Wastewater life cycle inventory initiative

WW LCI version 4.0 user manual

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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 in wastewater. 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

C O N T E N T S

Acronyms and abbreviations

APOS	Allocation at the point of substitution
BOD_5	Biological oxygen demand in five days
CAS	Chemical abstracts service
COD	Chemical oxygen demand
CSV	Comma-separated values
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
Fair	Fraction of chemical, in mass percentage, that undergoes volatilization in the WWTP
Fdeg	Fraction of chemical, in mass percentage, that undergoes degradation in the WWTP
Fsludge	Fraction of chemical, in mass percentage, that partitioning to sludge in the WWTP
GWP	Global warming potential
HL	Half-life (seconds)
IFA	International Fertilizer Association
Kd sed	Solid/liquid partition coefficients in sediments (dimensionless)
Kd soil	Solid/liquid partition coefficients in soil (dimensionless)
Kd susp	Solid/liquid partition coefficients in suspended solids (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}.
Koc	Soil organic carbon-water partitioning coefficient (dimensionless)
Kow	Octanol-water partitioning coefficient (dimensionless)
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
MW	Molecular weight (g/mol)
pKa	Acid dissociation constant (dimensionless)
QSAR	Quantitative structure-activity relationships
SS	Suspended solids = total suspended solids (TSS)
TSS	Total suspended solids
VSS	Volatile suspended solids
ISS	Inert suspended solids
Total-N	Total nitrogen
Total-P	Total phosphorus
WWTP	Wastewater treatment plant
AD	Anaerobic digestion
CHP	Cogeneration of heat and power
MCF	Methane correction factor

1   Introduction and purpose of this document

WW LCI is a model and tool programmed in MS Excel, designed to calculate life cycle inventories (LCIs) of municipal wastewater discharges and sanitation. The model addresses both centralized and decentralized wastewater and human excreta management, as well as sludge disposal and untreated discharges of wastewater and septic sludge. An overview of the individual processes covered by WW LCI is given in Figure 1. While the user provides as main input data a characterization of the generated wastewater, the tool already incorporates a set of average scenario conditions at the country level, by means of a database storing these country profiles. The outcome of the calculation is an LCI describing the management of the indicated wastewater under the established scenario, which is linked to ecoinvent data sets and can be imported to the software SimaPro and GaBi.
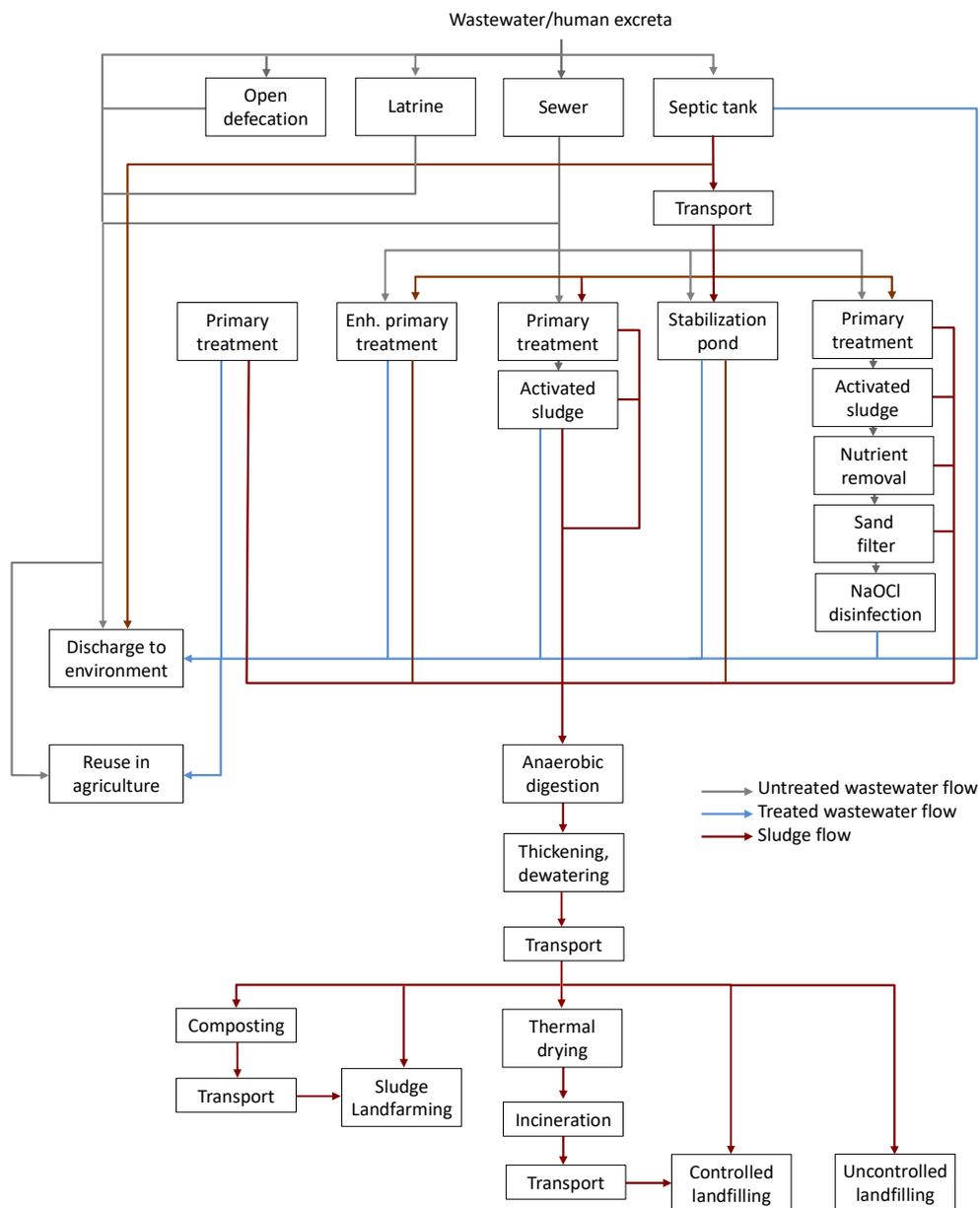
Figure 1. Overview of the processes included in WW LCI.

In this document we provide instructions to operate the Excel file where version 4 of WW LCI has been programmed. It is not a purpose of this document to describe the developed model from a scientific point of view. For the latter, the reader is instead referred to the model documentation (Muñoz 2021).

2   Accessing WW LCI

Accessing WW LCI requires registering as a member of the Wastewater Life Cycle Initiative. This can be done by contacting 2.-0 LCA consultants at info@lca-net.com. Once becoming a registered member, the user receives by email a username and password to access the members-only section of the Initiative, at: http://lca-net.com/clubs/wastewater/ (Figure 2). Once logged in, all files are available for download, including WW LCI.
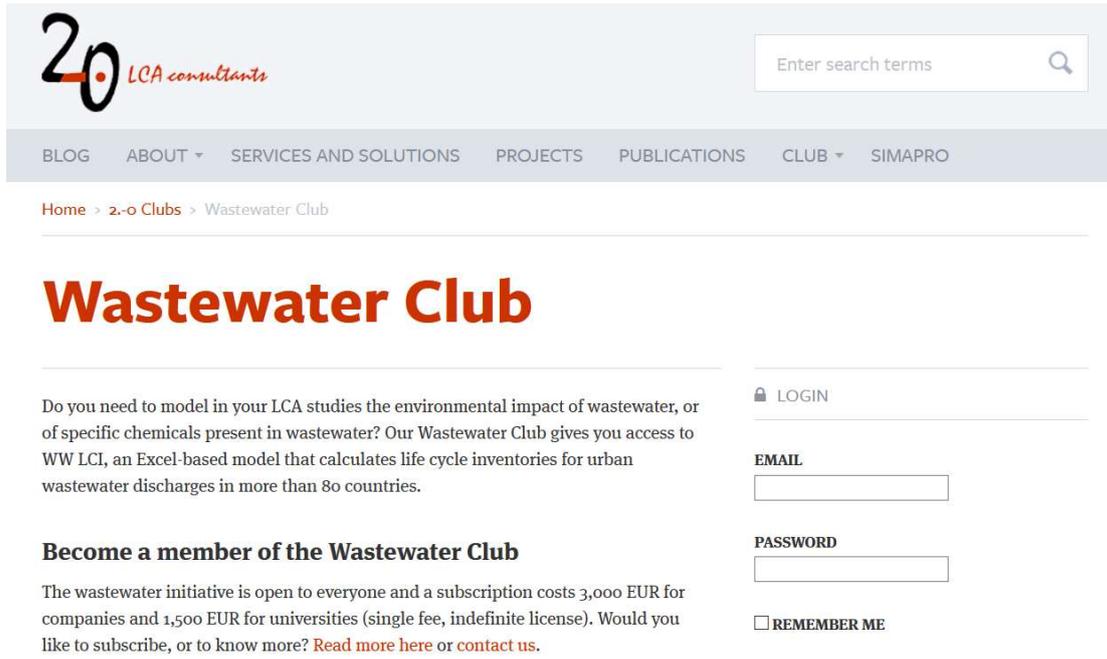
Figure 2. Screenshot of the 2.-0 LCA consultants' website showing the Wastewater LCI initiative section.

