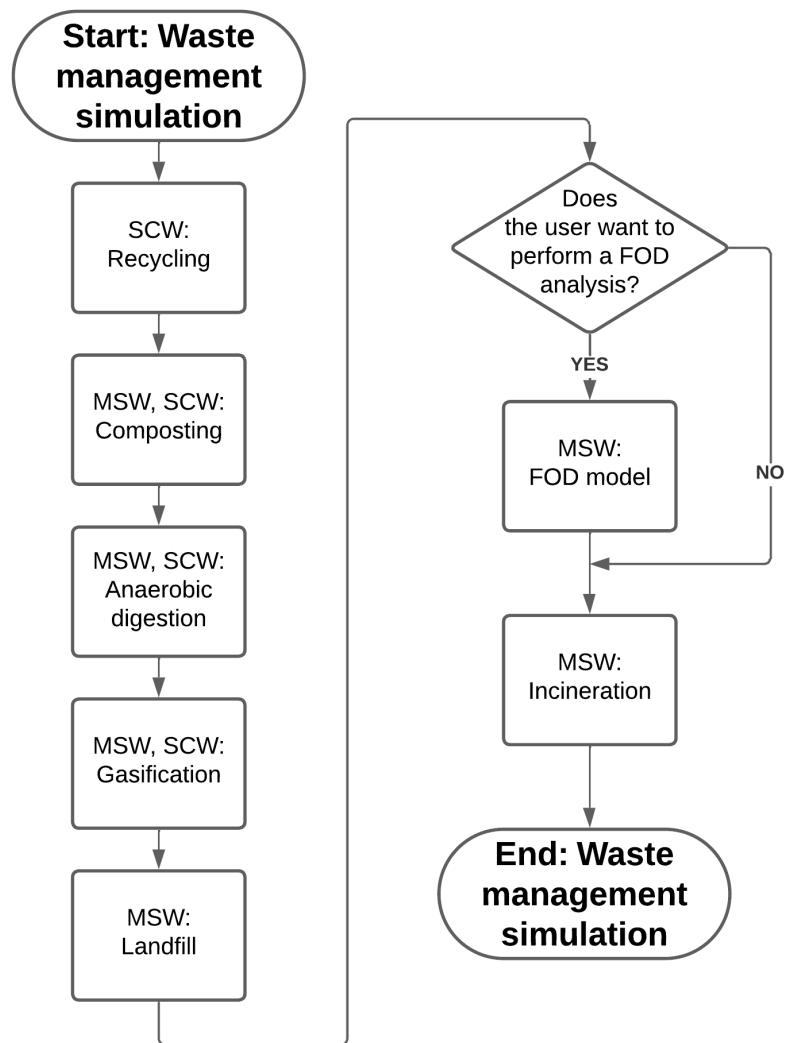
### 2.2.2 Biowaste treatment

Regarding the treatment of the Biowaste stream, the program uses the same logic/model as the one used in the MSW section. This means that the formulas from the Composting, AD, and Gasification sections are employed for this section of the SCW stream.

