Wastewater life cycle inventory initiative

WW LCI version 3.0: changes and improvements to WW LCI v2

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Preface

Together with Procter & Gamble, Henkel and Unilever, 2.-0 LCA consultants initiated in 2015 the Wastewater Life Cycle Initiative, with the aim of developing a model to calculate life cycle inventories of chemical substances sent down the drain, taking into account wastewater treatment, sludge disposal, and degradation in the environment. This project was established as a club to which anyone can subscribe. The Wastewater life cycle initiative is administrated by 2.-0 LCA consultants. For more information and subscription, please contact 2.-0 LCA consultants:
http://lca-net.com/clubs/wastewater/

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Front page picture: Overview of the wastewater treatment plant of Antwerpen-Zuid, located in the south of the agglomeration of Antwerp (Belgium). Source:
https://en.wikipedia.org/wiki/Wastewater_treatment#/media/File:WWTP_Antwerpen-Zuid.jpg

CONTENTS

Acronyms, abbreviations and units

A	Area
AD	Anaerobic digestion
BOD	Biochemical oxygen demand
CHP	Cogeneration of heat and power
COD	Chemical oxygen demand
C_p	Heat capacity of sludge (MJ/m^3/ºC)
CSV	Comma-separated values
d	Day
Deg_a	Fraction of chemical, expressed in mass percentage, expected to degrade in air
Deg_s	Fraction of chemical, expressed in mass percentage, expected to degrade in soil
Deg_{sed}	Fraction of chemical, expressed in mass percentage, expected to degrade in sediments
Deg_w	Fraction of chemical, expressed in mass percentage, expected to degrade in water
EU28	European Union with 28 Member States
F_{air}	Fraction of chemical, in mass percentage, that undergoes volatilization in the WWTP
F_{deg}	Fraction of chemical, in mass percentage, that undergoes degradation in the WWTP
F_{sludge}	Fraction of chemical, in mass percentage, that partitions to sludge in the WWTP
g	Gram
GHG	Greenhouse gases
GNI	Gross National Income
H	Hydrogen
H_2S	Hydrogen sulphide
HHV	High heating value
HRT	Hydraulic residence time
IMF	International Monetary Fund
IPCC	Intergovernmental Panel on Climate Change
Kd	Solid/liquid partition coefficient (dimensionless)
kdeg air	Decay constant in the atmosphere, in s^{-1}.
kdeg sed	Decay constant in sediments, in s^{-1}.
kdeg soil	Decay constant in soil, in s^{-1}.
kdeg water	Decay constant in water, in s^{-1}.
kg	Kilogram
Koc	Soil organic carbon-water partitioning coefficient (dimensionless)
Kow	Octanol-water partitioning coefficient (dimensionless)
Ktoe	Kilotonne oil equivalent
kWh	Kilowatt-hour
L	Litre
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LHV	Low heating value
m^2	Square metre
m^3	Cubic metre
MCF	Methane correction factor
Mgal	Megagallon
MJ	Megajoule
MW	Molecular weight (g/mol)
N	Nitrogen
NaOCl	Sodium hypochlorite
O	Oxygen (element)
O_2	Oxygen (molecular)
P	Phosphorus
Pa	Pascal
PE	Person equivalent
pKa	Acid dissociation constant (dimensionless)
Q	Flow (m^3/d)
QSAR	Quantitative structure-activity relationships
S	Sulfur
SS	Suspended solids
T	Temperature

TOC	Total organic carbon	VOC	Volatile organic carbon
U	Heat transfer coefficient ($W/m^2/ºC$)	VSS	Voltile suspended solids
		W	Water
US	United States	WWTP	Wastewater treatment plant
UV	Ultraviolet		

1 Introduction

WW LCI is a model and tool programmed in MS Excel, designed to calculate life cycle inventories of wastewater discharges in urban systems. The model addresses wastewater treatment at four levels: primary treatment (suspended solids settling), secondary treatment (aerobic biological treatment), tertiary treatment (nitrogen and phosphorus removal, sand filtration, disinfection through chlorination) and septic tanks (on-site primary treatment). Sludge disposal is also part of the model, including composting, landfilling, incineration and agricultural reuse. Emissions resulting from untreated discharges such as greenhouse gases (GHG), nutrients, etc., are also covered. The model incorporates a set of average scenario conditions at the country level, by means of a database storing these country profiles. Figure 1 shows an overview of the processes covered by the model.

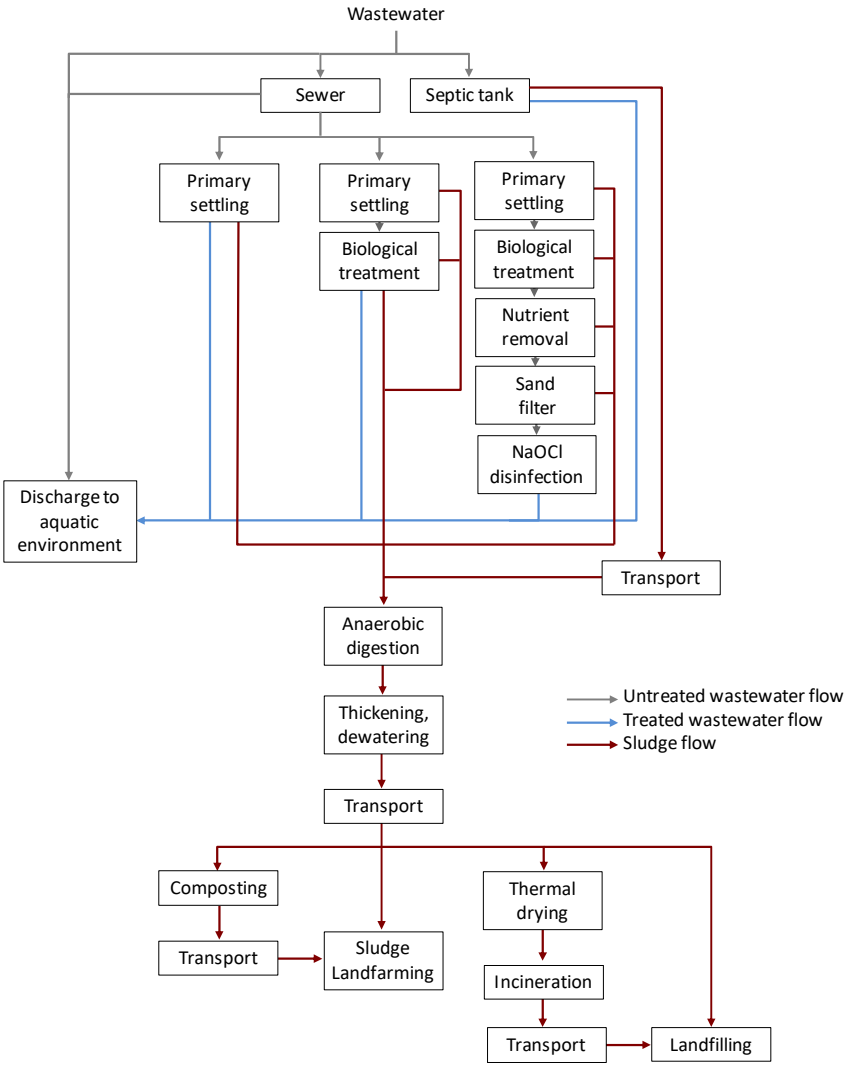

Figure 1. An overview of the processes included in WW LCI v3.

In this document we provide a description of the main new features introduced in the latest version of this tool, WW LCI v3. We do not address the basics of the model, as these have been extensively documented in previous articles, conference presentations and working papers. Also, it is not the goal of this report to

document to the last detail the new developments, but to provide a fair description, which can be then enhanced by accessing the spreadsheet, where all the data, calculations and data sources are traceable. Finally, the target reader of this document is a person already familiar with how WW LCI is implemented in Excel. For an introduction to the model starting from scratch, the reader is instead referred to the literature listed in Table 1. In the following sections we describe one by one all the changes introduced in the model, grouped in six chapters.

Table 1. List of available documentation on WW LCI.

Peer-reviewed articles
• Kalbar P, Muñoz I, Birkved M (2018) WW LCI v2: a second-generation life cycle inventory model for chemicals discharged to wastewater systems. Sci Total Environ, 622–623: 1649-1657.
• Muñoz I, Otte N, Van Hoof G, Rigarlsford G (2016) A model and tool to calculate life cycle inventories of chemicals discharged down the drain. International Journal of Life Cycle Assessment, 22 (6): 986-1004.
Conference presentations
• Muñoz, I (2017) Consequential LCI modeling of chemicals in wastewater: including avoided nutrient treatment. SETAC Europe 28th Annual Meeting, Barcelona, 27-28 November 2017.
• Kalbar P, Birkved M, Muñoz I (2017) A second-generation life cycle inventory model for chemicals discharged to wastewater. SETAC Europe 27th Annual Meeting, Brussels, 7-11 May 2017.
• Muñoz I, Van Hoof G, Rigarlsford G (2016) LCI model and tool for chemicals discharged down the drain. Case study on detergent formulations. 22nd SETAC Europe LCA Case Study Symposium, Montpellier, 20-22 September 2016.
• Muñoz I, Otte N, Van Hoof G, Rigarlsford G (2016) A model and tool to calculate life cycle inventories of chemicals discharged down the drain. 26th SETAC Europe Annual Meeting, Nantes, 22-26 May 2016.
Other documents by 2.-0 LCA consultants
• Muñoz I (2019) Wastewater life cycle inventory initiative. WW LCI version 3.0 user manual. 2.-0 LCA consultants, Aalborg, Denmark.

2 Changes to the coverage of wastewater components

2.1 Inclusion of conventional wastewater descriptors: COD, N, P, SS

WW LCI was designed to cover the modelling of chemical substances discharged in wastewater, where the individual substances discharged must be identified, as done in environmental risk assessment. An example would be to model a wastewater generated by a washing machine, where the individual ingredients in the detergent formulation are known. This is an innovative and unique approach, useful for LCA studies of consumer products washed down the drain, however, often the only information available to the LCA practitioner on urban (or industrial) wastewater composition is limited to generic pollution descriptors such as chemical oxygen demand (COD). In WW LCI v3 we have adapted the model to also accommodate this kind of generic descriptors, for those cases where the individual chemicals present in wastewater cannot be identified. Now the user is capable of obtaining an LCI for a wastewater based on four easily available measures, expressed in mg/L:

- COD
- Suspended solids (SS)
- Total nitrogen (N)
- Total phosphorus (P)

These parameters are now entered by the user in a new tab called 'CODNPSS input', where they are converted into a format that WW LCI can interpret. This conversion consists on translating the above-mentioned measures into four components, expressed in kg/kg wastewater:

- Organic matter, dissolved
- Organic matter, particulate
- Inert suspended solids
- Water

Each of these components corresponds to a row of input data in WW LCI. Both organic matter components are expressed as an empirical formula of the type $C_aH_bO_cN_dP_eS_f$ and this is done assuming typical fractionation ratios for urban wastewater, mainly obtained from Henze and Comeau (2008), except the O and H content, which is estimated assuming typical mass ratios in human excreta (Yacob et al. 2018) and the S content, which is roughly estimated based on the N/S ratio found in domestic wastewater (Jönssson et al. 2005). Inert suspended solids is calculated as the total SS content minus the volatile suspended solids (VSS) content, again taking typical fractionation of SS from Henze and Comeau (2008). Finally, water is used as a balancing term.

Calculations are prepared to adapt to the user's input data. For example, if the content of SS is 0 mg/L, then automatically the organic matter in particulate fraction becomes also zero, i.e. it is not possible to have no suspended solids while at the same time having some organic carbon in particulate form. Nevertheless, the calculations rely on typical ratios found in domestic wastewater. Thus, when a wastewater composition substantially deviates from the domestic type, the user should consider modifying the ratios taken as default by WW LCI.

As already mentioned, each of the four wastewater components corresponds to a row of data input to WW LCI. Besides the composition, other variables need to be defined for each component, which is done by default as follows:

- Kd: the solid/liquid partition coefficient in suspended solids of the WWTP is quantified for the two particulate fractions organic matter particulate and inert solids. This is done in order for the model to be able to consider the potential removal of these solids in the sand filter considered as part of tertiary treatment. We use a value of 1000 for this parameter, which leads to a removal efficiency of 71% of these solids in the sand filter, in agreement with the modifications we have made to the sand filter model (see section 3.2).
- Biogenic carbon: for the sake of simplicity, both organic matter fractions (dissolved and particulate) are assumed to contain only biogenic carbon. It is known that a fraction of the total organic carbon (TOC) in urban wastewater is of fossil origin, ranging from 4-14% (Law et al. 2013) to 25% (Griffith et al. 2009), but as a default we decide not to include this aspect. If desired, it is possible for the user to split these two fractions into four fractions with different carbon labelling, although this needs to be done manually.
- Fate factors in WWTP with secondary treatment (F_{air}, F_{deg}, F_{sludge}): as a default, we consider the two organic fractions to be readily degradable with F_{deg}=95%. In the particular case of particulate organic matter, we consider that the WWTP has a primary settling tank, whereby part of these solids are settled. We use in this case F_{sludge}=60% (see section 3.5) and F_{deg}=35%. In case the user is interested in modelling a WWTP with no primary settling, this can be established in the 'CODNPSS input' tab, automatically leading to F_{sludge}=0% and F_{deg} =95% for the organic particulate fraction. Inert suspended solids are attributed a removal through sludge, with F_{sludge}=95%.
- Anaerobic degradability: both organic fractions are considered anaerobically degradable, while inert suspended solids are not subject to any reactions in the anaerobic digester.
- Fate factors for WWTP with primary treatment only and septic tanks: we rely on the default assumptions made in WW LCI v3 for these cases (see section 3.5). It is possible though for the user to introduce specific factors for F_{sludge} in these treatment settings if he/she so desires.
- Fate factors in the environment: these facte factors are used by WW LCI to calculate emissions of GHG and nutrients for direct discharges, treated effluents and sludge application to soil. They should be obtained by means of the USES-LCA fate model embedded in WW LCI. The limitation in this case is that USES-LCA can only operate with specific chemical substances and not with generic fractions such as 'organic matter'. We have made an attempt to estimate these facte factors in USES-LCA, as explained in the Appendix, where we show the actual fate factors obtained.

As a result of all these calculations, the user obtains a table with chemical-specific data, describing the assessed wastewater. This table can then be copied and pasted in the 'WWTP input' tab, where it is read by WW LCI in the traditional way.

2.2 Inclusion of metals as wastewater components

One of the limitations of WW LCI v1 and v2 was the impossibility to model the presence, fate and LCI of metals discharged to urban wastewaters. This is now overcome by WW LCI v3, where the following metals can be introduced as wastewater components:

- Silver
- Aluminium
- Arsenic
- Cadmium
- Chromium
- Copper
- Mercury
- Manganese
- Nickel
- Lead
- Zinc
- Barium
- Cobalt
- Iron
- Magnesium
- Antimony
- Vanadium

Obtaining LCIs for metals in WW LCI v3 is a simple task, since they rely on a set of predefined chemical-specific data and fate factors, which are stored in a new spreadsheet tab 'Metals', the content of which is described below.

Physical-chemical properties required for metals are their molecular weight and Kd in suspended solids. These data have been obtained from the USEtox v2.02 inorganic substances database (USEtox 2018). In the particular case of Magnesium, the USEtox database does not provide a Kd and as an approximation we use the Kd of Cadmium, which has similar properties to Magnesium (Domènech 2018). Fate of these metals in WWTPs is established by a set of metal-specific removal factors (F_{sludge}). A pre-defined set of factors is used for WWTPs with primary treatment only and for septic tanks, while a different set of factors is used for WWTPs with secondary treatment. All factors are derived from Yoshida et al. (2015) except Arsenic, obtained from Cecchini et al. (2015). Finally, for tertiary treatment, removal through sand filtration relies on the existing sand filter model embedded in WW LCI, which estimates removal based on the Kd of each metal.