3   How to use WW LCI

3.1   Structure of the Excel file

WW LCI has in total 35 sheets, however only 21 are visible, and only 10 are intended to be manipulated by the user. Sheets intended for direct use are the following:

- Tier1-input
- Tier2-input
- USESLCA
- Scenario
- Ready to CSV
- Ready to GaBi
- Parameters
- Database
- Refs
- Uncert

These 10 sheets are marked in yellow background, as shown in Figure 3.
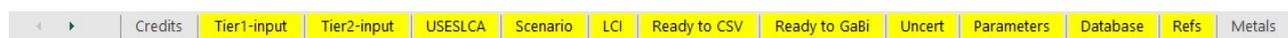
Figure 3. Sheets in yellow background in WW LCI are those intended to be manipulated by the user.

The second to fifth sheets (Tier1-input, Tier2-input, USESLCA, Scenario) allow the user to either enter data and choose from drop-down menus, in order to set up an assessment and obtain an LCI. In these sheets the following colour code is used:

| Green cells **not** to be filled in |
| Brown cells can be filled in |

Cells in green background might contain formulae and are not to be used, whereas cells in brown background can be safely filled in.

Sheets not intended for direct use are the following:

- Metals
- Sewer
- Reuse
- Env deg
- Energy&AD
- Pri
- Pond
- AS
- Tert
- Septic

- Sludge
- Landfill
- Incin
- Compost
- Landfarm
- Transpose
- LCI
- Credits

On the one hand, the first 17 sheets contain intermediate calculations and do not require any input from the user. They are kept visible to allow full transparency on the calculations. The last sheet, on the other hand, serves just as a frontpage for the file.

As mentioned above, there are also 13 hidden sheets (Figure 4). These sheets contain the necessary calculations for environmental multimedia fate modelling according to USES-LCA 2.0. Given their large number, their complexity, and the fact that they are not to be manipulated by the user, they are kept hidden. The user is free to unhide them, however care should be taken not to modify their content. In this document we do not describe these sheets further, and the interested reader is referred to the USES-LCA literature (Huijbregts et al. 2005; van Zelm et al. 2009), as well as to the original documentation of the Simplebox model (Brandes et al. 1996), which served as the basis for the development of fate modelling in USES-LCA.

It must be stressed that none of the (visible and hidden) sheets in WW LCI and their content are protected. The user should be careful not to modify the content of any cells other than those intended for that purpose, as explained in the following sections.

USESLCAsubst.db
USESLCAengine
USESLCAcorr.factors
USESLCAlevel 3
USESLCAlocal
USESLCAreg
USESLCAcont
USESLCAmod
USESLCAarctic
USESLCAtropic
USESLCA–STPinput
USESLCA–STPoutput
USESLCA–STPengine

Figure 4. Screenshot of the list of hidden sheets in WW LCI.

3.2 Conducting a Tier 1 assessment

A Tier 1 assessment applies when the only information available to the LCA practitioner on wastewater composition is limited to generic pollution descriptors such as chemical oxygen demand (COD). The model accommodates this kind of generic descriptors, for those cases where the individual chemicals present in

wastewater cannot be identified. In particular, in Tier 1 a wastewater is defined based on four easily available measures, expressed in mg/L: COD, TSS, Total-N, Total-P and a total of 17 metals.

3.2.1 Input data in 'Tier1-input'

The first step to perform a Tier 1 assessment in WW LCI is to introduce the wastewater composition in sheet 'Tier1-input', containing three tables intended to be populated or modified by the user:

- **Influent composition**: in this table (Figure 5), under column 'User data' the user enters the wastewater composition, in mg/L, for COD, N, P, TSS and metals. For COD, N and P it is possible to either provide the total value, or to specify the soluble and the suspended fraction separately. For TSS it is possible to specify the volatile (VSS) and inert (ISS) fraction separately. When only the totals for COD, N, P and SS are provided, the fractionation is estimated automatically, using typical ratios from domestic wastewater (see Figure 5). The result of this fractionation can be seen in the column 'Fractionation'. In the column 'User data' it is possible to enter the total for one parameter, while specifying the soluble and suspended fractions for other parameters. For example, we can enter COD total, SS total (TSS), but then specify the soluble and suspended fractions for N and P. It is important, though, that for each of the four measures, only one of the options for data entry is used, that is, we either 1) enter the total value or 2) enter the soluble and/or the suspended fraction. In case an incorrect combination of data is entered, an automated error flag will appear.

- **Organic carbon labelling**: as a default, organic carbon in wastewater is labelled as 100% biogenic. This percentage can be adjusted by the user to a lower value if necessary.

- **Primary settling in WWTP with secondary treatment by activated sludge**: as a default, 100% of wastewater treatment plants (WWTPs) applying activated sludge as biological treatment are assumed to include a primary settling tank. This percentage can be adjusted by the user to a lower value if necessary.

- **Ratios:** This table contains a list of ratios used to fractionate the wastewater. The values chosen are typical of domestic wastewater.

Influent composition		
Parameters	User data	Fractionation
Chemical oxygen demand, total, COD (mg O2/L)	500	500.0
COD, soluble (mg O2/L)		218.8
COD, suspended (mg O2/L)		281.3
Nitrogen, total, N (mg N/L)	30	30.0
N, soluble (mg N/L)		25.6
N, suspended (mg N/L)		4.4
Phosphorus, total, P (mg P/L)	6	6.0
P, soluble (mg P/L)		4.2
P, suspended (mg P/L)		1.8
Suspended solids, total, TSS (mg TSS/L)	250	250.0
Suspended solids, volatile, VSS (mg VSS/L)		200.0
Suspended solids, inert, ISS (mg ISS/L)		50.0
Metals (mg/L)		
Silver		
Aluminium		
Arsenic		
Cadmium	0.0050	
Chromium		
Copper		
Mercury	0.0010	
Manganese		
Nickel		
Lead		
Zinc		
Barium		
Cobalt		
Iron		
Magnesium		
Antimony		
Vanadium		

Figure 5. Defining wastewater composition in sheet 'Tier1-input'.

It is important to enter data for the four groups of measures (COD, N, P, SS) and only leave one or more empty or with a zero value if their concentration is known to be zero mg/L. Below we provide some rules of thumb to fill in data gaps i.e. to complete the four fields when one or more are missing and they are known to be >0.

Table 1. Estimating the four wastewater pollution measures, based on typical ratios in domestic wastewater (Henze and Comeau 2008).

Missing measure	Estimate
Total COD	= 2.1 · BOD$_5$
Total N	= 0.08 · COD
	= 0.15 · TSS
Total P	= (0.01 to 0.02) · COD
	= (0.02 to 0.04) · TSS
Total SS	= 0.5 · COD

The current implementation of the calculations allows the user to have N, P and SS (either as totals or as the sum of soluble and suspended) with a zero value, but COD must have a value above zero in all cases. Again, this can refer to total COD, soluble COD, suspended COD, or a combination of the last two. This flexibility in wastewater composition allows the user to deviate from typical domestic wastewater compositions.

3.2.2   Input data in 'Scenario'

In the sheet 'Scenario', the user establishes the context or conditions in which wastewater is managed. This includes both geographical conditions (such as climate) and technological conditions (sanitation systems in

place). This sheet contains three tables, although only the first one (Scenario data) requires input from the user:

- **Scenario data**: where the user sets the geography and wastewater/sludge treatment scenario, among other aspects.

- **Organics and inorganics excluding metals**: this table is automatically filled, based on the input data from sheet 'Tier1-input'. It reflects the composition of wastewater, physical-chemical properties and fate factors in the WWTP and the environment for all wastewater components except metals.

- **Metals**: equivalent to the table above, but intended only for the list of 17 metals supported by the model.

Figure 6. The 'Scenario' sheet in WW LCI.

The **Scenario data** table contains the following fields:

- **Type of assessment** (drop-down menu): the user can choose between Tier 1 or Tier 2. When Tier 1 is chosen, this will load the wastewater composition defined in sheet 'Tier1-input'.

- **Country** (drop-down menu): the user can choose from this drop-down menu from the list of covered countries. By choosing a country from the list, its scenario for wastewater management will automatically load in cells L10 to L87. Countries are listed according to their ISO two-digit code.

- **Country name**: this field is not to be manipulated by the user. It displays the above-chosen country by its name.

- **Choice of country data set** (drop-down menu): the user can choose whether to use the default country-specific scenario in cells L10 to L87, or to use his/her own. In order to use the default data, the option 'Database' must be chosen from the drop-down list, otherwise the option 'User-specific' must be chosen. After choosing 'User-specific' in the drop-down menu, the actual values shall be entered by the user in cells R10 to R87. The values in column R will automatically override the default ones in column L for as long as the option 'User-specific' is set.

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- **Type of discharge** (drop-down menu): the user can choose from four different types of discharges, namely 'Domestic, grey water', 'Domestic-faecal water', Domestic, grey & faecal water' and 'Industry'. This choice affects the wastewater/sanitation options involved in managing the discharge. See the model documentation (Muñoz 2021) for further details on these types of discharges.

- **Wastewater modelled as a mixture** (drop-down menu): this field establishes whether or not the list of components in wastewater are to be modelled as a mixture (yes) or only individually (no). As a default, this field is set to 'yes'.

If the user relies on default database data under 'Choice of country data set', then the fields below do not need to be modified. Otherwise, when the user chooses the 'User-specific' option, the fields below need to be individually defined, in column R:

- **Wastewater collection and treatment scenario**: this field is in fact a sub-table describing the scenario for wastewater management and sanitation in the chosen country, in percentages.