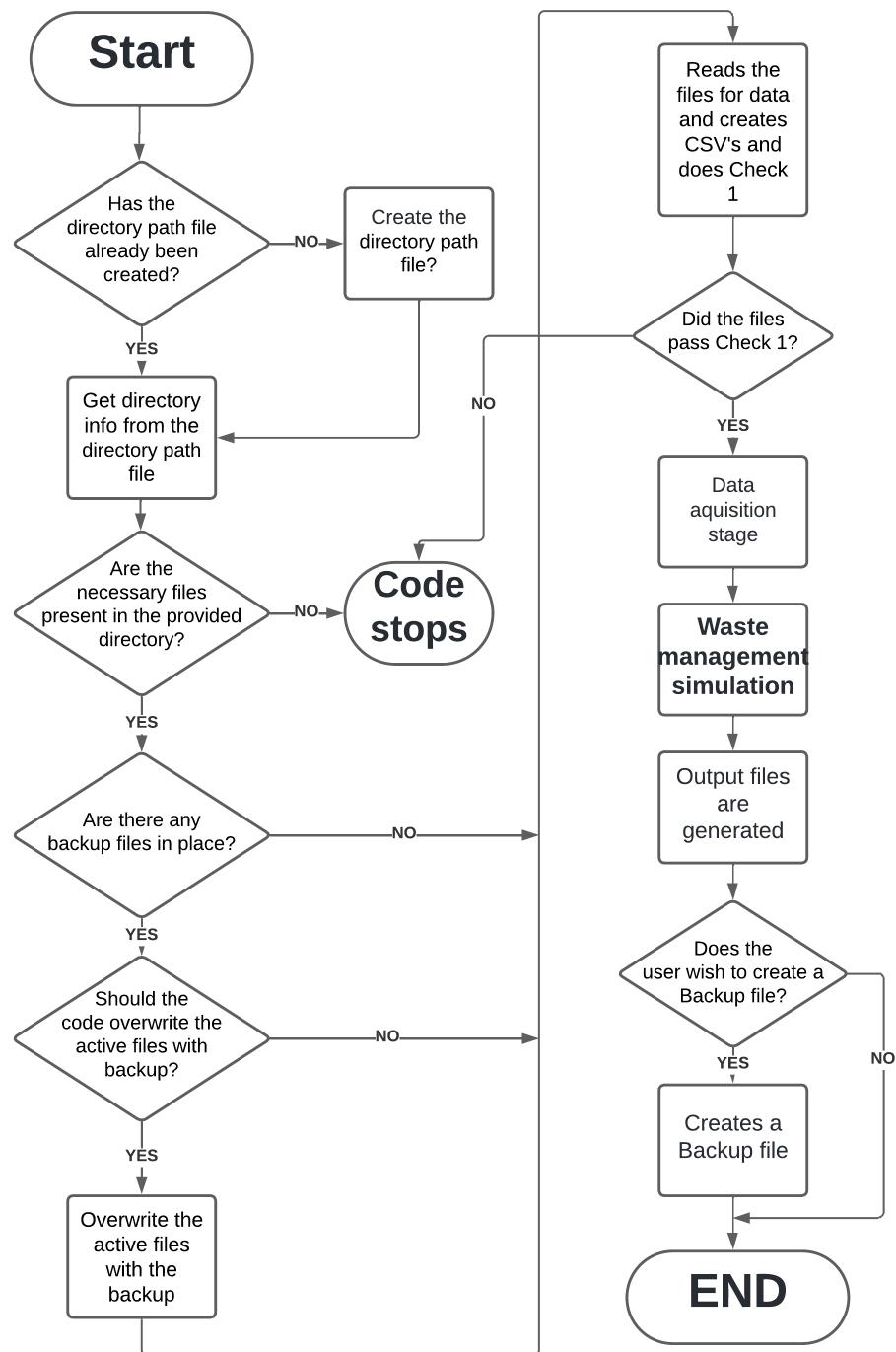
It is important to point out that there will be slight differences in the methodology when compared with the MSW, as the transportation emissions factors for the SCW stream differ from those in the MSW stream.

## 3 Program Manual

This section aims to provide explanations on how the program's code works and how the user can modify its functionalities without having to directly modify the code. However, before moving to those points, a generalized overview of how the code works will be provided. The overview of the code can be summarized by the following flowcharts:



**Figure 1:** Waste management simulation overview

**Figure 2:** Program Overview

Figures 1 and 2 are flowcharts that represent a detailed view of the Waste management simulation section and a general overview of the program, respectively. Understanding these diagrams is not necessary to use the program; however, if the user decides to modify the code itself, they should try to maintain this structure to preserve the program's functionalities.