From the point of view of the user, calculating individual LCIs for metals only requires choosing the target metal from a drop-down list in the 'WWTP input' tab. When metals are part of a given wastewater composition the only additional step is to enter the metal concentration in wastewater as a mass fraction (kg metal/kg wastewater). As always, WW LCI allows the user to modify the pre-defined data, for example the removal factors from literature can be overridden by better values the user might have.

3 Changes to wastewater treatment processes

3.1 Inclusion of credits from avoided nutrient treatment in WWTPs

This particular aspect was the subject of a presentation at the SETAC Europe 28th Annual Meeting (Muñoz 2017). The issue we address is related to the fact that in LCA we usually need to model wastewater compositions that deviate from the average. An example could be a single chemical discharged in wastewater, such as ethanol. Once in a WWTP (if built to apply biological treatment) ethanol is expected to be degraded by microorganisms that have certain requirements for nutrients such as nitrogen and phosphorus. In WW LCI biomass formed by biological treatment is characterized with the formula $C_5H_7NO_2P_{0.074}$, which means every time 5 mol organic carbon is taken in to build biomass, 1 mol N and 0.074 mol P are needed. In the case of ethanol (C_2H_6O), we see that its degradation requires N and P but this cannot be supplied by the compound itself. In industrial WWTPs this problem is overcome by adding nutrients from external sources, such as urea or phosphoric acid. In urban WWTPs there is no need for this, as these nutrients can be supplied by other wastewater streams with an excess of N and P and which end up in the same WWTP as our ethanol. The question at hand is, how this N and P deficiency should be modelled in consequential LCI terms. Basically, nutrients in urban wastewater are an example of 'not fully utilized' materials (Consequential LCA 2015), whereby additional demand for these nutrients displaces their disposal. Following with the ethanol example, if degradation of ethanol consumes N and P from other wastewater streams, the consequence is that these N and P no longer undergo treatment in the WWTP; this is what we call 'avoided nutrient treatment'. Although the example of ethanol might seem extreme, some wastewater mixtures can easily be nutrient deficient. In Muñoz (2017) we show that a particular washing detergent formulation is N-deficient by 94% and P-deficient by 100%, i.e. it lacks all the necessary P and most of the necessary N. In WW LCI v2 this kind of nutrient consumption, although registered by the model's stoichiometric calculations, did not have any LCI implications, analogous to the attributional 'recycled content' approach to products incorporating recycled materials, where the recycled material is free of any burdens.

In WW LCI v3 'avoided nutrient treatment' is systematically included, with no additional effort for the user. Since biological treatment in WW LCI relies completely on stoichiometry, the amount of N and P required by any chemical or chemical mixture is already being quantified by the existing calculations in the model, as shown in the chemical equation below, for ethanol:

$$C_2H_6O + 1.96\ O_2 + 0.22\ NH_4 + 0.016\ P\text{-}PO_4 \rightarrow 0.22\ C_5H_7NO_2P_{0.074} + 0.9\ CO_2 + 2.7\ H_2O$$

In this way, 1 mol ethanol requires 0.22 mol N and 0.016 mol P. In WW LCI v3 we quantify this consumption for treatment in WWTPs with secondary or tertiary treatment. In the final LCI for ethanol, we find two new inputs from technosphere, namely 'Ammonium, in wastewater' and 'Phosphate, in wastewater', both with a negative sign, meaning an avoided or substituted activity. The LCI for these two activities (that is, what is being avoided) is calculated in parallel, automatically, by the model, and it is especially interesting to note that these LCIs for ammonium and phosphate are not static, terminated LCIs, but dynamic ones as they change according to the scenario conditions: it is not the same to avoid 1 kg P treatment in a country where 100% of wastewater receives tertiary treatment than in a country where wastewater is discharged with no

treatment. In the first case what is being avoided is mainly P removal by means of coagulation with $FeCl_3$, in the second case we simply avoid the discharge of this P to the environment.

As already mentioned, these 'avoided nutrient' calculations are only applied to WWTPs with secondary or tertiary treatment. In WWTPs with primary treatment only, we consider there is no biological treatment, but only partitioning of substances to sludge (see section 3.5). In septic tanks there is no aerobic biological treatment either, but anaerobic degradation occurs in the bottom sludge layer. In the model we neglect any biomass formation during anaerobic digestion, as the gross biomass yield of anaerobic microorganisms is much lower than that of aerobic microorganisms (Von Sperling 2007, p. 94). This is even more the case for septic tanks, given the long solids residence time involved (up to years), which means the net biomass yield is even lower when compared to aerobic systems.

3.2 Sand filtration efficiency in tertiary treatment

In WW LCI v2 we introduced tertiary treatment by means of sand filtration, where solids removal is substance-specific and depends on the substance's Kd, either entered by the user or estimated by the model with the parameters Kow and pKa entered by the user. The equations incorporated in the model (see Kalbar et al. 2018) estimate the fraction of the substance expected to be partitioned to suspended solids in the WWTP tanks after secondary treatment. The fraction of substance partitioned to solids is considered as removed by the sand filter. This assumes that the sand filter completely removes all suspended solids from the effluent, which can be considered as too optimistic. In order to make the model more realistic we have introduced a suspended solids removal rate in the sand filter, which takes a value of 71% (Benth et al. 1981). This means that, given 1 kg of a substance in the effluent of the secondary treatment that partitions to suspended solids, the sand filter will remove 0.71 kg and 0.29 kg will be discharged with the filtered effluent, whereas in the previous version of the model 0 kg of the substance would be discharged in the filtered effluent.

3.3 Inclusion of electricity consumption in WWTPs as a function of plant size

It is well known that electricity demand in WWTPs is influenced by the size of the plants, meaning by size the plant's daily flow in m^3/d. Bigger plants show generally lower consumption on a per m^3 or person-equivalnet (PE) basis (CUAS 2015; Trapote et al. 2014). According to CUAS (2015) this is due to economies of scale in larger systems, leading to larger but more efficient equipment, better performing automation and regulation, and also to more and better-trained staff operating the plants. In WW LCI v3 we have addressed this topic, by adding what in the model is called the 'scale factor', which is a multiplier factor that increases the energy demand of the plant as its size decreases. In this section we describe how this scale factor was derived and implemented.

The relationship between kWh/m^3 and WWTP size was established using two studies covering plants in the US (Stillwell et al. 2010) and Spain (Albadalejo et al. 2017). Figure 2 below plots the data obtained from these studies, together with power regressions calculated in Excel. Data from the two studies were used as they cover WWTPs of different sizes, with the Spanish study reaching to smaller sizes while the US study reaches to bigger sizes. In WW LCI v3 we take a WWTP treating 2 million m^3/d as reference (we use this as the point beyond which higher efficiency is not considered). The regressions in Figure 2 predict that such a

plant has an electricity demand of 0.23 kWh/m^3 (based on ES data) and 0.30 kWh/m^3 (based on US data). In the model we take the arithmetic average of these two, namely 0.27 kWh/m^3.

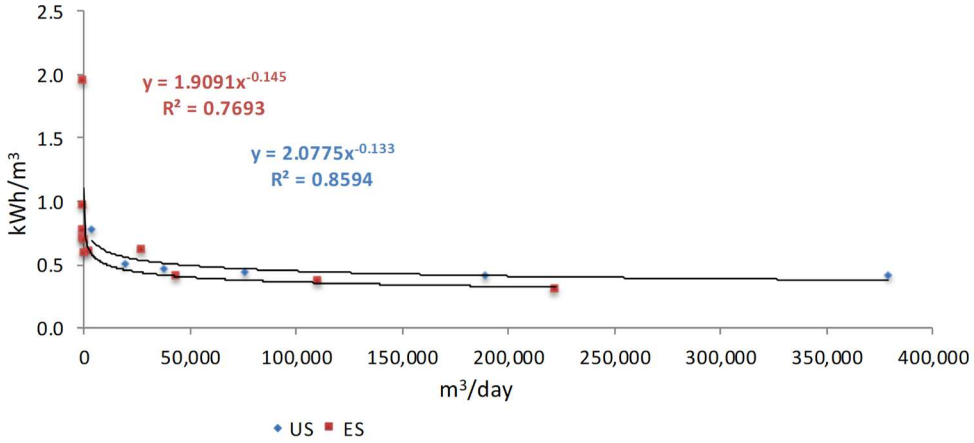

Figure 2. Electricity consumption in WWTPs (kWh/m³) as a function of daily wastewater flow (m³/d) in United States and Spain. Underlying data from Stillwell et al. (2010) and Albadalejo et al. (2017).

In Figure 3 below the energy demand of WWTPs as predicted by the two regressions calculated in Figure 2 is divided by the demand of the reference plant (0.27 kWh/m^3). We call this ratio the 'scale factor'. The reference WWTP is thus attributed a scale factor of 1, whereas smaller WWTPs have a scale factor above 1. It can be seen that both studies lead to very similar scale factors. For example, a WWTP treating 500,000 m^3/d gets a scale factor of 1.20 using the US regression and 1.22 using the Spanish study regression. We finally merge the scale factors of the two studies by means of a polynomic regression, as seen in Figure 3. This equation is the one used in WW LCI v3 to relate WWTP size with energy consumption.

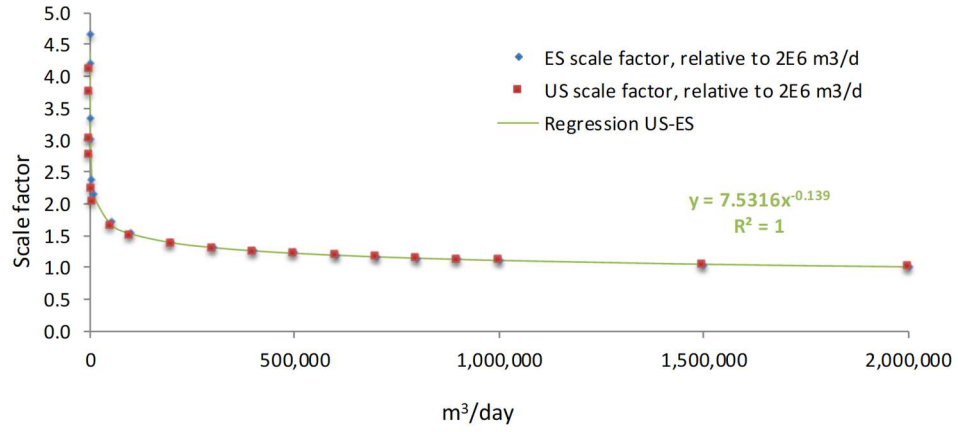

Figure 3. Derivation of a scale factor relating WWTP size with electricity consumption per m³, based on the data from Figure 2.

The procedure to calculate the specific energy consumption at the WWTP has been changed in WW LCI v3, although it is grounded in the same principles than in WW LCI v2, that is, we subdivide the WWTP into subprocesses, to which we attribute specific electricity consumption factors. These subprocesses are the following:

- Miscellanous: this includes building energy consumption (offices, labs, etc.) as well as pre-treatment and pumping of wastewater inside the plant. This miscellaneous demand is attributed to the wastewater components on a mass basis.
- Aeration: electricity consumed by blowers to supply oxygen for the biological treatment basin. This is attributed to the wastewater components based on the total oxygen consumption, which is stoichiometrically calculated by the model.
- Sludge treatment: electricity consumed by primary and secondary settling tanks, anaerobic digestion (if available), thickening and dewatering. This is attributed to the wastewater components based on the amount of dry solids they produce.

These three energy demand categories are further specified according to the treatment level. For example, a WWTP with primary treatment only does not incur in aeration energy needs, or a WWTP with tertiary treatment has higher sludge treatment energy needs as it includes the sand filter, among other additional processes. The electricity consumption factors used are shown in Table 2. Miscellaneous energy factors were derived from a distribution in percentages of electricity demand in different activities by a WWTP treating 100 megagallon/d (Stillwell et al. 2010). These percentages were converted into kWh/m^3 considering the electricity demand for the reference WWTP, of 0.27 kWh/m^3. The electricity demand for sludge treatment comes from the same source (Stillwell et al. 2010). In this case we assume that 1 m^3 produces 0.35 kg solids in the WWTP, based on 0.06-0.08 kg solids/PE in activated sludge plants (Andreoli et al. 2007) and a wastewater volume of 0.2 m^3/PE/d (Henze and Comeau 2008). Finally, the electricity demand for aeration is taken from Von Sperling (2007) as an average from different aeration methods (diffused air, mechanical aeration).

Table 2. Electricity consumption factors considered in WW LCI v3 for a reference WWTP treating 2 million m^3/d.

Operation	Unit	WWTP with primary treatment	WWTP with secondary treatment	WWTP with tertiary treatment
Miscellaneous	kWh/m^3	0.027	0.027	0.028
Sludge treatment, no anaerobic digestion	kWh/kg solids	0.086	0.112	0.181
Sludge treatment, with anaerobic digestion	kWh/kg solids	0.162	0.188	0.258
Aeration	kWh/kg O_2	0	0.714	0.714

The electricity demand factors in Table 2 refer to a WWTP treating 2 million m^3/d. For smaller plants we apply the scale factor to each one of these factors. For example, a WWTP with secondary treatment and anaerobic digestion of sludge treating 500,000 m^3/d has a scale factor of 1.21. Its electricity demand for sludge treatment is thus 1.21*0.188 = 0.227 kWh/kg solids. All these calculations are now placed in WW LCI v3 in a new tab 'EnergyWWTP', where they are transparently reported.

The specification of electricity consumption as a function of plant size involves at some point the definition by the user of the size of the plant or group of plants to be assessed. The database in WW LCI v3 now includes country-specific estimates of the distribution of WWTPs by size, which are automatically loaded as scenario data (see section 3.3). As usual, the user is allowed to modify these estimates to represent different conditions.

3.4 Inclusion of sewer and WWTP infrastructure specification in five classes

In WW LCI v2 wastewater infrastructure was covered as background system, using the ecoinvent data sets for sewers and WWTPs with a capacity of 4.7E+10 L/year, which is the biggest size available. In WW LCI v3 we go a step further, by incorporating in the model all five sewer and WWTP capacities available in ecoinvent:

- 4.7E+10 L/year for sewers/WWTPs treating ≥55,000 m^3/d.
- 1.1E+10 L/year for sewers/WWTPs treating between 28,000 m^3/d and 54,999 m^3/d.
- 5E+09 L/year for sewers/WWTPs treating between 5,500 m^3/d and 27,999 m^3/d.
- 1E+09 L/year year for sewers/WWTPs treating between 1,100 m^3/d and 5,499 m^3/d.
- 1.6E+08 L/year for sewers/WWTPs treating <1,100 m^3/d.

For all countries in the WW LCI database we provide a sewer size mix and a WWTP size mix. In practice, what we have calculated is the WWTP size mix, which is then matched with the equivalent sewer size mix. It must be highlighted that this mix not only influences the impact of infrastructure as such, but also the electricity consumption associated to the WWTPs, as explained in section 3.3. For each country, the sewer/WWTP mixes states 1) the percentage of wastewater treated under each one of the five infrastructure classes and 2) the average size of the WWTPs within each class. In the Excel tool, for each country mix we provide a short explanation and the data sources/assumptions made, although the actual calculation of the mixes is not shown. These calculations are available to the user upon request.