- **WWTP capacity**: this sub-table describes the size of the centralized WWTPs in the chosen country. The percentages express the percentage of wastewater treated in each of the five WWTP sizes out of the total wastewater treated in the chosen country, while the absolute figures quantify the average daily flow (in m^3/day) in each of the five WWTP sizes. For waste stabilization ponds, a specific field is provided, where the average daily flow of this particular type of plant in the country is provided, in m^3/day.

- **Primary treatment technology**: establishes the percentage of wastewater treated in WWTPs with primary treatment that applies either conventional primary settling or chemically-enhanced primary settling.

- **Secondary treatment technology**: establishes the percentage of wastewater treated in WWTPs with secondary treatment that applies either activated sludge systems or stabilization pond systems.

- **Nutrient removal**: quantifies the percentages of wastewater treated in WWTPs with nitrogen removal and phosphorus removal, respectively. N removal refers to nitrification followed by denitrification, while P removal refers to chemical precipitation using iron chloride. As a default, these percentages are set equal to the field 'Urban wastewater treatment - tertiary treatment (%)'. In case that 'User-defined' data are entered, the percentages provided by the user cannot exceed the sum of wastewater treated in WWTPs with secondary treatment and with tertiary treatment (sum of cells L14 and L15). This is because the model is not designed to consider any advanced nutrient removal for instance in septic tanks or in WWTPs with primary treatment only. Finally, the field 'Connection to WWTP with nitrogen removal, using methanol (%)' expresses what percentage of N removal is carried out using methanol as an external carbon source. This is zero as a default. The user can change this, entering any value between 0% and 100%, with 100% meaning that all WWTPs that conduct N removal do this using methanol.

- **Sludge treatment in WWTPs**: Provides the percentage of wastewater treated in WWTPs that apply on-site anaerobic digestion (AD) of sludge, and the percentage of wastewater treated in WWTPs

that apply both anaerobic digestion and use biogas for cogeneration of heat and power (CHP). The percentage of AD+CHP can only be lower or equal to the percentage of AD, since the former is a sub-set of the latter.

- **Wastewater discharge**: contains the percentage of wastewater either discharged to freshwater or to the sea. These percentages are applied to wastewater either discharged without treatment or in centralized WWTPs. Wastewater treated in septic tanks and through latrines is assumed to be discharged to groundwater, while open defecation assumes discharges to soil.

- **Wastewater reuse – treated/untreated**: establishes the percentages of treated and untreated wastewater used for irrigation in agriculture. Treated wastewater includes effluents from all types of centralized WWTPs and septic tanks. Untreated wastewater considers wastewater from either closed or open sewers, but excludes latrines and open defecation.

- **Wastewater reuse – Irrigation water supply mix**: establishes the percentage of freshwater supply from surface water, groundwater and from seawater (produced by desalination) substituted by wastewater reuse in countries where water supply for agriculture is not constrained. See the model documentation for further details (Muñoz 2021).

- **Wastewater reuse – Crop production mix**: establishes the most likely crops to be affected by a marginal increase in irrigation through wastewater reuse in countries where water supply for agriculture is constrained. See the model documentation for further details (Muñoz 2021).

- **Septic sludge management**: establishes the percentages of sludge removed from septic tanks that is subject to either safe or unsafe disposal. Safe disposal is modelled as co-treatment with wastewater in a WWTP, while unsafe disposal is modelled as direct discharge to surface waters.

- **Sludge disposal**: quantifies the percentage of sludge (in dry mass), including that produced by WWTPs and septic tanks, that is sent to any of the following off-site disposal options: composting, reuse in agriculture (landfarming), landfilling – controlled, landfilling – uncontrolled, and incineration with energy recovery. In reality, composting is not a final disposal option but a treatment. The produced compost is modelled as sent for landfarming.

- **Ambient temperature**: Shows the mean annual and monthly mean air temperatures in the chosen country. This information is used in the calculation of methane emissions from discharges, as well as in the heat energy balance in the WWTPs.

- **Methane correction factors**: MCFs reflect the fraction of wastewater degradation that occurs under anaerobic conditions, affecting, among others, methane emissions. We establish MCFs for open/stagnant sewers (MCF_{open}), direct discharges of treated and untreated wastewater to surface waters (MCF_w), latrines (MCF_{lat}), and also for open defecation (MCF_{open}). For closed sewers we establish a different factor, called degradation factor in closed sewers (Deg_{closed}), expressing the extent of degradation, always assumed to be under anaerobic conditions. See the model documentation for further details (Muñoz 2021).

At this point, WW LCI will automatically calculate the LCI of each wastewater component individually. If the option 'Wastewater mixture' is set to 'yes', then WW LCI will also combine all wastewater components and calculate the LCI of this mixture according to their concentrations.

3.2.3 Limitations of Tier 1 assessments

A limitation of a Tier 1 assessment compared to a Tier 2 assessment is that the LCIs obtained with the former do not allow to properly assess toxicity-related impacts from organic pollution in wastewater. This is because the pollution content is described with generic descriptors that are typically excluded from LCIA methods. For example, COD does not have characterization factors for aquatic ecotoxicity. This situation does not occur in Tier 2, since the organic load is in this case specified as a set of individual chemical substances, for which characterization factors might be available.

3.3 Conducting a Tier 2 assessment

A Tier 2 assessment corresponds to the original procedure to model wastewater discharges with WW LCI. In Tier 2, the individual substances discharged must be identified, as done in the field of environmental risk assessment. An example would be to assess a wastewater generated by the use of a washing machine, where the individual ingredients in the detergent formulation (content of surfactants A and B, builders C and D, bleaches E and F, water, etc.) are known, as are their proportions in weight. A Tier 2 assessment can be substantially more data-demanding than a Tier 1 assessment.

3.3.1 Input data in 'Tier2-input'

The first step to perform a Tier 2 assessment in WW LCI is to introduce the wastewater composition in sheet 'Tier2-input', containing two tables intended to be populated or modified by the user: 'Organics and inorganics excluding metals' and 'Metals'.

The table 'Organics and inorganics excluding metals' contains 30 open rows for introducing data on individual chemicals. The following fields need to be completed by the user:

- **Name**: name of the chemical. This is the name that will appear in the calculated LCI. If the LCI is to be imported to LCA software, where the chemical is to be classified by impact assessment methods (for example ecotoxicity), then the name used in the software for this chemical must be used, otherwise the chemical would not be recognized by the software in the impact assessment calculations. If a different name is used, then the chemical can only be classified in the software by adding the new name manually into the list of classified substances. See section 5.1 for details.

- **Mass in mixture (kg/kg wastewater)/Leave this column blank**: depending on whether the user chooses 'yes' or 'no' in the field 'Wastewater modelled as mixture' (see section 3.2.2), the heading of this field will have one of the two mentioned titles. When the substances entered in the table are to be modelled as a mixture, the user must enter in this field the fraction in mass that the chemical constitutes in the mixture. It should be noted that the sum in this field should add up to 1, otherwise a warning will appear in the Automated error flags box (see 3.4). Also note that chemicals can contribute to 0% in the mixture. In such a case their individual LCI will be obtained, but they will not contribute to the wastewater mixture LCI. Finally, if the user is not modelling a chemical mixture, then the 'Leave this column blank' message will appear in the column heading.

- **CAS number**: this field is optional.

- **Type** (organic/inorganic): the substance must be labelled as organic or inorganic in the drop-down list.

- **Composition** (no of atoms in a molecule): in this field the number of atoms of each element, related to the empirical formula of the chemical substance, must be entered. The following elements are supported: carbon, hydrogen, oxygen, nitrogen, sulfur, phosphorus, and chlorine. If the chemical substance contains other elements, their mass will be accounted for in mass balances based on the substance's molecular weight (see below).

- **Molecular weight** (g/mol): the molecular weight of the substance should be entered, including all its elements. For example, if a chemical substance has sodium in its molecule, the weight of the sodium atoms can be accounted for in the molecular weight, however since sodium is not supported by 'Composition' field, this will be treated by the model as an inert fraction of the substance.

- **Vapour pressure (Pa)**: to define the chemical's vapour pressure, in Pascal. This parameter is only used to define if the chemical substance is volatile during sludge composting. As a default, the model considers volatility only when vapour pressure is 10 Pa or higher.

- **Kow** (dimensionless): to define the chemical's octanol-water partitioning coefficient. In case there is no Kow available, this field can be left blank. This parameter is used to estimate the chemical's Kd (see below).

- **pKa** (dimensionless): to define, if applicable, the chemical's acid dissociation constant. This parameter is used to estimate the chemical's Kd (see below).

- **Kd** (dimensionless): to define the chemical's solid/liquid partition coefficients in the WWTP's suspended solids. This is used to calculate the chemical-specific removal in sand filters, as part of tertiary treatment. This field is only compulsory in the case that no Kow is available. The user can choose to either enter Kow+pKa (in this case Kd is automatically estimated with them), or Kd on its own. However, in the case that tertiary treatment is not relevant, or when a chemical has a Kd lower than 0.001, then these parameters can be skipped, since the sand filter only removes chemicals with relatively high Kd.

- **Biogenic carbon** (yes/no/n.a.): to define whether or not the chemical substance is derived from biogenic sources, e.g. biomass such as vegetable or animal sources (choose 'yes') or petrochemical sources (choose 'no'). In the particular case of inorganic chemicals either containing or not containing carbon, the 'n.a.' option must be chosen.