The code is structured in such a way that, generally speaking, each item in the flowchart corresponds to a section like this one:

```
1 # @@@@@@@@ check 1.1 @@@@@@@@ check 1.1 @@@@@@@@ check 1.1@@
2 # @@@@@@@@ check 1.1 @@@@@@@@ check 1.1 @@@@@@@@ check 1.1@@
3 # @@@@@@@@ check 1.1 @@@@@@@@ check 1.1 @@@@@@@@ check 1.1@@
4
5 percentage_total_MSW = 0
6 mass_MSW = []
7
8 for i in range(find_indices(inventory_data, 'A1')[0][0],
9     find_indices(inventory_data, 'AT1')[0][0]):
10    percentage_total_MSW += inventory_data[i][find_indices(
11        inventory_data, 'Mass %')[0][1]]
12    mass_MSW.append(inventory_data[i][find_indices(inventory_data,
13        'Mass (t)')[0][1]])
14
15 if percentage_total_MSW == 100 and round(mass_total_MSW, 3) == round(
16     inventory_data[1][0], 3):
17     print('Check 2 done')
18 elif percentage_total_MSW != 100 and round(mass_total_MSW, 3) ==
19     round(inventory_data[1][0], 3):
20     print('MSW percentage sum is not 100% =>' + str(
21         percentage_total_MSW))
22     sys.exit("Stopping execution. Failed Check 2")
23 else:
24     print('MSW mass sum does not match total mass')
25     sys.exit("Stopping execution. Failed Check 2")
```

### 3.1 How to use the Program

The first step is to download the necessary files from the GitHub repository. There the user will find the main code '**NT.py**' and a folder called '**files**'. Inside the '**files**' folder, there should be the two Excel files needed to run the simulations. It is fine if the user changes the directory of the Excel files as long as they are kept together and their names remain the same.

The second step is to run the main code for the first time (**Note:** some python libraries are necessary

for the code to work, they are at the top of the code). When this is done, a window should pop up prompting the user to choose the directory where the Excel files are located. Once the user have selected the desired directory, a new hidden file named '**directory\_file.json**' will be generated in the same directory where '**NT.py**' is located. The purpose of this file is to save the working directories so that in subsequent runs of the program, it does not ask the user to choose another directory. The program will then confirm if the Excel files are in the selected directory. If the files are not present, the program will stop, and the user will need to manually delete '**directory\_file.json**' before trying again. If everything is as expected, the message 'All required files found. Proceeding with execution...' will be printed on the console.

After that, the program should run a simulation using the default placeholder values set in the files. To finish setting up the program, the user should follow these steps:

- A window will pop up asking if the user wishes to make a 'time-dependent analysis.' The user should answer 'No.'
- A new pop-up window will ask the user about the incineration system. The user should answer 'No.'
- A final window will appear regarding the backup files. The user should answer 'Yes.'

If these steps are followed correctly, two new folders (**Output** and **Backup**) will become visible in the file directory. The purpose of these folders is discussed further below.

Now that the program is properly set up, the user may use it by setting up the excel files and running the code afterwards.

### 3.1.1 How to use/modify the '**Inventory\_data**' file

The '**Inventory\_data**' file is the main way the user can control the program. It stores the composition of the MSW and SCW streams and how they are to be split into each of the waste treatment techniques.

Upon opening the file, two main sections should be easily identifiable. The purple section refers to the MSW stream, while the green section relates to the SCW stream. These sections are independent of each other, so any changes made to one will not affect the results of the other.

Starting with the MSW section, there are three main points of interaction that the user must fill with their data. These regions are highlighted with a darker shade of purple. They are:

- In the MSW stream composition table (Figure 3), the user must fill the waste composition column (given as a percentage of mass on a wet basis).

- In the MSW stream destination table (Figure 4), the user has to specify how the waste should be split between the waste treatment techniques. This is done for every category, and the sum of the split percentages must total 100
- In the MSW total mass value box (Figure 5), the user should enter the total mass of MSW to be simulated.