The number of data sources to fill in this information at the country level is too long for an itemized discussion in this report, but all the references are available in the database. In short, we could describe the data sources as follows:

- For European countries we used the database Waterbase-UWWTD (European Environment Agency 2017). This database contains an inventory of European WWTPs including numerous descriptors, among which the design and actual treatment capacity, expressed as PE. The country mixes were derived from these data, by converting from PE to m^3/d, the latter based on wastewater production per person according to EUROSTAT (2018), AQUASTAT (2018) or other sources.
- For a few countries, such as US, New Zealand and Mexico we were able to use detailed inventories reporting on all the existing WWTPs in the country.
- In many cases we used technical reports, peer-reviewed articles, etc., which provided a more or less complete distribution of the existing WWTPs in a few capacity classes. In such cases it was necessary to assume a certain average size for each capacity. For example, if 20 plants were reported to be between 20,000 and 40,000 m^3/d, we typically took the average, 30,000 m^3/d to represent this capacity class.
- Finally, in some cases, e.g. Chile, Peru, Russia, it was not possible to obtain an actual mix, since the only data found were the total number of WWTPs and their total treatment capacity. In this case only one infrastructure class is used.

As always, these data can be modified in WW LCI by the user, either in the database itself or by choosing 'User-defined' input data in the 'WWTP input' tab. The quality of the data we provide is variable, i.e. of high

quality in some cases while poor in others. We welcome any feedback as well additional information allowing us to improve the current country data sets.

3.5 Fate factors in WWTPs with primary treatment only and in septic tanks

In WW LCI v2 both WWTPs with primary treatment only and septic tanks where assumed to achieve a certain extent of aerobic degradation, namely 30% of the equivalent extent assumed for WWTPs with secondary treatment. The main reason to take this into consideration in the model was based on the fact that these systems do remove biological oxygen demand (BOD). However, it seems reasonable to assume that the main mechanism by which BOD is removed in such cases is not biological degradation mediated by aerobic microorganisms, but the mere removal by settling of particulate organic matter. In WW LCI v3 both of these systems no longer achieve biological degradation. In practice, this means that any substance undergoing these treatments is subject to a fate factor for degradation (F_{deg}) of zero.

In these two types of treatment it was also taken as a default in WW LCI v2 that suspended solids removal efficiency was 30% of the equivalent value for a WWTP with secondary treatment, which we judge as rather low. Based on Von Sperling (2007b, p. 221) the absolute SS removal rates in primary treatments and septic tanks is 60%, while for secondary treatment this is 90%. Therefore, the ratio should rather be 60/90= 66.7%. Thus, the approach to quantify the fraction of a substance that is partitioned to sludge during primary treatment or in septic tanks remains the same as in WW LCI v2 (Kalbar et al. 2018, equations 2 and 8), but we change the relative solids removal efficiency from 30% to 66.7%.

Another assumption in WW LCI v2 for WWTPs with primary treatment only was that the fate factor F_{air}, expressing the fraction of substance entering the WWTP that is emitted to the atmosphere, was calculated as 30% of the equivalent value for a WWTP with secondary treatment. In WW LCI v3 we decided to neglect any emissions to air from primary treatment WWTPs, mainly due to the fact that there is little probability of air stripping in a settling tank with no aeration, compared to an aeration basin where air bubbles help volatile chemicals to escape to the atmosphere.

3.6 Specification of water emissions: freshwater, seawater, groundwater

In WW LCI v3 we now specify the type of water body to which wastewater and treated effluents are discharged. We differentiate three types of water bodies:

- Freshwater, represented as the sub-compartment ‘river’ in SimaPro.
- Coastal waters, represented as the sub-compartment ‘ocean’ in SimaPro.
- Groundwater

The groundwater sub-compartment is automatically chosen by the model when septic tanks are used. For any other treatment and for direct discharges a mix of freshwater/ocean discharge is used. This mix was established at the country level based on several sources:

- For most European countries we calculated this share based on the person-equivalents (PEs) discharged by WWTPs in each country according to the database Waterbase-UWWTD (European Environment Agency 2017). We considered discharges to freshwater and to land catchment of freshwater as emissions to ‘river’ and the remainder (coast, estuaries, etc.) as emissions to ‘ocean’.

- For Russia, Belgium and Ukraine we used data from Hauschild and Potting (2005, annex 1), reporting the fraction of wastewater discharged to inland waters or to the ocean.
- For Turkey we used actual reported distribution of wastewater discharges by the Turkish Statistical Institute (2014).
- For all the remaining countries we made the assumption that the percentage of discharges to the ocean is equal to the percentage of the country's population that lives in the coast. This is approximated with data from CIESIN (2012) reporting the percentage of population living within 10 km of the coast.

3.7 Inclusion of disinfection as part of tertiary treatment in WWTPs

In WW LCI v3 we introduce disinfection as an additional feature of WWTPs applying tertiary treatment. Here we refer to disinfection by means of dosing chemicals, in particular sodium hypochlorite (NaOCl). Although it would be possible to also include UV disinfection, at this point we have chosen not to include this process due to its relatively higher data demand at two levels: the LCI of the UV process itself (consumption of lamps, energy, etc.) and because once we have in the model two options for disinfection, this creates a need to determine in the WW LCI database a 'disinfection mix' for each country, implying a substantial effort in searching for country-specific penetration of these technologies.

The implementation of disinfection with NaOCl in WW LCI v3 is quite straightforward. For wastewaters treated in WWTPs with tertiary treatment, we consider a dose of 7.3 g $NaOCl/m^3$, based on a consumption of 3-4 g Cl_2/m^3 (Delft University of Technology 2013). Production of NaOCl is modelled in ecoinvent with the global market data set for NaOCl production, while the resulting increase in Na+ and Cl- ions in the effluent is at this point not included.

The functional unit in WW LCI is 1 kg of chemical substance discharged in wastewater, which means we attribute a consumption 7.3E-06 kg NaOCl/kg chemical compound passing through tertiary treatment. It must be highlighted that this treatment does not imply any physical or chemical changes (e.g degradation or physical removal) to the substances we assess with WW LCI. Since in LCA we do not address pollution of biological origin, the inclusion of disinfection in the model simply adds an environmental burden (the industrial production of NaOCl), while its potential human health benefits are unfortunately not captured.

3.8 Inclusion of hydrogen sulphide emissions from septic tanks

As seen in the chemical reaction in section 4.1, anaerobic digestion produces hydrogen sulphide (H_2S). In centralized WWTPs it is assumed that this is entirely converted to sulphur dioxide when the biogas is combusted. However, in septic tanks this H_2S is expected to be emitted to the atmosphere. Although WW LCI v2 already quantified H_2S in its anaerobic digestion calculations, this emission was not captured in the final LCI. In WW LCI v3 we have corrected this and included this emission as part of the final inventory for septic tanks. Rather than an improvement, this can actually be considered as an error correction in the existing model.

3.9 Inclusion of a COD emission flow

Although COD is typically not considered by any of the latest impact assessment methods (not even in the impact category of aquatic eutrophication), it is still an important pollution indicator. In WW LCI v3 we now allow the user to enter generic descriptors such as COD to obtain LCIs (see section 2.1) and therefore it makes sense to have COD too as a foreground flow in the final LCI results. We implemented this flow in the model based on the following chemical reaction, obtained from Wikipedia (2018):

$$\mathrm{C_nH_aO_bN_c} + \left(n + \frac{a}{4} - \frac{b}{2} - \frac{3}{4}c\right)\mathrm{O_2} \rightarrow n\mathrm{CO_2} + \left(\frac{a}{2} - \frac{3}{2}c\right)\mathrm{H_2O} + c\mathrm{NH_3}$$

It is highlighted that this oxidation reaction does not include the COD from oxidation of ammonia to nitrate, since dichromate (the chemical reagent used for COD determination) does not oxidize ammonia. From this chemical equation, COD is calculated for a given chemical substance as:

$$\text{COD (kg } O_2\text{/kg)} = \frac{32 \cdot (n + 0.25 \cdot a + 0.5 \cdot b - 0.75 \cdot c)}{MW}$$

Where n, a, b and c correspond to the sub-indexes shown in the COD chemical reaction above and MW is the molecular weight of the chemical substance, in g/mol. As an example, Diclofenac ($C_{14}H_{11}Cl_2NO_2$), with a MW of 296.15 g/mol has a COD of 1.62 kg O_2/kg.

3.10 Nitrogen and phosphorus removal as tertiary treatment by default

In WW LCI v2, the user was in charge of defining whether or not wastewater treatment was carried out in WWTPs with either N removal (through nitrification – denitrification) and/or P removal (through chemical coagulation with iron chloride). As in many other aspects related with data input, in WW LCI v3 we have made an effort to provide the user with as much default input as possible. Regarding nutrient removal, we have made the decision to automatically link these operations to tertiary treatment only. For example, in Denmark, 89% of the wastewater is treated in centralized WWTPs, with 2% in primary treatment WWTPs, 3% in secondary treatment WWTPs and 84% in tertiary treatment WWTPs. With the new settings, both N and P removal are only considered in the 84% of wastewater treated in tertiary treatment WWTPs. In fact, this is the way nutrient removal is understood by Eurostat (2018), the main data source we used to populate EU countries in the WW LCI database. In p. 74 of Eurostat (2018) tertiary treatment is defined as:

"Treatment (additional to secondary treatment) of nitrogen and/or phosphorous and/or any other pollutant affecting the quality or a specific use of water: microbiological pollution, colour etc.".

While secondary treatment is referred to as providing only BOD/COD removal:

"Treatment of wastewater by a process generally involving biological treatment with a secondary settlement or other process, resulting in a BOD removal of at least 70% and a COD removal of at least 75%".

It must be borne in mind, though, that in WW LCI v3 we populated the country database using numerous and diverse data sources, which might not be necessarily in agreement with the Eurostat definitions above. We implicitly assumed that any source of statistics on treatment levels in any given country referring to 'tertiary treatment' agrees with the Eurostat definition.

Finally, it must be highlighted that as usual, the WW LCI user can override the default settings and consider different penetration levels for N removal and P removal, respectively. In the example for Denmark, the user would be allowed to choose a P removal or N removal level from 0% to 87%. The limit of 87% is established by the sum of secondary + tertiary treatment, i.e. it is not possible to have primary treatment WWTPs (or septic tanks) with N or P removal.

3.11 Septic tank construction LCI

In WW LCI v2 we supplied the model with LCI data for construction of septic tanks based on the study by Pizzol et al. (2015), which offered data on septic tanks used in Denmark for allotment gardens. Although this study is transparent and complete, its main limitation for our purposes is that it represents a system with a very low capacity, namely 76.8 m^3/year or 210 L/day, which is around 1 PE or less. In WW LCI v3 we decided to replace these data with those from Magar (2016) describing a septic tank installed in Norway, for an average capacity of 8 PE (1,600 L/d). The LCI data available in this study cover the septic tank as a primary treatment, plus other more advanced unit operations, however we focused on the septic tank only. The study provides the total amount of materials, which are assumed to have a life span of 20 years. The excavated volume was not originally quantified; we added this as the volume of the tank itself (9.5 m^3) plus the volume occupied by the surrounding gravel (7 m^3). All activities were covered with ecoinvent data sets. In the case of the geomembrane, this was modelled as HDPE. We added a pipe extrusion process to approximate the manufacturing of the pipe and geomembrane. The end-of-life stage of the septic tank is not included in the LCI.

Table 3.Inventory data for construction of a septic tank with a capacity of 8 PE (1.6 m^3/day). Based on Magar (2016)

Activity	amount
Polyvinylchloride, kg/kg wastewater	1.05E-05
Geomembrane (as high-density polyethylene), kg/kg wastewater	2.91E-06
Glass fibre, kg /kg wastewater	3.25E-05
Gravel, kg/kg wastewater	9.09E-04
Excavation, m^3	1.41E-06
Geomembrane/pipe manufacturing (as extrusion), kg/kg wastewater	1.34E-05

3.12 Optional biological treatment with methanol

In WW LCI, nitrogen removal is modelled by means of nitrification followed by denitrification. The original WW LCI model, version 1, was designed to model the denitrification reaction considering the addition of methanol as a carbon source. The problem with this approach for N removal is that it seems to be rather infrequent. The methanol Institute (2018) claims that there are nearly 200 WWTPs in the US using methanol. The total number of urban WWTPs with advanced treatment, according to the Clean Watersheds Needs Survey in 2012 (USEPA 2018) is 4,971. If we assume that this is the number of plants applying N removal in the US, it means that only about 4% of the operating plants apply N removal with methanol.

In WW LCI v2 we introduced the option of using the carbon already available in wastewater for denitrification, but this was never documented. The original chemical reaction considered in WW LCI, when methanol is used, is the following (Muñoz et al. 2016):

$NO_3^- + 1.08\ CH_3OH + 0.9\ H^+ \rightarrow 0.06\ C_5H_7ON_2 + 0.47\ N_2 + 0.78\ CO_2 + 2.4\ H_2O$

In WW LCI v2, the option of no methanol addition was based on a simplification of the above reaction, as follows:

$NO_3^- + 6\ H^+ \rightarrow 0.5\ N_2 + 3\ H_2O$

This simplified chemical reaction still keeps stoichiometry and implies that denitrification results in no consumption of methanol, but also in no production of excess sludge or CO_2. In WW LCI v3 we keep these two equations, however, instead of leaving the user to always decide which option to apply, the default option is now the second one, i.e. not using methanol. The user is still allowed to modify this, by choosing to enter user-specific data rather than the default data.

4 Changes to sludge treatment and disposal processes

4.1 Full stoichiometry in anaerobic digestion

In WW LCI anaerobic digestion calculations are carried out for two processes: digestion of sludge generated by WWTPs and also digestion of sludge accumulated at the bottom of septic tanks. The chemical reaction was implemented in the model following a complete mass balance, but this balance was not entirely based on stoichiometry. This led in some cases to imbalances in the calculation of the composition of sludge sent to disposal. In WW LCI v3 we have addressed this limitation in order to make the anaerobic digestion calculations entirely stoichiometric. We have done this by applying the so-called Buswell equation (Buswell and Müller 1952), which can be expressed as follows:

$$C_cH_hO_oN_nS_s + \frac{(4c - h - 2o + 3n + 2s)}{4} H_2O \rightarrow \frac{(4c - h + 2o + 3n + 2s)}{8} CO_2 + \frac{(4c + h - 2o - 3n - 2s)}{8} CH_4 + n\ NH_3 + s\ H_2S$$

Where $C_cH_hO_oN_nS_s$ is the empirical formula of an anaerobically degradable organic compound. In centralized WWTPs the resulting products from anaerobic digestion are converted into emissions to air after combustion of these as biogas. In WW LCI v3 this is kept as in the previous versions of the model. In the case of septic tanks, in previous versions of the model the N in the products of the anaerobic digestion was modelled as nitrogen gas, whereas in WW LCI v3 we assume this N stays in the water phase as ammonium, which is discharged in the septic tank effluent.

4.2 Heat balance in anaerobic digestion and WWTP as a function of local climate

In WW LCI v2 a heat energy balance was calculated for each chemical substance entering a WWTP, taking into consideration the following:

- Heat energy demand was split into two components: for sludge digestion and for miscellaneous purposes (e.g. heating of buildings). These two components were defined based on data from the Swiss WWTP model by Doka (2007).
- Heat energy production was calculated from the amount of methane produced during anaerobic digestion of the specific chemical substance, and a heat recovery efficiency defined for a WWTP applying cogeneration of heat and power (CHP).

Based on these two terms, a balance calculation led to either a net heat surplus or a net heat demand. When a heat surplus occurred, this led to a substitution of natural gas as fuel, whereas a net heat demand led to a natural gas input.

In WW LCI v3 the basic approach above, of performing a heat balance for each chemical component in wastewater, does not change. However, we move away from our previous approach in the following aspects:

- Not all WWTPs apply anaerobic digestion. In the absence of the latter, the heat demand by the WWTP is much lower, since heating the digester is typically the main heat-consuming activity in a WWTP. We now account for situations where there is no anaerobic digestion. For each country, we

define the percentage of wastewater treated in WWTPs with anaerobic digestion. This is explained in section 4.3).