- **Fate in WWTP with 2ary tr. (activated sludge) (%) - Fair, Fdeg, Fsludge** (%): this field includes four sub-fields corresponding to the fraction of the chemical, in mass percentage, that undergoes the following fate paths in a WWTP including secondary treatment by activated sludge: volatilization (Fair), degradation (Fdeg), and partitioning to sludge (Fsludge). The remainder to close the balance constitutes the fraction of chemical in the treated effluent, therefore these three percentages do not necessarily need to add up to 100%, unless the fraction of chemical discharged in the effluent is 0%. These data about the fate of chemicals can be obtained by means of monitoring data,

published studies, modelling with such models as Simpletreat (Franco et al. 213a, 2013b) or from the estimates by the Technical Guidance Document on Risk Assessment (EC 2003), that we provide in the Appendix. The percentages in these fields must reflect the removal level expected in a WWTP applying secondary treatment by activated sludge. In Table 2 we provide tips for some specific chemicals of importance in wastewater.

- **Fate in WWTP with secondary tr. - Anaerobic deg?** (yes/no): in this field, the user defines whether or not the chemical substance is degradable under anaerobic conditions. This information can be obtained from anaerobic degradation test reports, or theoretically by means of quantitative structure-activity relationship (QSAR) models like the Anaerobic Biodegradation model (BIOWIN 7) included in the EPI Suite progam (USEPA 2009). Note that this field does not allow for the determination of the degree of degradability, but only a binary label, i.e. degradable/not degradable. This is because WW LCI considers the same degree of anaerobic degradation for all degradable substances.

- **Fate in WWTP with 1ary tr. only (%) – Fsludge** (%): this corresponds to the same type of fate factors previously described for an activated sludge WWTP, but referring to a WWTP with primary treatment only. In practice, by default in WW LCI it is assumed that Fair and Fdeg are zero in such a plant, therefore the user is allowed to provide only a value for Fsludge. However, even providing Fsludge is only optional. If no value is provided by the user, WW LCI estimates Fsludge for primary treatment based on the data provided by the user for a WWTP with activated sludge. See the model documentation in Muñoz (2021) for further details.

- **Fate in septic tank (%) – Fsludge** (%): this corresponds to the same type of fate factors described in the previous bullet, but referring to treatment in a septic tank. In practice, by default in WW LCI it is assumed that Fair and Fdeg are zero in septic tanks, therefore the user is allowed to provide only a value for Fsludge. However, even providing Fsludge is only optional. If no value is provided by the user, WW LCI estimates Fsludge for septic tanks based on the data provided by the user for a WWTP with activated sludge. See the model documentation in Muñoz (2021) for further details.

- **Fate in stabilization pond (%) - Fair, Fdeg, Fsludge** (%): this corresponds to the same type of fate factors described in the previous bullet, but referring to treatment in a waste stabilization pond (WSP). In practice, providing the three fate factors optional. If no values are provided by the user, WW LCI estimates them for WSPs based on the data provided by the user for a WWTP with activated sludge. See the model documentation in Muñoz (2021) for further details.

- **Fate in the environment – if emitted to freshwater, if emitted to seawater, if emitted to soil, if emitted to air – Deg_a, Deg_w, Deg_{sed}, Deg_s** (%): these parameters are intended to reflect the fate of the chemical substance if emitted to the environment, for example from a WWTP. The values for these parameters are obtained in the sheet 'USESLCA' (see section 3.3.2), and pasted as values in the corresponding cells in this table. However, it is not always necessary to fill all these fields. In particular, if a chemical substance is inorganic, these fields must be left blank.

Table 2. Tips on input data for certain chemicals.

Water
Water is by far the main component in a wastewater mixture. Input data for water must be entered in the 'Tier2-input' sheet just like for any other chemical (its composition, molecular weight, etc.). Water is modelled in WW LCI as entirely discharged in the effluent of the WWTP. Of course, some water could be evaporated from the WWTP. In this case the user can enter a value for the parameter Fair. Concerning water leaving the WWTP as sludge moisture, this is calculated as part of the LCI for chemicals producing sludge, and not as part of the LCI for the chemical 'water'.

Chemicals including phosphorus
When assessing inorganic chemicals with phosphorus, such as phosphate (PO_4^{3-}), if the WWTP includes P removal (as per the scenario settings), the factor Fsludge should not account for this P removal, otherwise the model will account for P removal twice. In the example of phosphate and similar chemicals, the value for Fsludge should be = 0, i.e. as if there was no P removal. The model will automatically account for P removal according to the parameter settings (the default P removal is 80% in a WWTP with tertiary treatment). For organic chemicals with phosphorus, it is important to remember that P is only available for P removal if this P is released from the parent molecule. This is the case for chemicals that degrade in the WWTP. Therefore, if a chemical has P in its molecule but Fdeg = 0, then the model will not apply P removal to this substance.

Chemicals including nitrogen
If inorganic species with N are assessed, such as nitrate, nitrite or ammonium, in all cases Fdeg must be set to zero, as these are already inorganic substances and will not degrade. Fsludge and Fair must be set to zero too. The model will automatically incorporate these substances into the calculations for biological treatment, and if N removal is included (as per the scenario settings), the nitrification and denitrification reactions will be applied, leading to a certain removal of each of these species. For organic chemicals including nitrogen, the only N available for N removal is the one released from the parent molecule. Therefore, if a chemical has N in its molecule but Fdeg = 0, then none of this N will be removed through nitrification-denitrification.

The table 'Metals' is an equivalent to the previously described table, however it is meant to cover 17 metals. Any other metal not included in that list is currently not supported by the model. This table is used in a different and simpler way. Below we describe the fields that need to be filled in by the user:

- **Name**: this is a drop-down menu, where the user chooses the target metal from the list of 17 elements available. When an element is chosen, the fields 'CAS number', 'Type', 'Molecular weight' and 'Kd' are automatically filled in.

- **Mass in mixture (kg/kg wastewater)/Leave this column blank**: this field is used as previously described for the table 'Organics and inorganics excluding metals'. Metal concentrations are expressed in kg metal/kg wastewater.

- **Fate in WWTP with 2ary tr. (activated sludge) (%) - Fsludge** (%): the fraction of metal partitioned to sludge in WWTPs is automatically calculated by the model based on predefined data stored in sheet 'Metals', however in this field the user is allowed to override these data for WWTPs with secondary treatment by activated sludge. The fate factors 'Fair' and 'Fdeg' cannot be filled in by the user, since all metals are considered in the model as non-degradable and non-volatile.

- **Fate in WWTP with 1ary tr. only (%) - Fsludge** (%): as in the previous bullet, applicable to WWTPs with primary treatment only.

- **Fate in septic tank (%) - Fsludge** (%): as in the previous bullet, applicable to septic tanks.

- **Fate in stabilization pond (%) - Fsludge** (%): as in the previous bullet, applicable to waste stabilization ponds.

3.3.2 Input data in 'USESLCA'

The sheet 'USESLCA' is used in a Tier 2 assessment to define substance-specific fate factors in the environment. In practice this sheet needs to be used only for organic chemicals. In this sheet we calculate the fate in the environment of chemicals that, for example, escape removal in the WWTP or are volatilized, resulting in their release to the environment. Substance-specific data are used by the USES-LCA model (hidden in several sheets) to estimate fate in the environment. The output of the USES-LCA calculations is summarized in this sheet as the fraction of the chemical that is expected to degrade in different environmental compartments (freshwater, seawater, air, soil, sediments).

Figure 7 shows a screenshot of this sheet. It contains three separate tables:

- **Substance-specific data**: the user enters physical-chemical properties, etc.

- **Input to USES-LCA**: the user picks a chemical from the entered list and a release compartment.

- **Fate in environment, based on USES-LCA output**: results from the USES-LCA model for the assessed combination of chemical and release compartment.

Using this sheet can be broken down into three steps, corresponding to using the three above tables.

Figure 7. Screenshot of the 'USESLCA' sheet.

The **Substance-specific data table** contains 30 open rows for introducing data for specific substances. The first step corresponds to filling the fields in this table, although some of them are automatically filled in from the content already provided in sheet 'Tier2-input'.

- **Name**: name of the chemical. By default, this field is automatically filled in from the 'Tier2-input' sheet.

- **CAS number**: this field is automatically filled in from the 'Tier2-input' sheet, if a CAS number has been provided.

- **ChemType** (organic/inorganic): this field is automatically filled in from the 'Tier2-input' sheet.

- **Neutral/Acid/Base** (B/-/A): to define from the drop-down list whether the chemical is a base (B), neutral (-) or an acid (A).

- **MW** (g/mol): to define the molecular weight of the chemical. This field is automatically filled in from the 'Tier2-input' sheet.

- **Vapour pressure 25 deg. C** (Pa): to define the chemical's vapour pressure, in Pascal. This field is automatically filled in from the 'Tier2-input' sheet.

- **Solubility 25 deg** (mg/L): to define the chemical's solubility in mg/L.

- **Melting point** (deg. C): to define the chemical's melting point, in degrees Celsius.

- **Kow** (dimensionless): to define the chemical's octanol-water partitioning coefficient. This field is automatically filled in from the 'Tier2-input' sheet. In case there is no Kow available, USES-LCA requires filling the 'Distribution coefficients' (see below).

- **Koc** (dimensionless): to define the chemical's soil organic carbon-water partitioning coefficient. This field is not compulsory however it is advised to enter a value if available.