Code	Category	Mass %	Mass (t)	Energy(MJ/Kg)	Total energy contribution (MJ/Kg)
A1	Paper/Cardboard	25	37878,750	16,51	4,128
A2	Textiles	10	15151,500	17,445	1,745
A3	Food waste	12	18181,800	4,652	0,558
A4	Wood	3	4545,450	18,608	0,558
A5	Garden and Park waste	15	22727,250	6,5128	0,977
A6	Rubber and Leather	4	6060,600	20,3525	0,814
A7	Plastics	20	30303,000	32,564	6,513
A8	Metal	1	1515,150	0,3489	0,003
A9	Glass	10	15151,500	0,13956	0,014
AT1	Total	100	151515		15,310

Figure 3: MSW stream composition table

Code	Mixed waste to MBT, composting %	Mixed waste to MBT, Anaerobic digestion %	Mixed waste to Incineration %	Mixed waste to Landfill %	Mixed waste to Gasification %	Total %
A1	20	20	60	0	0	100
A2	0	0	20	80	0	100
A3	55	30	0	0	15	100
A4	20	0	50	10	20	100
A5	80	20	0	0	0	100
A6	0	0	70	30	0	100
A7	0	0	20	70	10	100
A8	0	0	0	100	0	100
A9	0	0	0	100	0	100

Figure 4: MSW stream destination table

<b>Mixed Waste total mass (t)</b>
<b>151515</b>

Figure 5: MSW total mass value box

Regarding the SCW section, there are two main points of interaction that the user must fill with their data. These regions are highlighted with a darker shade of green. They are:

- In the SCW stream composition table (Figure 6), the user must fill in the mass of each category of the waste stream.

- In the SCW stream destination table (Figure 7), the user has to specify how the waste should be split between the waste treatment techniques. This is done for every category, and the sum of the split percentages must total 100

Code	Category	Mass (t)	Mass %
B1	Ferrous metal	1000	1,77
B2	Non-ferrous metal	12345	21,86
B3	PET	22000	38,96
B4	HDPE	124	0,22
B5	Glass	5000	8,85
B6	Paper/Cardboard	2000	3,54
B7	Biowaste (Food Waste)	4000	7,08
B8	Biowaste (Wood)	10000	17,71
B9	Biowaste (Garden and Park waste)	0	0,00
BT1	Total	56469	100,00

Figure 6: SCW stream composition table

Code	S.C. = Separately Collected				Total %
	S.C. waste to MBT, Gasification %	S.C. waste to MBT, composting %	S.C. waste to MBT, Anaerobic digestion %	S.C. waste to MBT, Recycling %	
B1	0	0	0	100	100
B2	0	0	0	100	100
B3	0	0	0	100	100
B4	0	0	0	100	100
B5	0	0	0	100	100
B6	0	10	0	90	100
B7	0	40	60	0	100
B8	10	40	50	0	100
B9	10	40	50	0	100

Figure 7: SCW stream destination table

After the user has entered all the values, the file is ready to be used by the program. Note: Don't forget to save the changes before running the code; otherwise, the changes won't be detected by the program.

### 3.1.2 How to use/modify the 'Assumptions\_data' file

The 'Assumptions\_data' file stores all the factors, constants, and assumptions used by the program. It is advisable to modify this file only if the user understands the theoretical basis behind the code's functionality.

The file consists of a collection of tables, of which there are two types: informative and assumption tables (Figure 8). The informative tables (colored purple) help the user understand the typical ranges used to fill certain values in the assumption tables. The assumption tables (colored light blue) are where the program retrieves its assumption values.