- When there is anaerobic digestion, the resulting methane can be either combusted in a flare, in a boiler, or in a CHP plant. We now include this in the model. This is explained in section 4.4).
- For the anaerobic digestion process, rather than relying on Swiss average conditions, we have built an anaerobic digestion heating model which provides country-specific calculations, by considering the average climate conditions (ambient temperature) in the country. This is implemented as the sum of 12 monthly heat balances, using the average monthly temperatures per country.
- With the above information, we calculate, for each wastewater component in a given country-specific situation: 1) whether this component provides a net heat surplus or net heat demand and 2) in any of these two cases, what is the marginal source of heat either substituted or consumed: biogas, natural gas or a combination of the two.

The new anaerobic digestion heating model is placed under the new 'EnergyWWTP' tab in the Excel spreadsheet, where all the calculations are available. This model is based on data and equations provided in Turovskiy and Mathai (2006) for a WWTP treating 37,800 m^3 wastewater/d and producing 5,443 kg primary sludge and 2,722 kg activated sludge per day, which are treated in two mesophilic digesters with 15 m diameter, where we assume a hydraulic residence time of 20 days. The total volume of the digester (as the sum of the two units) is 3,499 m^3. The underlying geometrical data by Turovskiy and Mathai (2006) allow us to calculate for each digester, in m^2, the floor area (180 m^2), wall area (561 m^2), and roof area (177 m^2). The total heat demand, in MJ/day is calculated as:

$$\text{Heat demand (MJ/d)} = \frac{\text{Losses + Sludge heating}}{0.9}$$

Where Losses is the heat demand to offset the sum of heat losses through the digester's wall, floor and roof, while Sludge heating is the heat required to increase the sludge temperature from ambient conditions to the 35ºC maintained in the digester. The 0.9 factor is meant to account for additional heating demand in the WWTP, i.e. the 'miscellaneous' component mentioned at the beginning of this section. This is quantified at 10% of the total heating demand of the WWTP as in Doka (2007). Losses for each one of the surfaces are calculated with the formula:

$$\text{Losses (MJ/d)} = \frac{U \cdot A \cdot (35 - T)}{1000 \cdot 24 \cdot 3.6}$$

Where U is the heat transfer coefficient ($W/m^2/ºC$) for either floor, wall or roof, A is the total area of each surface and T is the temperature (ºC) of either air (for losses through wall and roof) or soil (for losses through floor). Values for U are taken from Foley et al. (2010) as 5, 1.7 and 2 $W/m^2/ºC$ for wall, floor and roof, respectively. These values are assumed to be constant across countries.

Sludge heating is calculated with the formula:

$$\text{Sludge heating (MJ/d)} = Q \cdot C_p \cdot (35 - T)$$

Where Q is the sludge flow in m^3/d, C_p is the heat capacity of sludge in $MJ/m^3/ºC$ and T is the sludge temperature (ºC). Q is calculated as 87.5 m^3/d per digester and C_p for sludge is assimilated to that of water, i.e. 4.2 $MJ/m^3/ºC$.

As it can be seen, the formulae for Losses and Sludge heating depend on temperatures of three media: air, soil and sludge. In our model we differentiate these three temperatures, both in space and time. In space since each country is attributed its own average temperature profile and in time since we calculate each of the above heat requirements on a monthly basis, from January to December. Air temperatures for each country and month were obtained from Weatherbase (2018). Soil temperature (T_s) was estimated as a function of air temperature, using the following polynomial regression:

$T_s = 0.0163x^2 + 0.408x + 3.6511$ ($R^2 = 0.9295$)

This regression was obtained from published data on soil and air temperatures in Ottawa, Canada (Agriculture Canada 1975). In Figure 4 below it can be seen how this regression simulates reasonably well the actual soil temperatures in this location. The reason why Canada was chosen to obtain this regression is to reflect that soil is a very good insulator. In particular, The Ottawa data set used allows us to reflect this in the regression, as it covers a wide range of air temperatures, from very low (-11 ºC) to moderately high (20ºC).

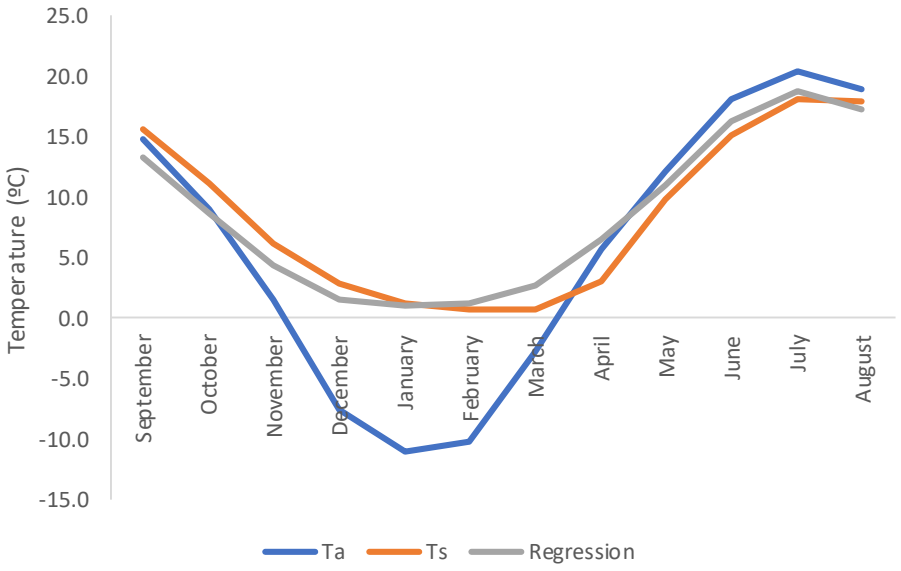

Figure 4. Air (Ta) and soil (Ts) temperatures in Ottawa from Agriculture Canada (1975) and simulation of Ts with our regression $Ts = 0.0163x^2 + 0.408x + 3.6511$.

The temperature of sludge at the input to the digester is approximated by the temperature of wastewater (Tww), which we also estimate as a function of air temperature, with the following equation:

$Tww = 0.0148x^2 + 0.1716x + 13.522$ ($R^2 = 0.8226$)

This equation was obtained from two separate sets of data: wastewater temperatures in the years 2005 and 2006 at the input of the WWTP in Zurich, Switzerland (Schmid 2008) and the average monthly air temperature in Zurich from Yr (2018). In the figure below, we plot the monthly average air temperature in Zurich (Ta), the wastewater temperature (Tww) and the prediction of wastewater temperature with our equation (Regression). It can be seen that the regression has an acceptable fit, and that wastewater has quite a constant temperature profile through the year, compared to air temperature.

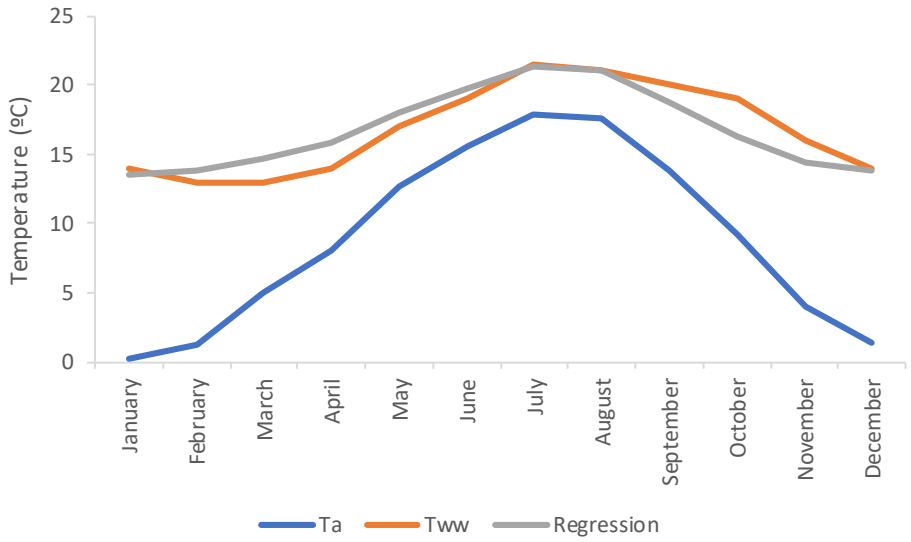

Figure 5. Air (Ta) and wastewater (Tww) temperatures in Zurich and simulation of Tww with our regression Tww = 0.0148x² + 0.1716x + 13.522. This regression is used in the model as a proxy for sludge temperature at the inlet of the anaerobic digester.

The presented equations and data allow us to calculate the heat demand by the WWTP. The following step is to calculate heat production in the defined system. This is done based on the following site-generic assumptions:

- Volatile solids content in primary and secondary sludge is 65% and 75%, respectively.
- VSS reduction in the digester is 50%.
- Specific biogas production is 1 m^3/kg VSS destroyed.
- Methane content in biogas is 65%.
- Methane net calorific value is 50 MJ/kg.
- The heat efficiency in a boiler is 80%
- The heat efficiency in a CHP system is 48%

The above assumptions and data are mainly taken from Turovskiy and Mathai, except the heat efficiencies, taken from Panepinto et al. (2016) and Wason (2016). From these data, it can be calculated that the modelled digester produces the following amount of heat, in MJ/d:

$$\text{Heat production (MJ/d)} = -59{,}568 \cdot (0.8 \cdot f_{boiler} + 0.48 \cdot f_{CHP})$$

Where fboiler is the fraction wastewater treated in WWTPs where biogas is burned in boilers and fCHP is the fraction of wastewater treated in WWTPs where biogas is burned in CHP systems. In this equation, heat

production takes a negative sign. The calorific value of the biogas produced (before combustion) in our digester model is -59,568 MJ/d.

With the approach presented so far, it is possible to build the heat energy balance for a WWTP, on a monthly basis. This is shown in Table 4 using Russia as an example. In these calculations, it is assumed that the WWTP has a CHP system. It can be seen that the plant is not self-sufficient in terms of heat energy, needing an input of external fuel in 9 out 12 months per year. Only in June, July and August there is enough self-produced heat to fully supply the plant. The balance is notably affected by the way the biogas is used. If instead of a CHP system (48% heat efficiency) a conventional boiler was considered (80% efficiency), the WWTP would be self-sufficient from March to November (not shown in the table). It must be highlighted that our monthly balance approach assumes that biogas production is constant over the months and that even if biogas storage capacity is available at the WWTP to buffer heat demand variations, this capacity is not capable of coping with inter-monthly variations.

Table 4. Summary of WWTP heat energy balance in Russia.

Month	Heat demand, MJ/d	Heat production, MJ/d	Net, MJ/d	NG days[a]
January	50,235	-28,592	21,642	31
February	49,720	-28,592	21,128	28
March	46,892	-28,592	18,299	31
April	41,204	-28,592	12,611	30
May	34,565	-28,592	5,972	31
June	28,156	-28,592	-437	0
July	24,695	-28,592	-3,898	0
August	26,914	-28,592	-1,678	0
September	33,007	-28,592	4,415	30
October	40,286	-28,592	11,693	31
November	46,578	-28,592	17,986	30
December	49,328	-28,592	20,735	31

[a] NG days is the number of days where the WWTP requires an external fuel input, taken as natural gas. The number of days equals the total number of days in the month.

The next question is: how do we use this average heat balance in WW LCI, on a wastewater component basis? We use it to obtain the following data:

- The country-specific heat energy demand for treating sludge in anaerobic digestion, in MJ/kg dry mass sent to digestion.
- The country-specific heat energy demand for miscellaneous purposes, in MJ/kg component in a WWTP.
- The country-specific marginal heat mix, composed of a percentage of biogas combustion and natural gas combustion.

The country-specific heat energy demand for treating sludge in anaerobic digestion, in MJ/kg dry mass sent to digestion, is calculated as:

$$\text{Heat sludge (MJ/kg dm)} = \frac{(\text{Losses} + \text{Sludge heating}) \cdot 0.9}{(5{,}443 + 2{,}722)}$$

Where 5,443 and 2,722 are the amounts, in kg dry mass, of primary and secondary sludge fed to the model digester on a daily basis. This energy demand is calculated on a monthly basis and an annual weighted

average is derived from the 12 months. The numerator is multiplied by 0.9 as in our model it is assumed that 90% of the heat energy demand in the WWTP is associated with the digester. In the example of Russia, Heat sludge is in average 4.32 MJ/kg sludge dry mass. In this way, in WW LCI v3, a wastewater component producing sludge in Russia is attributed this energy demand, which replaces the generic value for Switzerland, of 7.128 MJ/kg sludge dry mass (Doka 2007), used in WW LCI v2. As in WW LCI v2, the model then performs a specific heat balance for each component in wastewater, leading to a net demand or a net surplus per kg component.

The country-specific heat energy demand for miscellaneous purposes, in MJ/kg component in the WWTP, is calculated as:

$$\text{Heat misc. (MJ/kg ww)} = \frac{(\text{Losses} + \text{Sludge heating}) \cdot 0.1}{37{,}800{,}000}$$

Where 37,800,000 is the volume of wastewater (in L or kg) treated daily by the WWTP considered in the anaerobic digestion model. These miscellaneous purposes are assumed to demand 10% of the total heat used by the WWTP, whereby the 0.1 factor in the equation. In the example of Russia, we obtain a value of 1.04E-04 MJ/kg, which replaces the generic value of 9.9E-05 MJ/kg previously derived from Doka (2007) and used in WW LCI v2. This Heat misc. is a generic heat demand in the WWTP and as such it is attributed to all wastewater components entering the plant, on a mass basis. In those cases where the WWTP does not have anaerobic digestion, this parameter is calculated in the same way. As mentioned in the previous paragraph, the model performs a specific heat balance for each component in wastewater, including Heat misc., leading to a net demand or a net surplus per kg component.

Finally, the marginal heat mix is calculated as the contribution in percentage of two possible sources for heat: natural gas or biogas. The percentages of natural gas and biogas are calculated as:

$$\%\text{NG} = \frac{\text{NG days}}{365}$$

$$\%\text{Biogas} = 100\% - \%\text{NG}$$

Where NG days is the total number of days in the year where the plant requires an external input of fuel. In the example of Russia (Table 4) this sum equals 274 days, out of 365 days. In this way, the marginal heat mix for the Russian WWTP is 75% natural gas and 25% biogas.

This marginal heat mix is used as a reflection of the expected source of energy for a marginal heat demand in this WWTP. If we demand the treatment of 1 kg of sludge, we have seen that this requires 4.32 MJ for the anaerobic digestion process in an average Russian WWTP. For simplicity, let's assume that this sludge is inert, so that it is not able to produce any methane with which to offset this demand. The question is: where do the 4.32 MJ come from? The monthly energy balance (Table 4) shows that 75% of the time, the WWTP has a heat deficiency, thus, any marginal increase in heat demand must come from an external fuel. During 25% of the time, namely in the summer season, the opposite is true, i.e. the WWTP shows a heat surplus. In such a situation, a marginal increase in heat demand does not require an external fuel input, but

simply diverting some of the excess heat to the digester rather than dissipating it to the environment. The same thinking is applied in a case where a wastewater component shows a net heat surplus. This happens when this component generates anaerobically degradable sludge, which in turn produces more energy (as methane) than what is needed according to the calculations of Heat sludge and Heat Misc. This wastewater component has a credit and the environmental burdens of this credit are also calculated with the marginal heat mix. A marginal increase in heat availability in this Russian WWTP leads, 75% of the time, to substituting natural gas, whereas 25% of the time an increase in available heat simply involves more heat dissipation, with no environmental burdens associated.