- **Henry's Law Constant** ($Pa \cdot m^3/mol$): to define the Henry's law constant. If a chemical substance can be classified as non-volatile, and a Henry's Law constant is not available, the value 1E-20 can be entered in this field.

- **pKa** (dimensionless): to define, if applicable, the chemical's acid dissociation constant This field is automatically filled in from the 'Tier2-input' sheet.

- **kdeg air** (s^{-1}): to define the chemical's decay constant in the atmosphere, in s^{-1}. If the chemical is known not to be volatile, a value of 1E-20 can be entered.

- **kdeg water** (s^{-1}): to define the chemical's decay constant in water, in s^{-1}.

- **kdeg sed** (s^{-1}): to define the chemical's decay constant in sediments, in s^{-1}.

- **kdeg soil** (s^{-1}): to define the chemical's decay constant in soil, in s^{-1}.

- **Distribution coefficients - Kd sed, Kd soil, Kd susp** (dimensionless): to define the solid/liquid partition coefficients in sediments, soil and suspended solids, respectively. These fields are only compulsory in case there is no Kow available.

Most physical-chemical data described above are easily available. In case there are no measured values, the EPI Suite programme (USEPA 2009) provides QSAR to estimate them. Decay constants in air, water, soil and sediments are more difficult to obtain. They are usually found expressed as half-lives, rather than decay constants. In this case half-lives can be transformed into decay constants using Equation 1:

Decay constant = Ln2 / HL

Equation 1. Calculation of a decay constant.

Where HL is the half-life, in seconds. Usually, half-lives are expressed in hours or days, thus conversion to seconds is required for use in Equation 1. On the one hand, for half-lives in air, the AOPWIN model included

in EPI Suite can be used to get an estimate. Values for half-lives in water, soil and sediments are easier to find in published studies and chemical databases, especially values for water. In case only the value for the water compartment is reported, the following rules of thumb are suggested by the EPI Suite program (USEPA 2009):

- Half-life in soil can be approximated as twice that for water.

- Half-life in sediments can be approximated as nine times that for water.

The approach suggested above to estimate half-lives using EPI Suite is the method of choice to deal with this kind of data gaps in the USEtox model (Fantke 2015) and for this reason it is adopted. An alternative to this method, coming from an environmental risk assessment context, is the one defined in the Technical Guidance Document on Risk Assessment (TGDRA) by the European Commission (EC 2003), where half-lives in water, soil and sediments can be estimated based on biodegradability classes (readily biodegradable, inherently biodegradable, etc.) and log Kow (see section 2.3.6.5, p. 53 in the TGDRA).

Once the user has entered the data for the chemical substances under assessment, the second step is to use the 'Input to USES-LCA' table, which has two fields:

- **Row number** (enter a value from 1 to 30): Currently, fate calculations with USES-LCA can only be applied to one chemical at a time. For this reason, in this field the user must pick a row from the 'Substance-specific data' table. USES-LCA will calculate the fate of the chemical in the chosen row.

- **Emission compartment** (air/freshwater/seawater/agricultural soil): the user defines the emission compartment for the assessed chemical.

The results of USES-LCA fate modelling for the chosen chemical and release compartment are shown in the table 'Fate in environment', which shows values for the following parameters:

- **Substance**: Name of the chemical that has been assessed.

- **Deg$_a$, Deg$_w$, Deg$_{sed}$, Deg$_s$** (%): Fraction of the chemical substance, expressed in mass percentage, that is expected to degrade in the air, water, sediments, and soil compartments, respectively. The sum of these four parameters may not add up to 100% if the chemical is poorly degradable.

The third and final step is to copy the values obtained for Deg$_a$, Deg$_w$, Deg$_{sed}$, Deg$_s$ and paste them in the corresponding cells in the sheet 'Tier-2 input', under the field 'Fate in the environment (%)', according to the emission compartment considered (air, freshwater, seawater, soil).

Steps 2 and 3 need to be carried out for as many combinations of chemicals and emission compartments as needed.

3.3.3 Input data in 'Scenario'

After defining the wastewater composition in sheet 'Tier2-input', the scenario conditions for managing this wastewater are set up by the user in sheet 'Scenario'. In a Tier 2 assessment this sheet is managed in the same way as described for a Tier 1 assessment in section 3.2.2, with the exception of the field 'Type of

assessment' in the table 'Scenario data'. This field is a drop-down menu where the user must choose the option 'Tier 2'.

At this point, WW LCI will automatically calculate the LCI of each wastewater component individually. If the option 'Wastewater mixture' is set to 'yes' in the 'Scenario data' table, then WW LCI will also combine all wastewater components and calculate the LCI of this mixture according to their concentrations.

3.4 Automated error flags

To prevent errors, a set of automated warnings have been set up in sheets 'Tier1-input' and 'Scenario', as explained below.

3.4.1 Tier1-input

Six automated error flags have been implemented in this sheet. When data in the 'Influent composition' table are coherent, the box 'Automated error flags' shows the message 'No errors', otherwise the following messages can appear:

- **Enter either COD suspended or VSS, but not the two parameters at the same time**: VSS in wastewater involve a suspended COD and vice versa. If the user enters a value for VSS, then COD suspended is derived from this, with a default ratio of 1.406 kg COD_{susp}/kg VSS. If the user instead enters COD suspended, then the inverse of the mentioned ratio is used to derive VSS (1.406^{-1} kg VSS/kg COD_{susp} = 0.711 kg VSS/kg COD_{susp}). Entering the two parameters at the same time will lead to errors, as the user data might not respect the mentioned ratio and this leads to an error in the mass balance.

- **Choose to either use 'total' or specify the fractions, but do not use both at the same time**: for any of the four measures (COD, N, P, TSS), it is only allowed to enter either the total value, or to specify the fractions (soluble and suspended for COD, N, P; volatile and inert for TSS) but not both, even if they add up correctly.

- **User COD/TSS too low for a default VSS/TSS = 0.8; COD/TSS cannot be <1.125. Decrease VSS/TSS in cell B45 so that COD/TSS ≥1.125**: this flag appears if the user has entered values for total COD and total SS, where the ratio COD/TSS is lower than 1.125. This ratio appears as the product from our default values for the ratios VSS/TSS and COD_{susp}/VSS ($0.8 \cdot 1.406 = 1.125$ kg COD_{susp}/kg TSS). If the TSS entered by the user is high enough to exceed that ratio, this leads to a COD suspended value above the user COD total, which is not possible. If the user is certain about the data entered for COD and TSS, then the mass balance can be corrected by decreasing the VSS/TSS ratio in cell B45 up to a point where the COD/TSS ratio raises to (at least) 1.125. It must be highlighted that this flag has a live link to cell B45 (VSS/TSS) and B46 (COD_{susp}/VSS), which means that if the values in these cells are changed by the user, this will be reflected both in the flag text and in the error's logical formula. For example, if we change VSS/TSS from 0.8 to 0.7 and the error persists, the flag will read "User COD/TSS too low for a default VSS/TSS = 0.7; COD/TSS cannot be <0.984375. Decrease VSS/TSS in cell B26 so that COD/TSS ≥0.984375".

- **User COD/VSS lower than = 1.40625. Decrease default COD/VSS ratio in cell B46**: this flag appears if the user has entered values for total COD and VSS, where the ratio COD/VSS is lower than 1.406,

which is the default value for COD_{susp}/VSS. The problem caused by this is similar to the one described in the previous bullet, that is, the amount of VSS declared by the user, when converted to COD, exceeds the total COD declared by the user. If the user is certain about the data entered for COD and VSS, then the mass balance can be corrected by decreasing the default COD_{susp}/VSS ratio in cell B46 to match that of the user. It must be highlighted that this flag has a live link to cell B46 (COD_{susp}/VSS), which means that if the value in this cell is changed by the user, this will be reflected both in the flag text and in the error's logical formula. For example, if we change for COD_{susp}/VSS from 1.406 to 1.3 and the error persists, the flag will read "User COD/VSS lower than = 1.3. Decrease default COD/VSS ratio in cell B46".

- **COD cannot be zero**: the calculations in this sheet require that, as a minimum, COD total, COD soluble, COD suspended, or a combination of the last two is entered by the user.

- **TSS cannot be lower than COD suspended/1.40625. Increase default COD suspended/VSS ratio in cell B46 to match user ratio**: when the user enters a value for COD suspended and a value for TSS, where the latter is lower than the ratio COD suspended/1.40625, this leads to an error in the mass balance, since the VSS calculated from COD suspended (by dividing by the ratio 1.40625 kg COD_{susp}/kg VSS) will result in a higher value than the TSS declared by the user. If the user is certain about the data entered for COD suspended and TSS, then the mass balance can be corrected by increasing the ratio 1.40625 in cell B46 to match that of the user. As explained in previous bullets, the text and the formula in this flag is linked to the value in cell B46, so the flag text will change if the user modifies the value in cell B46.

3.4.2   Scenario data

A set of automated warnings have been set up in the box 'Automated error flags'. When all input data are coherent, this box shows the message 'No errors', otherwise any of the following errors can appear:

- **Wastewater mixture mass sum does not equal 1:** this error message should only appear in a Tier 2 assessment. The mass percentages attributed to each of the chemical substances present in the assessed mixture, in column B in tables 'Chemical-specific data' and 'Metals' are incomplete or do not add up to 1 kg components/kg wastewater.

- **WWTP capacity sum does not add up to 100%:** the percentages of wastewater treated in each of the five WWTP sizes in the 'WWTP capacity' sub-table do not add up to 100%.