<b>Table 2.2: Oxidation Factor (OX)</b>		<b>Table 2.3: Correction factor for greenhouse gases (CO<sub>2</sub>eq)</b>	
Type of Site	Oxidation Factor (OX) Default values	Correction factor for 1Kg of CH <sub>4</sub>	25
Managed, unmanaged and uncategorised SWDS	0,00	Correction factor for 1Kg of NO <sub>2</sub>	298
Managed covered with CH <sub>4</sub> oxidising material	0,10		

**Figure 8:** Example of the tables present in the 'Assumptions\_data' file

If the user wishes to modify any assumptions, they should only modify the assumption tables. Each table is numbered and its purpose is clearly identified, making it easy to find the values the user wants to change.

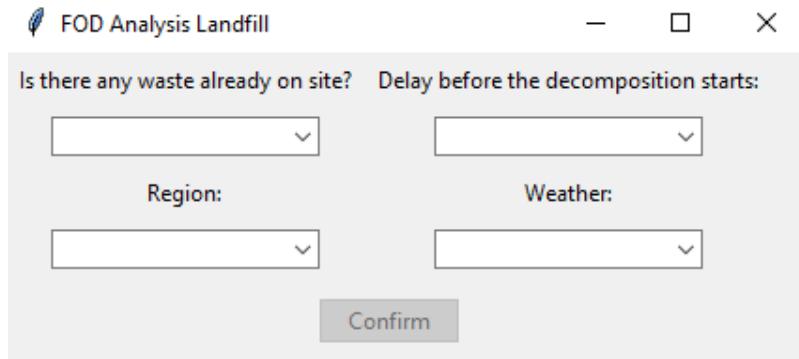
### 3.1.3 How to add new categories to the simulation

If the user needs to add a new category to either the MSW or SCW streams, it is very important that they follow these instructions carefully (Note: please read them all before starting to modify the files):

- In the Inventory file, they should add their new category lines between the last and second-to-last default categories. For example, if the user wants to add a new category to the MSW stream, they would create a new line between 'Metal' and 'Glass' in both the MSW stream composition table and the MSW stream destination table.
- In the Inventory file, any new line added must have the same style of cell formatting as the default ones, i.e., any Excel formula in the default cells should be replicated in the new lines.
- In the Assumptions file, the new categories must be added in the same order as they were implemented in the Inventory file, i.e., the order of the category lists must be the same in both files.
- In the Assumptions file, the only tables that need to be modified with the new categories are tables 1; 10 and 11

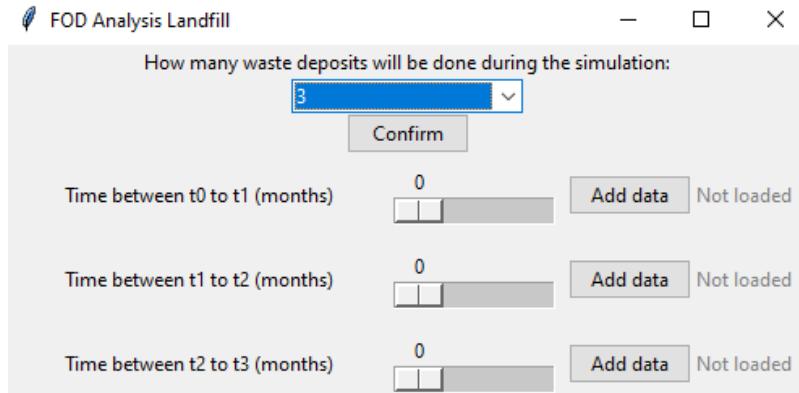
### 3.1.4 FOD Analysis

During the execution of the program, the user will be prompted to decide if they want to conduct a FOD analysis for the Landfill stream. If they answer 'Yes', the following window will pop up:



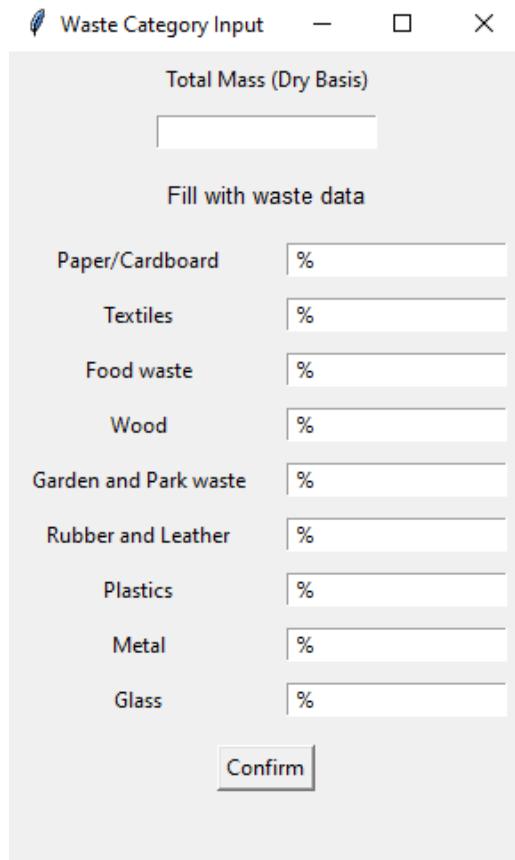
**Figure 9:** FOD: Initial conditions window

In this first window (Figure 9), the initial conditions of the simulation are set up. Here, the user must define conditions such as whether the Landfill already contains waste, the delay before the start of decomposition, and the climate conditions affecting the waste. After configuring these settings, the user should click 'Confirm' to proceed to the next step. A new window will then appear:



**Figure 10:** FOD: Simulation control window

In this second window (Figure 10), the user can specify the duration and other parameters of the simulation. Given that a landfill is a dynamic system, it is crucial to define how many additional waste depositions will occur during the simulation and their frequency. The user has the option to schedule up to nine additional waste depositions and set the interval between each deposition. By clicking the 'Add data' button, an auxiliary window will appear:



**Figure 11:** FOD: Initial conditions window

In this auxiliary pop-up window (Figure 11), the user can input data pertaining to the specific waste deposition. Once all the data for each extra deposition is entered, the user should click 'Confirm' in the main window to finalize the settings.

Note that there is a limit to the sliders that let the user choose the time between depositions. If the user wishes to have a longer time gap, they should define an extra deposition with 0 waste being deposited. This allows the use of the additional slider to increase the maximum value of the intended deposition.

### 3.1.5 Backup and Output folders

#### Backup Stage

After the simulation is finished, the program will ask the user if they wish to define a new backup stage. This means that the files used for the most recent simulation will become the new backup

stage. This feature is particularly useful if the user wants to permanently change any of the files and establish a new simulation baseline.

### **Output Stage**

The output file will be in CSV format and will include the time and date in its name, making it clear to the user which file belongs to each simulation.

## **4 Conclusion and Future work**

Waste management is a highly complex topic that requires numerous approximations and concessions to be effectively simulated on a large scale. The current model aims to provide results that are sufficiently accurate to assist politicians and decision-makers in setting goals and expectations for their related plans.

In the future, the program could be updated to incorporate more complex models, such as proper combustion simulations and higher-order approximations for the decay model. Another potential improvement could involve enhancing the program to suggest the most optimal distribution of waste streams, prioritizing specific aspects according to the user's needs.

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## Appendix

### A Parameters' Tables

**Table 2:** GHG emission factors for waste collection and transport [2]

<b>GHG emission factors for waste collection and transport</b>			
Separately collected waste	Separately collected metal to sorting and recycling	0.01	ton of $CO_2$ (eq)/ton material
	Separately collected plastic to sorting and recycling	0.015	ton of $CO_2$ (eq)/ton material
	Separately collected paper/cardboard to sorting and recycling	0.01	ton of $CO_2$ (eq)/ton material
	Separately collected glass to sorting and recycling	0.01	ton of $CO_2$ (eq)/ton material
	Separately collected biowaste to composting	0.008	ton of $CO_2$ (eq)/ton material
	Separately collected biowaste to AD	0.008	ton of $CO_2$ (eq)/ton material
Mixed Waste	Mixed waste to MBT	0.009	ton of $CO_2$ (eq)/ton material
	Mixed waste to incineration	0.008	ton of $CO_2$ (eq)/ton material
	Mixed waste to landfill	0.007	ton of $CO_2$ (eq)/ton material