A question that could be asked about this approach is why bother to calculate monthly balances rather than a global annual balance? The benefit of the monthly approach is that it allows us to calculate a more accurate marginal heat mix. We can easily show this with the Russian WWTP example. Based on the numbers in Table 4, it can be calculated that this plant requires 14.3 TJ per year, while it only produces 10.4 TJ per year. This points to an annual heat deficit of 3.9 TJ, whereby NG days = 365. On the other hand, the monthly balance gives us a higher resolution, where we see that in summer the plant is self-sufficient, leading to NG days = 274. Obviously, there is no reason why one should stop at the monthly resolution, one could do the same balances on a daily basis. This could maybe lead us to identify some further days in the year where the plant is also self-sufficient, while this is lost at the monthly resolution. However, collecting and processing 365 temperatures per country would be excessive for the purposes of WW LCI. Also, as we shorten the time frame, i.e. days instead of months, we are more likely to incur in errors if the plants have some kind of biogas storage capacity allowing them to alleviate demand variations.

4.3 Penetration of anaerobic digestion of sludge and cogeneration with biogas

In WW LCI v2 it was considered by default that WWTPs with secondary and tertiary treatment always have anaerobic digestion (AD) of sludge and energy recovery from biogas in a CHP system. This was also the case in the WWTP model prepared by Doka (2007) for ecoinvent v2. In reality, though, many WWTPs apply AD but do not have a CHP system and also many WWTPs do not have AD at all. In WW LCI v3 we have made an attempt to provide, for each country in the database, the following variables:

- The percentage of wastewater treated in WWTPs with AD.
- The percentage of wastewater treated in WWTPs with AD and CHP.

Quantifying these variables for dozens of countries was no easy task, and the results are not entirely satisfactory either, but we argue that they provide a reasonable estimate of how common these technologies are in the target countries. In this document it is not feasible for us to describe in detail how we managed to calculate these percentages for each country. Instead, we describe the main data sources, assumptions and limitations. The results of this analysis are part of WW LCI v3 and they are automatically used every time a country from the database is chosen for an assessment. The detailed calculations are available to the user upon request.

For European countries the percentage of AD was estimated based on two main variables: the annual amount of primary energy produced from biogas in WWTPs and the annual amount of sludge produced. Biogas production in 2016, expressed as ktoe, was obtained from the Biogas Barometer (EurObserv'ER 2017), which publishes this information for the EU28, disaggregated by country and for three sectors

(landfills, sewage, and other e.g. municipal solid waste, agricultural waste). The percentage of sludge treated with AD (%AD) was calculated as:

$$\%AD = \frac{Sludge\_to\_AD}{0.375 \cdot Sludge\_to\_AD + Final\_sludge}$$

Where Sludge_to_AD is our estimate of the amount of raw sludge sent to anaerobic digestion (kg dry mass/year) and Final_sludge is the declared amount of sludge sent for disposal (kg dry mass/year). The value of 0.375 is the ratio of kg total solids destroyed per kg solids sent to anaerobic digestion, which originates from assuming 0.75 kg VSS/kg raw sludge and 50% destruction of VSS in the AD process. The parameter Sludge_to_AD is calculated as:

$$Sludge\_to\_AD\ (kg\ dm/year) = Biogas \cdot 8.625$$

Where Biogas is the annual biogas production as primary energy, in MJ/year, and 8.625 is our estimate of biogas energy produced per unit of raw sludge sent to the AD process, in MJ/kg dry mass. This factor originates from taking the above factor of 0.375 kg solids destroyed/kg dry mass and further assuming 1 m^3 biogas/kg solids destroyed and a net calorific value of 23 MJ/m^3 biogas. Besides the theoretical nature of this calculation procedure, another limitation or source of uncertainty is related to the original data on biogas production and sludge production. Concerning the former, the Biogas Barometer reports biogas production by the sewage sector, but this includes not only municipal but also industrial WWTPs. We tried to compensate this by including industrial sludge production from Eurostat in our calculations, however for most countries industrial sludge is not reported (Eurostat 2018b). Secondly, for reasons we ignore, sludge production for the same country sometimes varies substantially from year to year, even in countries where wastewater infrastructure is already developed and no significant changes should be expected. For example, in Austria in 2014 the amount of sludge (in dry mass) decreased by 11% compared to 2011. In our calculations we did not take these fluctuations into account, always choosing the latest data point available. Last but not least, it must be highlighted that the two sets of data referred to different years, with the biogas data referring to 2016 (latest available), while sludge production ranged from 2009 to 2015 depending on the country.

This approach led to coherent results for 27 out 28 countries, defining coherent results as a value for %AD that does not exceed 100%. The exception was Bulgaria, where we obtained %AD = 101%. In the database we set this to 100%, however we think this is overestimated, maybe due to either the inclusion of biogas production from industrial WWTPs, inaccurate data on sludge production or unrealistic assumptions from our side in the energy and mass balance of the AD process.

The penetration of CHP systems, in the case of EU countries, was based on figure 6 in Kampman et al. (2016), reporting percentage of biogas used for electricity, heat and biomethane. Here we assumed that only use for electricity production represents CHP systems. One limitation of these data is that it reflects the utilization of biogas by the entire biogas industry in each country, which might deviate from the specific WWTP sector.

The calculation procedure presented in the above paragraphs was also applied to Brazil, Korea and Norway, but using IEA (2017) for quantifying annual biogas production and utilization of biogas in CHP systems, while several other sources were used to quantify (sometimes crudely estimate) annual sludge production. For other countries we used technical reports, peer-reviewed literature, conference presentations, etc., often requiring additional assumptions from our side. For example, for US we used the study by ERG (2011) prepared for the USEPA, where it is stated that 60% of wastewater is treated in WWTPs with AD, however the penetration of CHP systems is quantified as installed capacity in MW. We estimated the capacity of the WWTPs with these installed MW assuming 26 kW/Mgal wastewater, based on the theoretical model they present to study the potential of CHP systems in the country. This estimated capacity can be then expressed as a percentage of the country's WWTP capacity as a whole. Another example is Canada, where we only found data for the State of Ontario (Environmental Commissioner of Ontario 2017, p. 138), which we took as a proxy for the entire country. In addition to this, the data for Ontario are reported in percentage of facilities, without weighting for their capacity. In developing countries, data availability for this topic is not good either. In many countries the wastewater treatment sector is in such an early stage of development that the lack of information is just a reflection of the lack of this kind of infrastructure in the first place; in many cases we assumed there is 0% AD, for example Tanzania and Pakistan. In other countries, the lack of AD and CHP infrastructure is supported by actual reports, for example in Saudi Arabia (Saudi Arabian Water Environment Association 2013) while in other countries where AD is applied, it was necessary to get down to the level of investigating which individual facilities have installed AD systems, as was the case for Ukraine and Russia, among others.

Overall, our percentages of AD and CHP, shown in Table 5 can be considered as a starting point, in spite of the substantial uncertainty. It is probably realistic to accept the difference in %AD between US (60%) and Egypt (15%), but not so much between US (60%) and Finland (43%). On top of this, the percentage of CHP is even more uncertain, as it adds up the uncertainty of the existence of CHP systems on top of that related to the existence of AD.

Table 5. Estimates for the penetration of anaerobic digestion and cogeneration in urban wastewater treatment.

Country	Wastewater treatment in WWTPs with	
	AD	AD + CHP
Argentina	0%	0%
Austria	22%	15%
Australia	38%	21%
Bosnia Herzegovina	100%	0%
Bangladesh	0%	0%
Belgium	60%	50%
Bulgaria	100%	100%
Brazil	11%	8%
Canada	29%	7%
Switzerland	89%	21%
Chile	10%	0%
Colombia	58%	42%
China	0%	0%
Costa Rica	0%	0%
Cyprus	0%	0%
Czech Republic	70%	67%
Germany	53%	36%
Denmark	50%	25%
Estonia	0%	0%
Egypt	15%	0%
Spain	25%	25%
Ethiopia	0%	0%
Finland	43%	10%
France	17%	14%
United Kingdom	95%	87%
Greece	55%	55%
Croatia	60%	43%
Hungary	47%	38%
Indonesia	0%	0%
Ireland	18%	18%
Israel	5%	5%
India	0%	0%
Iran	6%	6%
Iceland	0%	0%
Italy	23%	9%
Japan	0%	0%
Republic of Korea	24%	10%
Lithuania	61%	34%
Luxembourg	83%	48%
Latvia	46%	31%
Montenegro	0%	0%
Former Yugoslav Republic of Macedonia	0%	0%
Malta	55%	30%
Mexico	15%	15%
Malaysia	0%	0%
Nigeria	0%	0%
The Netherlands	43%	21%
Norway	63%	6%
New Zealand	20%	20%
Peru	2%	0%
Philippines	0%	0%
Pakistan	0%	0%
Poland	43%	37%
Portugal	4%	4%
Romania	0.12%	0.05%
Serbia	0%	0%

Country	Wastewater treatment in WWTPs with	
	AD	AD + CHP
Russia	9%	9%
Saudi Arabia	0%	0%
Sweden	96%	3%
Slovenia	32%	32%
Slovakia	86%	73%
Thailand	0%	0%
Turkey	37%	35%
Taiwan	0%	0%
Tanzania	0%	0%
Ukraine	36%	36%
United states	60%	27%
Vietnam	0%	0%
South Africa	57%	0%

4.4 Fugitive methane emissions from biogas flaring at WWTPs.

In WW LCI v2, fugitive emissions of methane from combustion of biogas in WWTPs were calculated with an emission factor of 1E-04 kg methane/MJ, from Dalemo et al. (1997). With a net calorific value for methane of 50 MJ/kg, this represents a fugitive emission rate of 0.5%. In WW LCI v3 we aim at clearly differentiating two situations: 1) combustion of the biogas in boilers or CHP systems and 2) combustion in flares. The reason to differentiate these two situations is that while the first one represents a very efficient combustion, the second one does not. According to a study by Willis et al. (2013) in the US, the combustion efficiency of flares is much lower, being affected by a low exit velocity of the fuel and environmental factors such as wind velocity, atmospheric pressure and humidity. They calculated this efficiency for two WWTPs in the US as 95.5% and 94.5%. Based on these data, we take an average value of 95%, meaning an emission factor for flares of 0.001 kg methane/MJ. For combustion in boilers or CHP systems, we take the emission factor from the ecoinvent data set for cogeneration with biogas (heat and power co-generation, biogas, gas engine), which is calculated as 5.2285E-04 kg methane for 1 m^3 biogas with 22.73 MJ net calorific value, leading to an emission factor of 2.3E-05 kg methane/MJ, representing a fugitive emission rate of 0.12%. Other emissions to air from these two combustion systems remain unchanged from WW LCI v2.

In order to implement these new emission factors in WW LCI v3, we consider the following:

- In WWTPs with CHP systems, the marginal combustion process is 100% in the CHP system and 0% flaring. This is justified by the fact that when CHP systems are installed, these are kept running as far as possible. Even if there is an excess of heat for the digesters, the plant will try to maximize the electricity output. This is backed by ERG (2011), stating that *"…CHP results in more beneficial use of the digester gas. For example, the Town of Lewiston, NY, indicated that prior to implementing CHP, its boiler used only 40 to 50 percent of the gas, whereas with the CHP system, gas utilization reached 98 percent*".
- When a WWTP does not have a CHP system but only a boiler for heat production, the marginal combustion process is established based on the same procedure described in section 4.2, i.e. when a plant produces heat in excess, a marginal increase in biogas production leads to increased flaring, whereas when the plant has a heat deficit, a marginal increase in biogas production leads to increased combustion in the boiler.

The weighted emission factor for fugitive emissions of methane in a country is finally calculated as:

$$E_{CH4} = 2.3E\text{-}05 \cdot \frac{\%CHP}{\%AD} + 0.001 \cdot \left(1 - \frac{\%CHP}{\%AD}\right) \cdot \%NG_{boiler}$$

Where E_{CH4} is the country-specific fugitive methane emission factor, in kg methane/MJ. %CHP is the percentage of wastewater treated in WWTPs with AD and CHP systems and $\%NG_{boiler}$ is the percentage of days in a year that a WWTP with AD and boiler relies on an external fuel (natural gas).

4.5 Determination of moisture content in dewatered sludge

In this section we document a feature already available in WW LCI v2, but implemented after the publication by Kalbar et al. (2018). Thus, we take the opportunity in this document to report it.

In WW LCI v1 the moisture content of sludge was specific for each chemical substance assessed with the model, depending on whether the chemical was converted into sludge biomass, or on whether the sludge was constituted by the chemical itself being partitioned to the solids phase, or both. Also, for the chemical 'water', the amount of this substance ending up in dewatered sludge was calculated specifically, using as a default a factor of 0.4% partitioning to sludge (which needed to be entered by the user in the sheet 'WWTP input', under F_{sludge}) and a water removal factor during dewatering. Although we initially thought this approach was good for individual chemicals, during our testing with chemical mixtures we realized that it led to strange results: the sludge moisture was dependent on the amount of water in the chemical mixture. In this way, a very concentrated wastewater ended up with a sludge that had little moisture, whereas a dilute wastewater appeared to have a very moist sludge. In reality, the sludge produced by urban WWTPs is not found to be affected so much by the concentration of pollutants in wastewater, but by the dewatering technology, being typically between 20%-40%. We changed the modelling of moisture content in sludge, as follows:

- For the chemical 'water', the amount of sludge is set to zero. WWTPs do not create sludge because of the component 'water' in wastewater, but because of the pollution that goes along with it. Although some water ends up in the dewatered sludge, in the model this water flow is not attributed to 'water' as input chemical. As opposed to WW LCI v2, in WW LCI v3 the user does not need to use the value F_{sludge}= 0.4% in the 'WWTP input' sheet when modelling this chemical. All fate factors for 'water' can be left blank instead.
- For all other chemical substances, the amount of sludge (in dry mass) is chemical-specific, but the moisture content of the dewatered sludge is fixed, according to the parameter 'Solids in dewatered sludge (%)' in the 'Parameters' sheet. The default value for this parameter in WWTPs is 30% (it is different for septic tanks). Thus, a chemical creating 0.3 kg sludge in dry mass will use 0.7 kg water to make 1 kg sludge in wet weight leaving the WWTP for disposal. For each chemical a water balance is established in the WWTP and depending on the overall balance, this amount of water can be reflected in the LCI as a negative water emission, meaning that this is a volume of water "removed' from the water phase.

4.6 Inclusion of the complete life cycle of polyelectrolyte used by WWTPs

In WW LCI v3 we introduce the consumption of polyelectrolyte as an aid for sludge dewatering. We consider a consumption of 3.5 g per kg of sludge in dry mass (Andreoli et al. 2007, table 5.5). The production of this chemical is modelled by means of the ecoinvent's global market data set for polyacrylamide. However, the model does not stop here, since the polyelectrolyte becomes a component in sludge for disposal. This means we need to be able to model what happens to this component when the sludge is subject to different disposal options. We have solved this by incorporating polyelectrolyte in the complete mass flow analysis of WW LCI, but including it only in those activities related to sludge disposal.

Polyelectrolyte is considered in the model to have the formula of acrylamide (C_3H_5NO). Its carbon is labelled as fossil and the substance is considered as not readily degradable in landfills or during composting. When sludge or compost from sludge is used as a fertilizer in agriculture, an emission of acrylamide to soil is displayed in the inventory. The fate of acrylamide once in soil is determined according to USES-LCA fate factors, just like with any other substance present in wastewater. The physical-chemical properties of acrylamide needed to run USES-LCA can be seen in the tab 'USESLCA input', at the bottom row of the main table. These data were obtained from the USEtox 2.02 database on organics (USEtox 2018), except Koc and melting point, which were taken from the USES-LCA 2.0 database (Van Zelm et al. 2009).

The LCI of any wastewater discharge that generates sludge displays a new input from technosphere, called 'polyelectrolyte production and disposal with sludge', that includes polyelectrolyte production (with the ecoinvent global market data set) and its end of life as one more component of wastewater sludge. This LCI is not a static, terminated LCI, but a dynamic one as it changes according to the sludge disposal scenario.

4.7 Calculation of sludge calorific value

In this section we document a feature already available in WW LCI v2, but implemented after the publication by Kalbar et al. (2018). Thus, we take the opportunity in this document to report it.