- **Septic sludge disposal scenario does not add up to 100%**: the percentages of septic sludge sent to either safe or unsafe disposal in the 'Septic sludge management' sub-table do not add up to 100%.

- **Population connection profile not correct or sum does not equal 100%:** the percentages of wastewater collection and treatment in sub-table 'Wastewater collection and treatment scenario' are incomplete or do not add up to 100%.

- **Wastewater discharge scenario does not add up to 100%:** the percentage of discharge to inland waters and sea water in sub-table 'Wastewater discharge' do not add up to 100%.

- **Percentage of anaerobic digestion cannot exceed 100%**: percentage of AD is set above 100%.

- **Percentage of CHP cannot be higher than percentage of anaerobic digestion**: the percentage of AD+CHP in sub-table 'Sludge treatment in WWTPs' is a sub-set of the percentage of AD, so it cannot be higher, but just lower or equal to the percentage of wastewater treated in WWTPs with AD.

- **Ambient temperature profile incomplete**: one or more of the temperatures are missing in sub-table 'Ambient temperature'.

- **Percentage of N removal cannot exceed sum of secondary + tertiary treatment percentages**: the percentage of wastewater treated in WWTP with N removal in sub-table 'Nutrient removal in WWTPs' cannot be higher than the sum of cells L14 and L15, establishing the percentage of wastewater treated in WWTPs with secondary and tertiary treatment, respectively.

- **Percentage of P removal cannot exceed sum of secondary + tertiary treatment percentages**: the percentage of wastewater treated in WWTP with P removal in sub-table 'Nutrient removal in WWTPs' of cells L14 and L15, establishing the percentage of wastewater treated in WWTPs with secondary and tertiary treatment, respectively.

- **Methane correction factors must be between 0 and 1**: the value of one or more of the values in sub-table 'Methane correction factors' is above 1 or negative. All values must be between 0 and 1.

- **Wastewater reuse needs to be between 0% and 100%**: the percentages of treated and untreated wastewater reuse in sub-table 'Wastewater reuse' do not add up to 100%.

- **Irrigation water supply mix must add up to 100%**: the percentages of surface water, groundwater and desalinated water in sub-table 'Wastewater reuse' do not add up to 100%.

- **Crop production mix must add up to 100%**: the percentages of different crops in sub-table 'Wastewater reuse' do not add up to 100%.

- **Irrigation supply mix and crop production mix cannot coexist, choose one set only**: the irrigation supply mix applies when freshwater resources are not constrained. In such a case the crop production mix must be set to zero. When freshwater resources are constrained, the irrigation supply mix must be instead set to zero.

- **Introduce irrigation supply mix or crop production mix**: this error appears if percentages of either treated or untreated wastewater reuse have been declared, but no irrigation supply mix or crop production mix has been defined to quantify the effect of wastewater reuse.

- **Untreated wastewater reuse is not possible if there is no untreated wastewater**: this error appears if a percentage of untreated wastewater reuse is declared, but in sub-table 'Wastewater collection and treatment' the percentage of untreated wastewater is zero (sum of cells L11 and L18).

- **Treated wastewater reuse is not possible if there is no treated wastewater**: this error appears if a percentage of treated wastewater reuse is declared, but in the sub-table 'Wastewater collection and treatment' the percentage of treated wastewater is zero (sum of cells L13, L14, L15 and L17).

- **Secondary treatment technology must add up to 100%**: the percentages of wastewater treated in by activated sludge and stabilization ponds in sub-table 'Secondary treatment technology' do not add up to 100%.

- **Define the stabilization pond average capacity in m3/day**: this error appears if a percentage of wastewater has been declared as treated by waste stabilization ponds in sub-table 'Secondary treatment technology', but no capacity for this type of plants has been declared in sub-table 'WWTP capacity'.

- **Primary treatment technology must add up to 100%**: this error appears if the percentages of conventional and chemically-enhanced primary treatment in sub-table 'Wastewater reuse' is higher than 100%.

- **Increase % of WWTPs with larger capacity, to account for anaerobic digestion. Plants <1,100 m3/day do not have anaerobic digestion**: This error appears when the declared percentage of wastewater treated in WWTPs with AD is higher than the percentage of wastewater treated in WWTPs with capacities above 1,100 m^3/day, which are the ones with the option of AD in the model. WWTPs with capacities below 1,100 m^3/day are assumed not to feature AD in any case.

- **Sludge disposal scenario sum does not equal to 100%**: the sum of percentages for sludge disposal does not add up to 100%.

3.5 Life cycle inventory results

There are three sheets showing the LCI results with different formats, as described below.

3.5.1 LCI

The sheet 'LCI' (Figure 8) is structured as an inventory table where the columns correspond to chemical substances in wastewater and the rows correspond to the exchanges of the assessed product system with the technosphere and the environment. The functional unit in this LCI table is 1 kg of the pertinent substance released in wastewater according to the scenario conditions established in the 'Scenario' sheet. In case the user is modelling a chemical mixture, then this sheet will show in column AZ the LCI associated to the mixture. The exchanges in this inventory table are arranged according to the following structure:

- **Inputs**
  - From technosphere
    - To WWTP
    - To sludge transport
    - To sludge composting
    - To sludge landfilling
    - To sludge incineration
- **Outputs**
  - To nature
    - Emissions from closed sewer
    - Emissions from WWTP
    - Emissions from environmental degradation
    - Emissions from sludge composting
    - Emissions from sludge landfilling
    - Emissions from sludge incineration

- Emissions from sludge application to soil and wastewater reuse
  - To technosphere
    - From WWTP
    - From sludge landfilling
    - From sludge incineration
    - From sludge application to soil and wastewater reuse

The table might show negative values, especially in the 'Outputs of technosphere' section. These are interpreted as credits.

Figure 8. Screenshot of the 'LCI' sheet.

3.5.2 Ready to CSV

The sheet 'Ready to CSV' (Figure 9) is arranged in the format required for exporting the LCIs to SimaPro (see section 4.1). The sheet is structured as an inventory table where the columns correspond to chemical substances in wastewater and the rows correspond to the exchanges of the assessed product system with the economic system and the environment. The exchanges in this inventory table are arranged according to the following order:

- Inputs from technosphere, excluding activities considered as waste treatment processes by SimaPro.

- Air emissions

- Water emissions

- Soil emissions

- Activities classified as waste treatment processes by SimaPro.

The functional unit in this LCI table is 1 kg of the pertinent chemical substance released in wastewater according to the scenario conditions previously established. In case the user is modelling a chemical

mixture, this sheet shows, besides the LCI of each individual chemical, the LCI associated to the mixture, reflecting the composition previously established. The mixture LCI is shown in column AZ. The results might show negative values for certain flows, which are interpreted as credits.

Besides the LCIs for wastewater discharges, this sheet also contains, in columns BA to BD, several inventories to model the global marginal market for N fertilizers, used to account for substituted fertiliser through agricultural reuse of sludge, compost and wastewater. Further details about this are included in the model documentation Muñoz (2021).

Figure 9. Screenshot of the 'Ready to CSV output' sheet.

In this sheet the heading of each column contains the name of the assessed chemical substance, according to the following structure:

Name of chemical, in wastewater {country}

The only exception to this is the LCI for the wastewater mixture (column AZ), which is labelled as:

Wastewater mixture {country}

In row 6 a comments section for each data set is provided, which describes in more detail the data set, namely the particular scenario conditions under which the LCI has been calculated. Below we show an example for the chemical diclofenac, discharged in Denmark:

Inventory for Diclofenac, in wastewater {DK}. WASTEWATER SCENARIO: Domestic, faecal water discharge. 0% primary treatment. 2% secondary treatment. 89% tertiary treatment. 9% septic tank. 0% only sewer collection and discharge. 0% no sewer collection and discharge. 0% latrines. 0% open defecation. SLUDGE TREATMENT: 49.66% of sludge treated in WWTPs with anaerobic digestion, 24.83% of sludge treated in WWTPs with anaerobic digestion and cogeneration. 100% septic sludge is safely treated in WWTPs and 0%

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is unsafely discharged. WASTEWATER REUSE SCENARIO: 0% treated wastewater reuse and 0% untreated wastewater reuse. SLUDGE DISPOSAL: 0% composting. 67.77% landfarming. 1.28% landfilling-controlled. 0% landfilling-uncontrolled. 31% incineration. WW LCI by 2.-0 LCA consultants, version 4.0, March 2021.

This provides basic information about the LCI data set when imported into SimaPro, that can be seen as meta-data.

The exchanges names in the table rows are in accordance with data sets from the consequential unit process model in ecoinvent 3.6, as incorporated in SimaPro. The names can be manually changed to reflect any of the other systems models in this database, or any other database.

Although the main purpose of this table is the conversion to a CSV file, it also allows for analysis of the obtained LCIs. This can be done by means of the filters applied in row 7. Also, in column BE the activity originating the exchange can be identified, e.g. wastewater treatment, sludge landfilling, etc.

3.5.3   Ready to GaBi

This sheet contains the LCI results for wastewater and for the global marginal market for N fertilizers, used to account for substituted fertiliser through agricultural reuse of sludge, compost and wastewater (see the model documentation for details). The data are presented in a format for export to the GaBi software (see section 4.2). Besides formatting, the information in this sheet differs from that in the 'Ready to CSV' sheet in the following aspects:

- The only LCI reported is that for a wastewater mixture, and not for individual wastewater components declared by the user.