**Table 3:** *DOC contents (MSW) [4]*

DOC contents MSW compo- nent	Dry matter content in % of wet weight	DOC content in % of wet waste	DOC content in % of dry waste			Total content in % of dry weight	Fossil carbon fraction in % of total carbon	Max	
			Default	Min	Max				
Paper/Cardboard	90	40	36	45	44	40	50	46	42
Textiles	80	24	20	40	30	25	50	25	50
Food waste	40	15	8	20	38	20	50	38	20
Wood	85	43	39	46	50	46	54	50	50
Garden and Park waste	40	20	18	22	49	45	55	49	-
Rubber and Leather	84	39	39	47	47	47	67	67	-
Plastics	100	-	-	-	-	-	75	67	-
Metal	100	-	-	-	-	-	NA	NA	-
Glass	100	-	-	-	-	-	NA	NA	-

**Table 4:** Methane Correction Factor (MCF) [4]

<b>METHANE CORRECTION FACTORS (MCF)</b>	
<b>Type of Site</b>	<b>Methane Correction Factor (MCF) Default Values</b>
Managed (anaerobic)	1.00
Managed (semi-aerobic)	0.50
Unmanaged (deep or high water table)	0.80
Unmanaged (shallow)	0.40

**Table 5:** Oxidation Factor (OX) [4]

<b>Oxidation Factor (OX)</b>	
<b>Type of Site</b>	<b>Oxidation Factor (OX) Default values</b>
Managed, unmanaged and uncategorised SWDS	0,00
Managed covered with CH <sub>4</sub> oxidising material	0,10

**Table 6:** Correction factors for greenhouse gases

<b>Correction factor for greenhouse gases (CO<sub>2</sub> eq.)</b>	
Correction factor for 1 Kg of CH <sub>4</sub>	25
Correction factor for 1 Kg of NO <sub>2</sub>	298

**Table 7:** Recommended Default Half-Life Values (YR) [4]

RECOMMENDED DEFAULT HALF-LIFE VALUES (YR)									
Type of waste	Boreal and Temperate (MAT greater than 20°C)				Tropical (MAT less than 20°C)				Moist and Wet (MAP greater than 1000 mm)
	Dry (MAP/PET less than 1)	Wet (MAP/PET greater than 1)	Default	Min	Max	Default	Min	Max	
Paper/textiles waste	17	14	23	12	10	14	15	12	17
Wood/straw waste	35	23	69	23	17	35	28	17	35
Other (non-food) organic putrescible/ Garden and park waste	14	12	17	7	6	9	11	9	14
Food waste/Sewage sludge	12	9	14	4	3	6	8	6	10
Bulk Waste	14	12	17	7	6	9	11	9	14

**Table 8:** Default Composting parameters used by the program

Parameters for the Composting section	
fraction of DOC that can decompose under anaerobic conditions (DODf)	0,5
Methane Correction Factor (MCF)	0,01
CO2/C mass ratio	44/12
CH4/C mass ratio	16/12
Oxidation Factor (OX)	0
fraction of CH4 in generated gas(F)	0,5

**Table 9:** Default AD parameters used by the program

Parameters for the Anaerobic digestion section	
fraction of DOC that can decompose under anaerobic conditions (DODf)	0,5
Methane Correction Factor (MCF)	1
CO2/C mass ratio	44/12
CH4/C mass ratio	16/12
Oxidation Factor (OX)	0
Methane Recovery Factor (R)	1
fraction of CH4 in generated gas(F)	0,5