In WW LCI v1 (and the first releases of WW LCI v2) the calculation of the calorific value of sludge was leading in many cases to underestimated values. This was partly based to the lack of a fully stoichiometric balance in the anaerobic digestion process (now solved as described in section 4.1), as well as to an incorrect consideration of water in the calorific value calculations.

In WW LCI v3 the low heating value (LHV) of sludge, in MJ/kg, is calculated with the following formulae:

$$LHV = HHV - 2.447 \cdot (W + 9H)$$

$$HHV = 34.016 \cdot C - 9.8324 \cdot O + 124.265 \cdot H + 6.276 \cdot N + 19.079 \cdot S$$

Where HHV is the high heating value (HHV), in MJ/kg, W is the moisture content in sludge, in kg water/kg, H is the hydrogen content in sludge, excluding that from moisture, in kg H/kg, C is the carbon content in

sludge, in kg C/kg, O is the oxygen content in sludge, excluding that from moisture, in kg O/kg, N is the nitrogen content in sludge, in kg N/kg and S is the sulfur content in sludge, in kg S/kg.

The second equation calculates the total heating value of the fuel, whereas the first one adjusts this value by subtracting the latent heat of evaporation for water (44.03 kJ/mol) initially present in the fuel or formed during combustion. The HHV equation is obtained from Muñoz et al. (2007).

4.8 Sludge drying

In this section we document a feature already available in WW LCI v2, but implemented after the publication by Kalbar et al. (2018). Thus, we take the opportunity in this document to report it.

Sludge is not a good fuel unless it is dried to a certain level. In WW LCI v.1 we assumed that dewatered sludge was directly incinerated. We now consider an additional thermal drying step before incineration (in the incineration plant itself), where we account for the specific heat and electricity demand to evaporate water in the sludge, based on the following data from Doblado (2004):

- 3.6 MJ thermal energy are used per kg water evaporated.
- 0.1 kWh electricity are used per kg water evaporated.

As a default, sludge is dried from 30% dry mass to 90% dry mass. Then the dry sludge is fed to the incinerator. An overall drying+incineration energy balance is established, which might lead to a net energy surplus or not depending on the composition of the sludge, which dictates its calorific value as explained in the previous section.

4.9 Inclusion of uncontrolled landfilling of sludge

A common issue in LCA is that, due to the lack of appropriate inventory data, we often represent economic activities with surrogates that can be considered as poor substitutes, given that they represent completely different realities. The whole area of waste management is a clear example of this: for example representing the management of electronic scrap waste in a developing country with LCI data from Switzerland. Although WW LCI itself is part of the solution to this problem, at least in the area of urban wastewater, we are also affected by this issue, and one of the affected areas is landfilling of sludge. WW LCI v2 calculates an LCI for landfilling of sludge based on the sanitary landfill model developed by Gabor Doka for ecoinvent v2 (Doka 2007). This model represents a modern landfill built with Swiss standards, including bottom liner, waste compaction, landfill gas capture with energy recovery, soil covers and managed renaturation after operation. Facilities like the one just described can only be expected, besides Switzerland, in the world's advanced economies, yet this is the model we have applied in WW LCI for any country in the world sending sludge to landfills. In WW LCI v3 we have attempted to address this, by adapting Doka's model to represent an unmanaged landfill, whereby WW LCI now supports the two landfill systems: controlled and uncontrolled.

The adaptation was done by changing certain settings in the original sanitary landfill model, programmed by Gabor Doka in Excel. The LCI results with these new settings were then imported to WW LCI in the tab 'Sludge landfill LCI calc'. Below we describe the main changes made:

- We excluded all inputs from technosphere originally included in the model (infrastructure, auxiliary materials, etc.).
- We corrected methane production by assuming a lower production, following the IPCC's guidance on MCF for landfills (Pipatti et al. 2006, Table 3.1). We chose an MCF of 0.8, corresponding to 'Unmanaged solid waste disposal sites – deep and/or with high water table'. The original ecoinvent model corresponds to a 'Managed – anaerobic' landfill, with an (implicit) MCF of 1, therefore we implemented the MCF of 0.8 by reducing methane production by 20% in the original model. This methane gap is corrected in the landfill gas balance by adding the corresponding amount of CO_2, so that the total carbon released in the gas stays the same.
- We set to zero the methane capture. This means all the methane produced in the landfill escapes to the atmosphere.
- Leachate collection and treatment is set to zero. This only affects the landfill emissions through leachate during the first 100 years, which is the period under which the landfill is assumed to be controlled. The Long-term emissions, i.e. those taking place after 100 years, stay the same as in the original ecoinvent model.
- Land occupation in the uncontrolled landfill is calculated assuming a landfill height of 10 m, a waste density of 1000 kg/m^3 and an operational life of 15 years. This leads to an occupation of 0.0015 m^2year per kg waste. We use the flow 'Occupation, dump site' in the LCI.

Once we have two options for landfilling, the next step is to decide how to choose one or the other, or how to combine them. This is explained in section 4.11.

4.10 Inclusion of volatilization in sludge composting

The implementation of sludge composting in WW LCI v2 included two possible options for the fate of substances present in sludge, namely partial degradation or persistence in the compost. A third option of relevance is the direct emission to air in the case of volatile substances. Compost piles can reach temperatures of up to 60-70 ºC, conditions which promote volatilization. We think this is an important fate to take into account in the model, since neglecting volatilization leads to erroneously assuming that such volatile substances are finally emitted to soil with the produced compost, when in reality they might have been simply emitted to the atmosphere from the compost pile.

In WW LCI v3 we have included volatilization in sludge composting, based on data from the composting LCI model by Sonesson (1996), who assumed that volatile organic carbon (VOC) is lost from the compost pile by 98.7%, and that this is due to volatilization (75%) and degradation (25%). In the model we apply these factors for substances which are both volatile and degradable, whereas in the case of volatile but non-degradable substances we choose to totally attribute the losses (98.7%) to volatilization. We define volatile substances following the criterion by the EU VOC Solvents Directive (1999/13), which defined VOC by their vapour pressure, i.e. a substance is volatile if its vapour pressure is 10 Pa or more at 293.15 K. Vapour pressure is already a required parameter in the model, in order to model fate of substances in the environment (in sheet 'USESLCA input'), therefore this does not involve additional data search effort for the user.

Table 6 below shows a summary of the applied fate factors in the sludge composting model, for the four supported combinations of degradability and volatility.

Table 6. Fate of chemical substances in sludge composting as a function of volatility and degradability.

Degradability	Volatility	
	Volatile	Non-volatile
Degradable	Fraction volatilized = 98.7% · 75% = 74% Fraction degraded = 98.7% · 25% = 24.7% Fraction in compost = 1.3%	Fraction volatilized = 0% Fraction degraded = 65% Fraction in compost = 35%
Non-degradable	Fraction volatilized = 98.7% · 100% = 98.7% Fraction degraded = 98.7% · 0% = 0% Fraction in compost = 1.3%	Fraction volatilized = 0% Fraction degraded = 0% Fraction in compost = 100%

4.11 Inclusion of a controlled/uncontrolled landfill mix

We have not found any statistics or studies covering sludge landfilling practices in different countries. In order to overcome this problem, we have attempted to estimate these practices, assuming that the level of control in landfilling of sludge in a country is correlated with the level of economic development, which we measure as the gross national income (GNI) per capita, with data from the World Bank (2018). We expect developed countries to rely on controlled landfills, whereas developing countries are expected to rely mainly on uncontrolled landfills. We have established the following key GNI levels:

- We define a GNI level of 35,000 USD per capita as the point at which 100% of the landfilling activity takes place in controlled facilities. This leaves out certain countries classified as advanced economies by the IMF, such as Italy (31,020 USD per capita) Spain (27,180 USD per capita) or Greece (18,090USD per capita). There is evidence, though, that landfilling of solid waste in these countries still happens (probably to a low extent) under uncontrolled conditions (see Revuelta 2017; Reuters 2014; Perchard 2016).
- We define a GNI level of 2,500 USD per capita as the point below which 0% of the landfilling activity takes place in controlled facilities. Under this threshold we find countries such as India (1,820 USD per capita) Vietnam (2,170 USD per capita) or Ukraine (2,390 USD per capita).

Based on the two coordinates above (x, y): (35000, 1), (2500, 0) and (0, 0) we defined a logistic curve with the online calculator at AAT Bioquest (2018), leading to the curve in Figure 6, where we show how several countries fit into this model. This function allows us to calculate the percentage of controlled landfilling, whereas the difference between this and 100% is the percentage of uncontrolled landfilling.

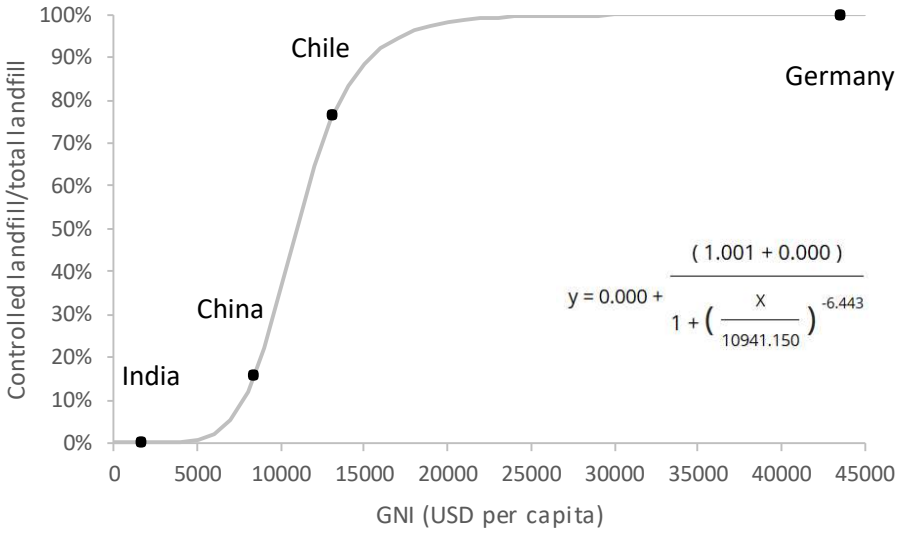

Figure 6. Curve used to estimate the 'landfill mix'. As GNI increases, so does the percentage of sludge to controlled landfills respect to total landfilling. Regression equation obtained with the online calculator at AAT Bioquest (2018).

The uncertainty of this approach is quite low in our opinion for those countries with GNI under 2,500 USD per capita or above 35,000 USD per capita, but rather high for those located in between. Also, another source of uncertainty in this approach is that landfilling as such is modelled with two extremes: a state-of-the-art Swiss landfill and what could be defined as an open dump. In reality, between these 'black and whites' there are 'shades of grey', since there are landfills which are not state of the art but might have some improvements over an open dump, such as a daily soil cover, or collection of methane for flaring. The latest approach by ecoinvent for solid waste (Doka 2018), which inspired us to address this topic, actually includes three landfill levels: open dump, unsanitary landfill and sanitary landfill. We admit such an approach is clearly better, since besides 'black' and 'white', at least there is a 'grey' option. For the purposes of WW LCI, though, including three landfill options was judged at this point as excessive, given that in many countries landfilling of sludge is not so relevant. In spite of these limitations, we think our approach still provides a better answer than our previous approach, where a modern sanitary landfill was considered in all countries. Last but not least, this landfill mix is provided to the WW LCI user as a way of having a mix by default. The sludge disposal scenario as a whole, including the share of controlled/uncontrolled landfill, can be modified by the user to represent other specific conditions.

5 Changes to the calculation of methane emitted from untreated and treated wastewater

5.1 Methane emissions from direct discharges through open sewers

The IPCC guidelines on GHG emissions for wastewater treatment and discharge (Doorn et al. 2006, Table 6.3) propose an MCF of 0.5 for direct discharges through stagnant sewers, which are further described as 'open and warm'. This is explained as follows:

"Sewers may be open or closed. In urban areas in developing countries and some developed countries, sewer systems often consist of networks of open canals, gutters, and ditches, which are referred to as open sewers." Also: "Wastewater in closed, underground sewers is not believed to be a significant source of CH_4. The situation is different for wastewater in open sewers, because it is subject to heating from the sun and the sewers may be stagnant allowing for anaerobic conditions to emit CH_4" (Doorn et al. 2006, p. 6.6).

From our point of view, the implementation of this approach in WW LCI faces two challenges:

1. How do we identify the existence of open, stagnant sewers in different countries?
2. Is it reasonable to apply the same MCF to open, stagnant sewers in countries with completely different climate?

The difficulty related to the first question is that national statistics and reports on the status of sanitation in different countries provide figures on the access of population to sewers, but not on their state of preservation or on whether the available sewers are open or closed. Further, in the WW LCI database we quantify direct discharges through sewers which are not connected to WWTPs and through so-called independent collection systems, which in practice refer to a situation where population have neither access to a sewer nor to on-site treatment (e.g. septic tanks). The question is, if we stick to how the MCF is proposed to be applied by the IPCC report, direct discharges through sewers are potentially eligible for an MCF of 0.5, while direct discharges without a sewer are not. We argue that reality might be closer to the opposite assumption, that is, that when discharges take place through sewers (as reported in sanitation statistics, etc.), the likelihood of methane formation is lower than when no sewer is available and improvised, poorly maintained drainage structures are used (see Figure 7).

Figure 7. Images of open sewers. Top left: Bangkok, Thailand; Top right: Bangalore, India; Bottom left: Kinshasa, Democratic Republic of Congo; Bottom-right: Ramadi, Iraq. All images from: https://www.crookedbrains.net/2008/01/open-sewers-of-world.html.

Our interpretation is that access to sewers, as reported in country statistics, sanitations reports, etc., most likely corresponds to what the IPCC calls 'Flowing sewer (open or closed)', with an MCF of zero, whereas it is the absence of a public sewer what most likely will lead to stagnant, anaerobic drainage. This, we think, is the most reasonable way to incorporate the MCF for open sewers in WW LCI v3. In summary, we choose to consider this MCF only when direct discharges take place in the absence of sewers, a situation which in WW LCI is classified as 'Independent wastewater collecting systems - without treatment'.

Furthermore, we differentiate two situations, which are substance-dependent:

- The organic substance discharged through open sewers is anaerobically degradable.
- The organic substance discharged through open sewers is not anaerobically degradable.

Anaerobic degradability is an input parameter that the user of WW LCI must provide in the 'WWTP input' tab. We only apply the MCF for open sewers in the first case, that is, when there is a relatively high likelihood that the affected substance undergoes degradation in anaerobic conditions, based on its chemistry.

In summary, we apply the MCF for open sewers to an organic substance in wastewater when:

1. It is discharged without treatment through an independent collection system, and
2. It is declared by the WW LCI user as an anaerobically degradable substance.

If these two conditions are not met, the MCFs for direct discharges through closed sewers apply instead (described in section 5.1) and thus methane production for the affected organic substance is the same through open and closed sewers.

The second question we faced when implementing this MCF is whether it makes sense that all countries should be attributed the same MCF value, of 0.5. We contacted Michiel Doorn (lead author of the IPCC report on wastewater treatment and discharge, Doorn et al. 2006) to discuss this issue. To the question of whether or not climate is an important variable, for example to differentiate emissions in countries like Russia and India, Mr Doorn kindly replied, stating:

"You are right that a hot climate would enhance rapid anaerobic conditions to manifest, as would stagnant water" and also "I agree with you that Russia would be very different than India for reasons of climate and perhaps infrastructure. Basically, the MCF was an educated guess" (Doorn 2018).