- The number of exchanges reported is the same, but each flow is reported only once. For example, CO_2 emissions from different sources are added up in a single, total figure, given that GaBi does not allow the repetition of flows.

Another limitation is that uncertainty factors, which can be exported to SimaPro from the 'Uncert' sheet (see section 3.6.1) are currently not available for export to GaBi.

3.6   Other sheets in WW LCI

3.6.1   Uncert

This sheet contains the assessment of uncertainty for each flow in the LCI, using the pedigree matrix. In WW LCI each flow is attributed a mean value and an uncertainty factor, attempting to quantify its variation assuming a lognormal distribution, as done in the ecoinvent database (Weidema et al. 2013). The uncertainty factor corresponds to the square of the geometric standard deviation (σ_g^2), reflecting the 95% confidence interval. As an example, for a value of $\sigma_g^2 = 1.5$, the lower bound of the confidence interval is calculated as the mean divided by 1.5, while the upper bound is calculated as the mean times 1.5. These bounds are expected to contain 95% of the measured values.

Figure 10. Screenshot of the 'Uncert' sheet.

The data in this sheet are organized with the same format as in the 'Ready to CSV' sheet, with the difference that the values shown, instead of mean values, correspond to the uncertainty factors. The underlying assessment of data quality (basic uncertainty, reliability, completeness, temporal correlation, geographic correlation and technological correlation) is shown in columns BB to BM, where the user can modify the default values assigned to each flow.

The uncertainty factors can be exported as part of the LCI results to the software SimaPro (see section 4.1.2), but currently not to GaBi.

3.6.2 Parameters

This sheet (Figure 11) provides an overview of all variables used in WW LCI. Each variable is defined, and default values are provided, together with a reference and/or description. All these parameters and the corresponding comment fields can be modified by the user.

Figure 11. Screenshot of the 'Parameters' sheet.

	Value	Definition/comments/source
Parameters for degradation in the environment		
MCF_w if direct discharge from closed sewer, worst case	0.15	Fraction of water compartments in the environment under anaerobic conditions, worst case. Applies to direct discharges from closed sewers and treated effluents. Based on IPCC (2006c)
$MCF_{open sewer}$ if direct discharge from open sewer, worst-case	0.75	Fraction of open sewer under anaerobic conditions, worst case. Applies to direct discharges only from open sewers (warm climate, stagnant). Based on IPCC (2006c), table 6-3 and Doorn and Liles (1999)
MCF_{sed}	0.5	Fraction of sediments compartments in the environment under anaerobic conditions. Muñoz et al. (2013)
MCF_{def}	0.043	Fraction of organic matter in human faeces degrading under anaerobic conditions after open defecation. Estimate based on Winrock International India (2008)
f_{ox}	0.5	Fraction of methane formed in sediments compartments that is oxidized to carbon dioxide. Muñoz et al. (2013)
f_{CH4}	0.6	Fraction of carbon converted to methane when degraded under anaerobic conditions (Muñoz et al. (2013)
EF_{air}	0.01	N2O emission factor for the air compartment: fraction of N in the air compartment that is converted to N-N2O through re-deposition in soil and water (kg N-N2O / kg N). Muñoz et al. (2013)
EF_s	0.01	N2O emission factor for the soil compartment: fraction of N in soil that is converted to N-N2O (kg N-N2O / kg N). Muñoz et al. (2013)
EF_w	0.005	N2O emission factor for the water compartment: fraction of N in water that is converted to N-N2O / kg N). Muñoz et al. (2013)
EF_{sed}	0.005	N2O emission factor for the sediments compartment: fraction of N in sediments that is converted to N-N2O (kg N-N2O / kg N). Muñoz et al. (2013)
T-dependence of methane production in open sewers: Tdep = a $^{(T-b)}$ 'a' parameter	1.05	Function used to estimate the effect of ambient temperature on potential CH4 emissions from direct discharges lacking connection to sewer (Chaosakul et al. 2014)
T-dependence of methane production in open sewers: Tdep = a $^{(T-b)}$ 'b' parameter	20	Function used to estimate the effect of ambient temperature on potential CH4 emissions from direct discharges lacking connection to sewer (Chaosakul et al. 2014)
Parameters for WWTP infrastructure	**Value**	**Definition/comments/source**
$Infra_{AS}$	0.84	Ratio infrastructure mass in WWTP with secondary treatment without anaerobic digestion of sludge to infrastructure in a WWTP with secondary treatment and anaerobic digestion of sludge. Estimate.
WWTP infrastructure input for WWTPs > 55,000 m3/d (unit/m3)	6.06E-10	Amount of WWTP infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 4.7E10L/year
WWTP infrastructure input for WWTPs 28,000-55,000 m3/d (unit/m3)	1.99E-09	Amount of WWTP infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1.1E10L/year
WWTP infrastructure input for WWTPs 5,500-28,000 m3/d (unit/m3)	5.69E-09	Amount of WWTP infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 5E9L/year
WWTP infrastructure input for WWTPs 1,100-5,500 m3/d (unit/m3)	2.66E-08	Amount of WWTP infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1E9L/year
WWTP infrastructure input for WWTPs <1,100 m3/d (unit/m3)	1.75E-07	Amount of WWTP infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1.6E8L/year
Sewer infrastructure input for Sewers > 55,000 m3/d (km/m3)	1.24E-07	Amount of sewer infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 4.7E10L/year
Sewer infrastructure input for Sewers 28,000-55,000 m3/d (km/m3)	1.68E-07	Amount of Sewer infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1.1E10L/year
Sewer infrastructure input for Sewers 5,500-28,000 m3/d (km/m3)	2.18E-07	Amount of Sewer infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 5E9L/year
Sewer infrastructure input for Sewers 1,100-5,500 m3/d (km/m3)	2.82E-07	Amount of Sewer infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1E9L/year
Sewer infrastructure input for Sewers <1,100 m3/d (km/m3)	3.76E-07	Amount of Sewer infrastructure attributed to 1 m3 wastewater, according to Ecoinvent 3, average sewage, plant capacity 1.6E8L/year
Parameters for conventional primary treatment WWTP	**Value**	**Definition/comments/source**
$Infra_{PRIM-AD}$	0.46	Ratio infrastructure mass in WWTP with primary treatment and anaerobic digestion of sludge to infrastructure in a WWTP with secondary treatment and anaerobic digestion of sludge. Estimate.
$Infra_{PRIM}$	0.31	Ratio infrastructure mass in WWTP with primary treatment without anaerobic digestion of sludge to infrastructure in a WWTP with secondary treatment and anaerobic digestion of sludge. Estimate.
Suspended solids removal rate in conventional primary treatment (%)	60%	Typical SS removal in conventional primary treatment is 60% (Von Sperling 2007 vol 1, p.221 table 4.9)
Fsludge in Primary Treatment compared to full WWTP with secondary treatment	67%	Typical SS removal in enhanced primary treatment is 60% and 90% in WWTP with activated sludge (Von Sperling 2007 vol 1, p.221 table 4.9)
Fdeg in Primary Treatment compared to full WWTP with secondary treatment	0%	Assumption. Main removal process for COD, SS, etc. in a primary settling tank is removal of particulate matter
Fair in Primary Treatment compared to full WWTP with secondary treatment	0%	Assumption. Little volatilization expected in a primary settling tank.
WWTP infrastructure relative to a WWTP with secondary/tertiary treatment (unit/m3)	30%	Physical infrastructure of a WWTP with primary treatment compared with a WWTP with secondary/tertiary treatment. Assumption
Parameters for chemically-enhanced primary treatment WWTP	**Value**	**Definition/comments/source**
Suspended solids removal rate in enhanced primary treatment (%)	75%	Typical SS removal in conventional primary treatment is 75% (Von Sperling 2007 vol 1, p.221 table 4.9)
Fsludge in Primary Treatment compared to full WWTP with secondary treatment	83%	Typical SS removal in enhanced primary treatment is 75% and 90% in WWTP with activated sludge (Von Sperling 2007 vol 1, p.221 table 4.9)
FeCl3 consumption (kg/kg SS removed)	0.15	Average from two plants: el Salitre in Bogotá, Colombia (Kingsley 2011) and Point Loma in San Diego, US (City of San Diego 2016)
Chemical P removal level (%)	25%	Assumption
FeCl3 excess for P removal (kg added/kg theoretical stoichiometric requirement)	1.5	Assumes iron chloride consumption for chemical phosphorus removal requires an additional 50% in excess (Paul et al. 2001)
Polyelectrolyte consumption (kg/kg SS removed)	0.002	Average from two plants: el Salitre in Bogotá, Colombia (Kingsley 2011) and Point Loma in San Diego, US (City of San Diego 2016)
Parameters for secondary treatment by activated sludge	**Value**	**Definition/comments/source**
Y, COD based	0.5	Coefficient of biomass production (g VSS/g COD removed), p. 94 in Von Sperling (2007, vol. 2)
kd	0.085	Endogenous respiration coefficient or bacterial decay coefficient (day-1), p. 92 in Von Sperling (2007, vol. 2)
SRT biological treatment, activated sludge system	5	Solids retention time in biological treatment (days). Values for activated sludge range between 4 to 10 days. For extended aeration goes to 18 to 30 days (Von Sperling, vol 1)
COD content in VSS	1.42	Chemical oxygen demand of volatile solids (biomass) with an empirical composition of C5H7NO2 (g COD/g VSS), from Von Sperling (2007, vol 5. p. 28)
N-N2O (kg emitted per kg N biodegraded)	0.005	Fraction of nitrogen input converted to N-N2O. Average from Dalemo (1997) (0.15%) and Doka (2007) (0.68%)

Figure 11. Screenshot of the 'Parameters' sheet.