**Table 10:** Default Incineration parameters used by the program

Parameters for the Incineration section	
Energy recovery efficiency (%)	21,2
CO2/C mass ratio	44/12
Oxidation Factor (OX)	1
Default CH4 emission factor (Kg/Gg MSW wet weight)	60
Default N2O emission factor (Kg/Gg MSW wet weight)	56

**Table 11:** CH<sub>4</sub> Emission Factors for Incineration of MSW

CH <sub>4</sub> Emission Factors for Incineration of MSW	
Type of incineration/technology	CH4 Emission Factors (kg/Gg waste incinerated on a wet weight basis)
Continuous incineration	0,2
Semi-continuous incineration	6
Batch type incineration	60

**Table 12:** *N<sub>2</sub>O Emission Factors for Incineration of MSW*

<b>N<sub>2</sub>O Emission Factors for Incineration of MSW</b>	
Type of incineration/technology	CH4 Emission Factors (kg/Gg waste incinerated on a wet weight basis)
Continuous incineration	47
Semi-continuous incineration	41
Batch type incineration	56

**Table 13:** *Default Landfill parameters used by the program*

<b>Parameters for the Landfill section</b>	
fraction of DOC that can decompose under anaerobic conditions (DODf)	0,5
Methane Correction Factor (MCF)	0,5
CO <sub>2</sub> /C mass ratio	44/12
CH <sub>4</sub> /C mass ratio	16/12
Oxidation Factor (OX)	0,1
Methane Recovery Factor (R)	0,5
fraction of CH <sub>4</sub> in generated gas(F)	0,5
Fraction of collected methane flared	0,5
Flare efficiency	0,45
CO <sub>2</sub> /CH <sub>4</sub> mass ratio	44/16

**Table 14:** Default Recycling parameters used by the program

Parameters for the Recycling section				
Type of waste	Emission factors (t CO <sub>2</sub> (eq)/t recycled material)	Material recovery factors (t recycled material/t material recycled)	Energy consumption factors (MJ/t material recycled)	Emission factors for waste collection and transport (t CO <sub>2</sub> (eq)/t recycled material)
Ferrous metal	-1.521	0.85	6	0.01
Non-ferrous metal	-9.108	0.9	20	0.01
PET	-0.53	0.75	40	0.015
HDPE	-1.8	0.8	50	0.015
Glass	-0.287	0.9	10	0.01
Paper/cardboard	-0.634	0.75	15	0.01
Biowaste (Food Waste)	N/A	N/A	N/A	N/A
Biowaste (Wood)	N/A	N/A	N/A	N/A
Biowaste (Garden and Park waste)	N/A	N/A	N/A	N/A

**Table 15:** Default Gasification parameters used by the program [9]

Parameters for the Gasification section					
	H <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>	N <sub>2</sub>
syngas from Municipal solid waste	10,63	4,06	23,8	1,34	60,14
syngas from Animal waste	14,16	7,25	18,28	2,51	57,77
syngas from Ground nut shell	17,92	13,01	17,6	4,12	47,33
Mass conversion efficiency			0,75		

**Table 16:** *DOC contents (SCW) [4]*

MSW compo- nent	DOC contents			DOC content in % of dry waste			Total carbon content in % of dry weight			Fossil carbon fraction in % of total carbon		
	Default	Min	Max	Default	Min	Max	Default	Min	Max	Default	Min	Max
Ferrous metal	100	-	-	-	-	-	-	-	-	NA	NA	NA
Non-ferrous metal	100	-	-	-	-	-	-	-	-	NA	NA	NA
PET	100	-	-	-	-	-	-	-	-	NA	NA	NA
HDPE	100	-	-	-	-	-	-	-	-	NA	NA	NA
Glass	100	-	-	-	-	-	-	-	-	NA	NA	NA
Biowaste (Food waste)	40	15	8	20	38	20	50	38	20	50	-	-
Biowaste (Wood)	85	43	39	46	50	46	54	50	46	54	-	-
Biowaste (Garden and Park waste)	40	20	18	22	49	45	55	49	45	55	0	0