Based on this, we decided to incorporate climatic conditions as part of the determination of the MCF for open sewers. Chaosakul et al. (2014) proposed a model for methane production in sewers, as a function of wastewater temperature, the area of biofilm formed in the sewer surface and the sewer's hydraulic retention time (HRT). The effect of temperature in this model can be isolated as the coefficient $1.05^{(T-20)}$, where T is the wastewater temperature (ºC). The MCF proposed by the IPCC ranges between 0.4 and 0.8; we take a value of 0.75 as a worst case (Doorn and Liles 1999). By this, we mean that an average MCF of 0.75 is only attributed to the warmest country, which happens to be Mali according to Weatherbase (2018), with a mean annual air temperature of 28.2 ºC. We calculate the climate-weighted MCF for open sewers in country 'i' as:

$$MCF_{open,\,i} = 0.75 \cdot \frac{1.05^{(T_i - 20)}}{1.05^{(28.2 - 20)}}$$

Where T_i is the mean annual air temperature in country 'i', which we obtain from Weatherbase (2018). Here we need to highlight that while the original model from Chaosakul et al. (2014) uses wastewater temperature, we use air temperature instead. Usually, wastewater in sewers is warmer than air (see Figure 5) and it is subject to less temperature variability, but this is typically the case in closed, underground sewers, whereas here we address open sewers, which are expected to be subject to wider temperature variations and closer to the air temperature. For this reason, we take air temperature as a proxy for

wastewater temperature in this particular context. With this approach, the MCF for open sewers can be plotted as a function of temperature as shown in Figure 8. We can see that in Russia the MCF is 0.18, while for India this increases to 0.62.

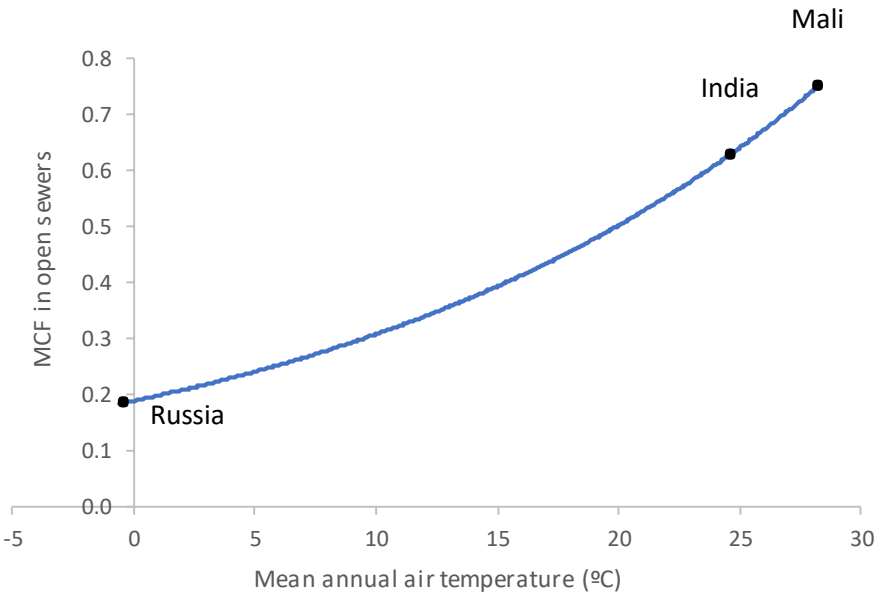

Figure 8. MCF for open sewers as a function of mean annual temperature, as implemented in WW LCI v3.

We consider that our approach for emissions from open sewers improves on the default generic value proposed by the IPCC, although still has some limitations. The MCF is related only to climate (mean air temperature), whereas other factors could be relevant, like the status of infrastructure as pointed out to us by Michiel Doorn. Also, our approach does not include emissions from closed sewers, which are known to exist, in spite of the IPCC guidelines proposing an MCF of zero for this situation (see Chaosakul et al. 2014; Guisasola et al. 2007). Unfortunately, including such emissions from closed sewers in WW LCI would imply extensive work, since they would require a full stoichiometric balance for the chemical transformations in the sewer, the results of which would have to be linked to the WWTP calculations. In the case of open sewers this is not necessary, since any emissions from the latter are directed to the environment and not to a technosphere process.

5.2 Methane emissions from direct discharges through closed sewers and from treated effluents

In WW LCI, when a substance is discharged to the aquatic environment either through the sewer or as a treated effluent, its degradation in the different environmental compartments (water, air, soil) is evaluated with USES-LCA. The most common situation is that substances discharged to the aquatic environment eventually degrade mostly in this same compartment (unless the substance is very volatile, very hydrophobic or very persistent). In WW LCI v2 the degradation of chemicals in the water compartment was considered to take place 90% of the time under aerobic conditions and 10% of the time under anaerobic conditions, the latter leading to some methane formation. This was based on Muñoz et al. (2013), which in

turn was based on the IPCC's methane correction factor (MCF) of 0.1 for 'sea, river and lake discharge', justified by the IPCC as 'Rivers with high organics loadings can turn anaerobic' (Doorn et al. 2006, Table 6.3). However, in our interpretation of this parameter in the IPCC report we missed the heading just above this MCF, reading 'Untreated system'. This means the MCF of 0.1 is meant only for cases where organic matter is discharged to the environment without any previous treatment, whereas in our model we have been applying it to all discharges of organic matter, regardless of whether or not they have been subject to treatment.

We have attempted to make these two views meet: on the one hand, even if we treat a wastewater, its impact in the receiving environment might not be zero as the IPCC suggests, but it could also be associated to a MCF lower than 0.1. The IPCC attributes the MCF of direct discharges to the 'high organics loadings' in receiving waters, and one could argue that this is correlated to the (lack of) development of the local wastewater treatment sector, i.e. the lack of WWTPs leads to high organic loadings in rivers. Thus, it seems reasonable to expect lower MCF values in river basins, estuaries, etc., where wastewater is properly treated, and vice versa. In WW LCI v3 we propose the MCF for the water environment to move from a static value of 0.1 to a variable, dependent on the country-specific status of the wastewater treatment sector, the latter measured as the percentage of COD removed. Based on Doorn et al. (2006, Table 6.3), the MCF is expected to range from 0 to 0.2. We take a value of 0.15 as the worst case and 0 as the best case. Assuming a linear relationship between MCF and COD removal, we can express MCF as:

$$MCF_{w,i} = 0.15 \cdot \left(1 - \frac{0.35 \cdot \%_{prim\text{-}sep} + 0.90 \cdot \%_{sec} + 0.95 \cdot \%_{tert}}{0.95} \right)$$

Where $MCF_{w,i}$ is the methane correction factor for direct discharges through closed sewers or treated effluents in country 'i' and $\%_{prim\text{-}sep}$, $\%_{sec}$ and $\%_{tert}$ are the percentages of urban wastewater in country 'i' treated in septic tanks or WWTP with primary treatment only, WWTP with secondary treatment and WWTP with tertiary treatment, respectively. These percentages are obtained from the WW LCI database. The factors 0.35, 0.90 and 0.95 represent typical COD removal levels (expressed as a fraction from 0 to 1) achieved by the corresponding treatment options, obtained from Von Sperling (2007b, table 4.9).

This simple function allows us to go beyond the site-generic MCF_w of 0.1 as suggested by the IPCC for direct discharges, while still keeping the principle that in a context where wastewater is treated properly, the impact in the aquatic environment should be lower. A country where 100% of urban wastewater is treated with tertiary treatment obtains a MCF_w of 0, in line with the IPCC factor for aerobically treated wastewater, whereas the opposite leads to a value of 0.15. Also, it is interesting to note that this approach fits coherently with the approach for open sewers. If we compare the worst case for MCF_w of 0.15 with the lowest MCF_{open}, which corresponds to Russia and equals 0.18, we see that according to the model, even in the most extreme cases, discharging untreated wastewater through a closed sewer is better (in methane formation terms) than discharging through an open sewer.

5.3 Summary of MCF choices

Figure 9 below attempts to provide a clear picture of which MCF is used in WW LCI v3 in each of the wastewater discharge situations currently supported by the model, as described in the two previous

sections. Organic substances in wastewater, once discharged to the aquatic environment, either untreated or after treatment, can undergo degradation in the water column, sediments, air, or soil. The extent of each of these degradation routes is assessed in WW LCI by manually running the USES-LCA fate model, leading to the degradation fractions Deg_a, Deg_w, Deg_{sed} and Deg_s. When USES-LCA predicts degradation in the water column or in sediments, we apply methane correction factors, chosen as displayed in the figure. We can simplify the explanation of the figure by stating that the MCF for sediments (receiving a generic value of 0.5 as in WW LCI v2) and the country-specific MCF_w (section 5.2) apply in all cases, except when, as explained in section 5.1, we have an anaerobically degradable organic substance channelled through independent collection without treatment. We identify this situation as having degradable organic matter in an open sewer. In this case we apply MCF_{open}, indistinctly to the fraction of substance expected to degrade in the water column or in sediments.

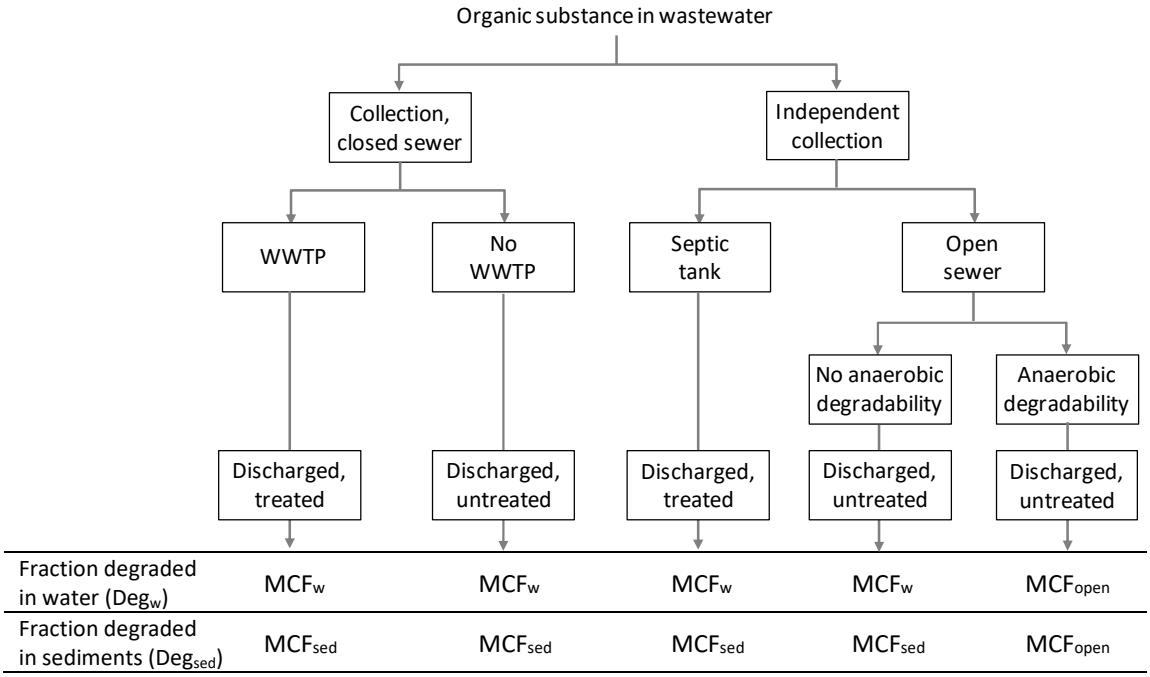

Figure 9. Diagram showing the use of methane correction factors (MCFs) in WW LCI v3 for each of the wastewater discharge situations supported by the model

6 Other changes

6.1 Inclusion of sub-compartments for all emissions

For emissions to air, water and soil inventoried in WW LCI v3, other than those discussed in section 3.6, we have now specified the corresponding sub-compartment:

- For air emissions: high population/low population.
- For water emissions: river/groundwater/groundwater-long term.
- For soil emissions: agricultural.

The sub-compartment for emissions to air occurring in the WWTP has been chosen taking the same assumptions as in ecoinvent for this same activity (urban wastewater treatment), that is, that emissions take place in a high-population density location. Emissions associated to landfilling and incineration also mirror the implementation of these activities in ecoinvent. In fact, the emission sub-compartments were already provided by the original models developed by Doka (2007). For emissions during composting, we use the same sub-compartments as in the ecoinvent data set for biowaste composting, which considers emissions to take place in a high-population density location. Finally, the only emissions to soil reported by WW LCI v3 in its foreground system are those related to sludge landfarming, which we label as emissions to agricultural soil.

6.2 Inclusion of seawater as emission compartment in USES-LCA

As described in section 3.6, now in WW LCI v3 it is possible to specify whether an emission in wastewater takes place in freshwater or in seawater. The evaluation of degradation of substances once discharged to the environment is done with USES-LCA, the fate model embedded in WW LCI. In WW LCI v2 any emission to the aquatic environment was modelled in USES-LCA as an emission to continental freshwater. In order to be consistent with the new differentiation of freshwater vs. seawater discharges, we have added continental seawater as an additional emission compartment when we use USES-LCA. This can be seen in the tab 'USESLCA input', row 42, where the existing drop-down menu now displays 'seawater' as an emission compartment. When we choose this option, the USES-LCA fate model (hidden in several tabs) now considers that the emission takes place through continental seawater.

The output from USES-LCA is a set of fractions (Deg_a, Deg_w, Deg_{sed}, Deg_s), expressing the share of degradation for a given organic substance in different environmental compartments (air, water, sediments, soil). Even though we have added one more emission compartment (seawater), the number of compartments where degradation is evaluated remains the same four, i.e. we do not further specify if degradation takes place in freshwater vs. seawater, or in freshwater sediments vs sea sediments. This is because the calculations in which these fractions are used (based on Muñoz et al. 2013) do not differentiate between seawater and freshwater.

The implications for the user of this development are mainly that, when assessing a given chemical with WW LCI, if the wastewater scenario involves seawater discharges as well as freshwater discharges, this means that the user needs to run the USES-LCA simulation for the seawater compartment as well, and (as usual) paste the simulation results in the corresponding section of the 'WWTP input' tab.

6.3 Ecoinvent 3.4 as background database

The background system in WW LCI v3 has been linked to the latest ecoinvent database version available in the SimaPro software, namely v3.4. All activities are linked to the consequential system model in this database.

6.4 Corrected market data set for nitrogen fertilizer in ecoinvent

As a default, WW LCI links to ecoinvent's market data set for nitrogen fertilizer. However, we realized in 2014 that this market mix has too high contributions from calcium nitrate and calcium ammonium nitrate. The consequence of this is that the impact of N fertilizer use is higher than it should be, leading in WW LCI to overestimating the benefits from reusing sludge in agriculture.

Due to this issue, for WW LCI v3 we have prepared an alternative market mix for N fertilizers, that is available for the user to get more accurate LCI data on this process. We extracted global N consumption from IFASTAT (2019) for years 2016, 2007 and calculated a marginal N fertilizer mix by looking at the trend for each fertilizer in this period; only those fertilizers with a positive growth trend in this period become part of the marginal mix, to which they contribute according to how much they have grown in that period.

Table 7. Calculation of a marginal and average global mix for N fertilizer use, based on IFASTAT data.

Product	2007 (thousand tonnes)[a]	2016 (thousand tonnes)[a]	2007-2016 trend (thousand tonnes)	Contribution to trend if positive (thousand tonnes)	Marginal mix 2007-2016	Average mix 2016
Ammonia dir. applic. (N)	12,177	11,850	-327	-	0%	4%
Ammonium nitrate (N)	15,149	20,149	4,999	4,999	11%	6%
Ammonium sulphate (N)	8,313	10,590	2,277	2,277	5%	3%
Calc. amm. nitrate (N)	10,174	10,140	-34	-	0%	3%
Nitrogen solutions (N)	13,894	17,234	3,341	3,341	7%	5%
Other N straight (N)	19,813	8,530	-11,282	-	0%	3%
Urea (N)	135,353	151,517	16,163	16,163	35%	48%
Ammonium phosphate (N)	16,125	21,736	5,611	5,611	12%	7%
N K compound (N)	389	1,650	1,262	1,262	3%	1%
N P K compound (N)	44,960	54,769	9,808	9,808	21%	17%
Other NP (N)	4,466	7,750	3,285	3,285	7%	2%
Total	280,813	315,915	35,102	46,746	100%	100%

[a] IFASTAT (2019).

As it can be seen in Table 7, on the one hand, according to the IFASTAT data, calcium nitrate is not even recorded as one of the main fertilizers. On the other hand, regardless of whether one takes a marginal or an average approach, the main N fertilizer globally is urea, followed by multi-nutrient NPK fertilizers.

The global marginal mix for N fertilizers in Table 7 is the one we recommend for use with WW LCI. Nevertheless, for those users interested in an attributional approach, we also provide the average mix for 2016, however in this case the ecoinvent market mix we provide does not exactly match the one shown in Table 7, since the attributional mix in ecoinvent also includes inputs of organic fertilizers (manure, compost, etc.), which are not part of IFASTAT data. In our procedure to create a corrected average market data set we left the default inputs of organic fertilizers as they are in the original ecoinvent market data set (0.31 kg

organic N/kg market N), and replaced the inputs of inorganic fertilizers (0.69 kg/kg market N) with the average mix in Table 7. In Table 8 below we summarize how the individual fertilizers in the market mix were modelled.

Table 8. Modelling of N fertilizer mix in ecoinvent.

Product	Ecoinvent data sets used in marginal mix	Ecoinvent data sets used in average mix
Ammonia dir. applic. (N)	Not applicable	Ammonia, liquid, as N {RoW}| market for | APOS, U. We correct the data set to express it as N-equivalents (0.823 kg N/kg ammonia). We add transports in the market data set.
Ammonium nitrate (N)	Ammonium nitrate, as N {GLO}| market for | Conseq, U	Ammonium nitrate, as N {GLO}| market for | APOS, U
Ammonium sulphate (N)	Ammonium sulfate, as N {GLO}| market for | Conseq, U	Ammonium sulfate, as N {GLO}| market for | APOS, U
Calc. amm. nitrate (N)	Not applicable	Nitrogen fertiliser, as N {RER}| calcium ammonium nitrate production | APOS, U. We add transports in the market data set.
Nitrogen solutions (N)	Nitrogen fertiliser, as N {RoW}| urea ammonium nitrate production | Conseq, U. We add transports in the market data set.	Nitrogen fertiliser, as N {RoW}| urea ammonium nitrate production | APOS, U. We add transports in the market data set.
Other N straight (N)	Not applicable	As a proxy we use Nitrogen fertiliser, as N {GLO}| nutrient supply from ammonium chloride | APOS, U.
Urea (N)	Urea, as N {GLO}| market for | Conseq, U. We add CO_2 emissions from mineralization of carbon in urea (0.73 kg CO_2/kg urea).	Urea, as N {GLO}| market for | APOS, U. We add CO_2 emissions from mineralization of carbon in urea (0.73 kg CO_2/kg urea).
Ammonium phosphate (N)	We create a specific data set, based on Phosphate fertiliser, as P2O5 {RoW}| monoammonium phosphate production | Conseq, U. This fertilizer has 11% N and 52% P_2O_5. Demanding 1 kg N results in a co-product of 4.73 kg P_2O_5. We add transports in the market data set.	Nitrogen fertiliser, as N {RoW}| monoammonium phosphate production | APOS, U
N K compound (N)	We create a specific data set, based on Potassium nitrate {GLO}| market for | Conseq, U. Demanding 1 kg N results in a co-product of 3.54 kg K_2O.	Nitrogen fertiliser, as N {GLO}| nutrient supply from potassium nitrate | Cut-off, U
N P K compound (N)	We create a specific data set for a NPK fertilizer with 15% N, 15% P_2O_5 and 15% K_2O, based on Phosphate fertiliser, as P2O5 {GLO}| market for | Conseq, U, Ammonium nitrate, as N {GLO}| market for | Conseq, U, Potassium fertiliser, as K2O {GLO}| market for | Conseq, U. Demanding 1 kg N results in a co-product of 1 kg P_2O_5 and 1 kg K_2O.	We create a specific data set for a NPK fertilizer with 15% N, 15% P_2O_5 and 15% K_2O, based on Phosphate fertiliser, as P2O5 {GLO}| market for | APOS, U, Ammonium nitrate, as N {GLO}| market for | APOS, U, Potassium fertiliser, as K2O {GLO}| market for | APOS, U. Allocation to N based on energy requirements as done in Nemecek and Kägi (2007), resulting in 69% of the burdens allocated to N.
Other NP (N)	Same as Ammonium phosphate (N)	Nitrogen fertiliser, as N {RoW}| monoammonium phosphate production | APOS, U

6.5 Changes to the CSV maker

As mentioned in sections 3.6 and 6.1, the new inventories produced by WW LCI v3 specify the emission sub-compartment. However, our CSV conversion tool did not support this feature, whereby all emissions where imported to SimaPro as emitted to an unspecified sub-compartment. We have modified the Excel macro in order for the converter to read sub-compartments. This new feature does not involve any changes to the way the CSV conversion tool is used.

7 Updates to the country database

7.1 Update of existing data

We have updated the statistics on wastewater collection and treatment and sludge disposal for numerous countries existing countries, such as most of the EU member states, for which we have used the latest Eurostat data. For some other countries in the database such as Brazil or Russia we replaced the existing data with other more recent and/or complete sources.

7.2 New descriptors per country

The number of new variables included in the database have been more or less explicitly described in the previous sections, where we have described how this new information is used. The actual list of new variables is the following:

- Mean annual and monthly temperatures (ºC): used in the WWTP heat balances (see section 4.2) as well as in the calculation of the MCF for open sewers (see section 5.1).
- Wastewater discharge in inland waters (%): percentage of wastewater produced that is expected to be discharged in freshwater ecosystems. This is used in the calculation of the percentage of effluents discharged either in freshwater or seawater (see section 3.6).
- Wastewater treatment plant capacity profile: the percentage of wastewater treated in five different WWTP capacity classes, and an estimate of the average capacity (m3/d) in each of these five classes. This information is used to quantify the use of WWTP and sewer infrastructure (see section 3.4), as well as the 'scale factor' used to estimate electricity consumption in WWTPs as a function of plant size (see section 3.3).
- Controlled/uncontrolled landfilling: includes the GNI per capita for each country, from which the percentage of controlled landfilling over total landfilling is estimated, as explained in section 4.11.
- Anaerobic digestion and cogeneration: an estimate of the percentage of wastewater treated in WWTPs with anaerobic digestion and the percentage of wastewater treated in WWTPs with anaerobic digestion and cogeneration (see section 4.3).
- Methane correction factors (MCF) for open sewers and environmental waters: country-specific methane correction factors as described in sections 5.1 and 5.2, used to calculate methane emissions from wastewaters discharged with and without treatment.

7.3 New countries

The number of countries covered by the database has increased from 56 to 81, representing 89% of the world's population. This coverage can be seen in Figure 10 and Table 9. The list of data sources used to cover all the new countries is too long to include in this document, however in the 'Database' tab in WW LCI each and every source is referenced. In general, the type of sources and their quality is widely variable. We used from recent and accurate statistics to older technical reports and articles. Most of the data sources, that is, more than 90% of them, were published in the last 10 years. Also, as described in this document, some of these primary data were further processed to obtain our target parameters (for example the landfill mix, or the percentages of AD and CHP). The user is advised to check the quality of the data, especially if an assessment requires comparing countries, since the quality of the respective country

data sets might differ. At 2.-0 LCA consultants we welcome any comments or suggestions to improve this database, which aims at eventually having a global coverage.

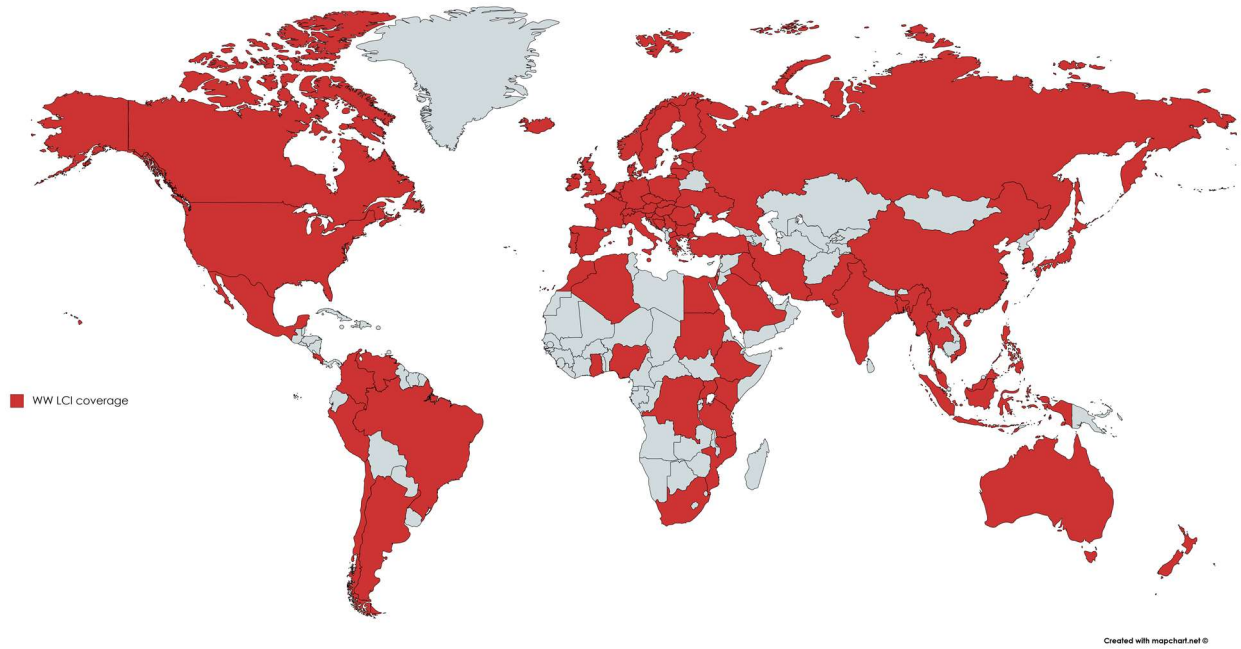

Figure 10. Geographical coverage of the WW LCI database as of January 2019.

Table 9. List of countries covered in the database.

Europe		Asia and Pacific	America	Africa
Austria	Lithuania	Afghanistan	Argentina	Algeria
Bosnia Herzegovina	Luxembourg	Australia	Brazil	Democratic Republic of the Congo
Belgium	Latvia	Bangladesh	Canada	Egypt
Bulgaria	Montenegro	China	Chile	Ethiopia
Switzerland	Macedonia, FYR	Indonesia	Colombia	Kenya
Cyprus	Malta	Israel	Costa Rica	Morocco
Czech Republic	The Netherlands	India	Mexico	Nigeria
Germany	Norway	Iran	Peru	Ghana
Denmark	Poland	Iraq	United states	Tanzania
Estonia	Portugal	Japan	Venezuela	South Africa
Spain	Romania	Republic of Korea		Sudan
Finland	Serbia	Malaysia		Uganda
France	Sweden	Mozambique		
United Kingdom	Slovenia	Myanmar		
Greece	Slovakia	New Zealand		
Croatia		Philippines		
Hungary		Pakistan		
Ireland		Russia		
Iceland		Saudi Arabia		
Italy		Thailand		
		Turkey		
		Taiwan		
		Ukraine		
		Vietnam		

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Appendix: Environmental fate of organic matter in urban wastewater

In section 2.1 we have proposed to split the organic content in urban wastewater into two fractions: dissolved and particulate. Once discharged in the aquatic environment or in soil (via sludge) in WW LCI we determine the environmental fate of substances by means of the USES-LCA model embedded in the spreadsheet. The problem with this model is that it requires the identification of individual chemical substances, as done in environmental risk assessment, whereas in our case, we are trying to model a generic organic matter contained in domestic wastewater. In terms of discharges to the aquatic environment, according to Von Sperling (2007b, p. 85) "settleable suspended solids tend to settle in the water body, forming a sludge layer at the bottom. The dissolved matter, together with the suspended solids of small dimensions (hardly settleable) remains in the liquid mass ". This suggests that dissolved organic matter stays in the water column, while particulate organic matter seems to be mainly partitioned to environmental sediments, although small-size suspended solids are expected to remain in the water column. In addition to the latter, particulate organic matter is labile, meaning that during the time it takes for it to potentially settle, degradation can occur to some extent. In this appendix we attempt to define values for Deg_w and Deg_{sed} attributable to particulate and dissolved organic matter once discharged to either inland waters, coastal waters, and agricultural soil. For this we use the fate model USES-LCA.

We have characterized both disolved and particulate organic matter with the physical-chemical data and degradation rates shown in Table 10. We set to zero vapour pressure and Henry's Law constant since we neglect any volatilization. In the case of particulate organic matter we also set solubility to zero, as we want to represent a material in suspension rather than dissolved. For the rest of parameters (Kow, Koc, degradation rates) we use data from ethanol to model dissoved organic matter and from oleic acid to model particulate organic matter. Ethanol is used as model of a highly degradable and soluble substance, while oleic acid represents a hydrophobic, yet degradable substance. Data for ethanol were obtained from Muñoz et al. (2016) while data for oleic acid were taken from the original USES-LCA database (not embedded in WW LCI).

Table 10. Key input data used for organic matter in the USES-LCA fate model.

Parameter	Organic matter, dissolved	Organic matter, particulate
ChemType	Organic	Organic
Neutral/Acid/Base	Neutral	Neutral
Vapour pressure (Pa)	1E-20 (as a proxy for zero)	1E-20 (as a proxy for zero)
Solubility 25 deg (mg/L)	1E+06 (same as ethanol)	1E-20 (as a proxy for zero)
Kow	0.49 (same as ethanol)	4.37E+07 (same as oleic acid)
Koc	1.04 (same as ethanol)	1.17E+04 (same as oleic acid)
Henry's Law Constant ($Pa \cdot m^3/mol$)	1E-20 (as a proxy for zero)	1E-20 (as a proxy for zero)
kdeg air (s^{-1})	2.45E-06 (same as ethanol)	5.66E-05 (same as oleic acid)
kdeg water (s^{-1})	9.25E-07 (same as ethanol)	5.35E-07 (same as oleic acid)
kdeg sed (s^{-1})	1.03E-07 (same as ethanol)	5.94E-08 (same as oleic acid)
kdeg soil (s^{-1})	4.62E-07 (same as ethanol)	2.67E-07 (same as oleic acid)

With these settings, the results from USES-LCA are shown in Table 11. It can be seen that the dissolved organic matter emitted to freshwater/seawater is expected to almost entirely degrade in the water column, whereas particulate organic matter degrades by 21% in sediments when originally discharged to

freshwater. When an emission to soil occurs, particulate organic matter degrades almost entirely in soil, while dissolved organic matter is expected to leach to groundwater by approximately 15%.

Table 11. Environmental degradation profile for particulate organic matter, estimated with USES-LCA.

Organic matter fraction and emission compartment	Deg_a	Deg_w	Deg_{sed}	Deg_s
Organic matter, dissolved:				
Freshwater	0.00%	99.92%	0.07%	0.00%
Seawater	0.00%	100.00%	0.00%	0.00%
Agricultural soil	0.00%	15.66%	0.01%	84.30%
Organic matter, particulate:				
Freshwater	0.00%	76.55%	20.94%	0.00%
Seawater	0.00%	99.17%	0.83%	0.00%
Agricultural soil	0.00%	0.23%	0.06%	99.63%

The values in Table 11 are used by default in WW LCI v3, in the tab 'CODNPSS input'. The user can modify these values if required.