3.6.3 Database

The sheet 'Database' (Figure 12) contains statistics and other data about wastewater management, sludge disposal, etc., in all supported countries. These data are used to populate the 'Scenario data' table in the 'Scenario' sheet. These default data can be modified by the user if necessary.

Figure 12. Screenshot of the 'Database' sheet.

3.6.4 Refs

This sheet contains all the references cited in any of the other sheets in WW LCI, listed alphabetically.

3.7 Intermediate calculation sheets

As previously mentioned, there are a number of visible sheets, not intended to be manipulated by the user. It must be stressed that these sheets are not protected, thus care should be taken not to modify their content.

- **Sewer**: includes the calculation of emissions associated to closed sewers.

- **Metals**: includes basic data on the 17 metals supported by WW LCI, including removal factors from literature.

- **Env deg**: calculates emissions associated to the release of chemical substances to the environment without treatment.

- **Energy&AD**: includes all the underlying data to calculate electricity and heat energy balances by the WWTPs. Section 1 calculates electricity consumption for different WWTP activities. Section 2 calculates the heat energy balance for anaerobic digestion of sludge.

- **Pri**: performs the mass and energy balance associated to the activities taking place in a WWTP with only primary treatment.

- **Pond**: performs the mass and energy balance associated to the activities taking place in a waste stabilization pond.

- **AS**: performs the mass and energy balance associated to the activities taking place in a WWTP with primary and secondary treatment through activated sludge.

- **Tert**: performs the mass and energy balance associated to the activities taking place in a WWTP with primary, secondary treatment and tertiary treatment.

- **Septic**: performs the mass and energy balance associated to septic tanks, as well as the transport of septic sludge to a WWTP, where it is treated.

- **Reuse**: calculates the substituted amounts of irrigation water and crops as a result of treated and untreated wastewater reuse.

- **Sludge**: calculates the composition of sludge leaving the WWTPs, the sludge transport service, and the inventory of exchanges associated to landfilling and incineration of sludge.

- **Landfill**: contains the underlying data for modelling controlled and uncontrolled landfilling of different chemical elements.

- **Incin**: contains the underlying data for modelling incineration of different chemical elements.

- **Compost**: performs the mass and energy balance of sludge composting.

- **Landfarm**: calculates the emissions and substituted mineral fertilizers associated to application of sludge, compost and reused wastewater in agriculture.

- **Transpose**: aggregates the contribution to the final LCI from the previous sheets.

4 Exporting and importing LCIs

Although WW LCI can be used as a stand-alone tool, linking it to other activities in the life cycle of products is desirable. Currently, it is designed to export data in CSV format for import to SimaPro, as well as directly from Excel format to the GaBi software. In this section we explain the procedure to export and import LCIs.

4.1 SimaPro

4.1.1 Exporting LCIs in CSV format, without uncertainty factors

Before performing the export, the CSV file converter needs to be downloaded from the 2.-0 LCA consultants' website:

- Login to the members-only section of the Initiative, at: http://lca-net.com/clubs/wastewater/ as explained in section 2.

- Download the file CSV converter (Figure 13).

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CSV converter

CSV converter Macro file to convert life cycle inventories into comma separated value (CSV) files for import to SimaPro.

Figure 13. Screenshot of the CSV converter file link in the 2.-0 LCA consultants' website.

Once the CSV converter file is downloaded, the steps to perform the export are as follows:

- Open the file 'CSV converter'. When prompted, click on 'Enable Macros'.

- In the WW LCI excel file go to the sheet 'Ready to CSV output' and copy the range A1:BD801.

- in the CSV converter paste the data range as values (this is done in the menu Edit\Paste Especial... and ticking the box 'Values' (Figure 14). It is important that the pasted data range starts in cell A1 in the CSV converter workbook.

Figure 14. Screenshot of the 'Paste Special' window in Excel.

- The pasted data includes not only the LCIs for wastewater, but also the LCIs associated to the marginal nitrogen fertilizer mix, in columns BA to BD. It is necessary to export these fertilizer LCIs (and import them into SimaPro) at least on the first export-import operation. Once they are available in SimaPro, columns BA to BD are no longer necessary and can be removed.

- When not all available columns for chemical substances are used, the data range will contain one or more columns with empty data. These columns must be deleted. As an example, in Figure 15 columns U to AH can be deleted. When these columns are deleted, the comments originally placed in column BE will move to a previous column. This can be corrected manually in order to make sure that the comments make it into SimaPro. Otherwise, the CSV conversion will still work, but the comments will be lost.

Figure 15. Screenshot of the CSV converter file after pasting a data range with LCIs. Empty columns can be deleted.

- A second, optional step, is to clean the data range to remove unnecessary zeroes. Select rows 8 to 801 starting at column E and finishing at the last column with data.

Figure 16. Screenshot of the CSV converter file. Selecting rows to delete unnecessary zeroes.

- Then go to to Edit\Replace... and type a value of zero in the 'Find what' field. Also, check the boxes 'Match case' and 'Find entire cells only' (Figure 17). Then click 'Replace All' and finally click 'Close'. The data range should now only display values $\neq$ 0 (as in Figure 18). As previously mentioned, this step is optional. On the one hand, if zeroes are not removed, LCIs imported to SimaPro will contain inventory flows with zeroes. On the other hand, if zeroes are removed, these inventory flows will not be present at all in the import to SimaPro.
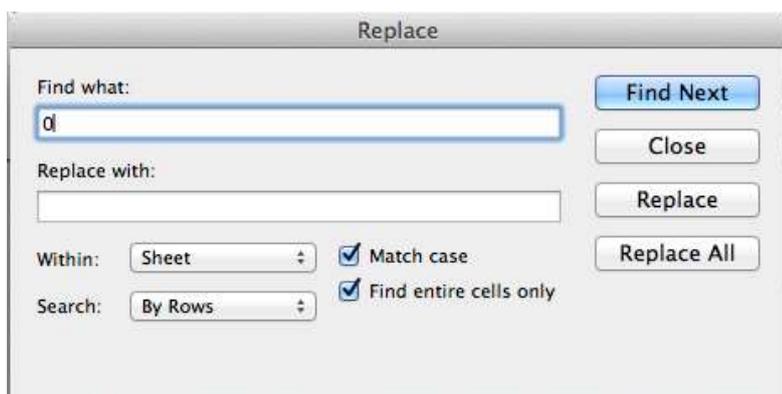
Figure 17. Screenshot of the 'Replace' window and the required settings to delete unnecessary zeroes.

Figure 18. Screenshot of the CSV converter file after deleting unnecessary zeroes.

- A third and again optional step is to remove entire rows where the flow name in column B is zero (see example in Figure 19). If these rows are not removed, during the import operation to SimaPro a substance '0' with mass properties will be created and will appear in the imported LCIs. Although this in practice has no implications when it comes to perform calculations in Simapro, it is meaningless information and as such can be kept out.

Figure 19. Screenshot of the CSV converter file with rows where the flow name is '0'.

Now the data range in Excel is ready to be converted to CSV format. This is done as follows:

- Go to Tools\Macro\Macros...

- The Macro 'MakeFileCSV' should be visible in the Macro window (Figure 20). Click on 'Run'.
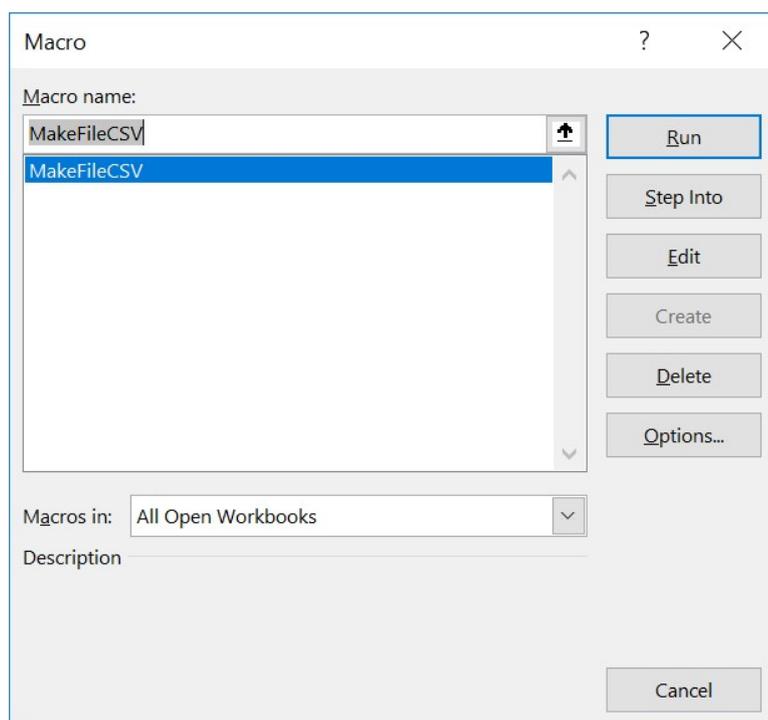
Figure 20. Screenshot of the Macro window in the CSV converter file.

To the question 'Do you want to include uncertainties?' (Figure 21). Click 'No'.
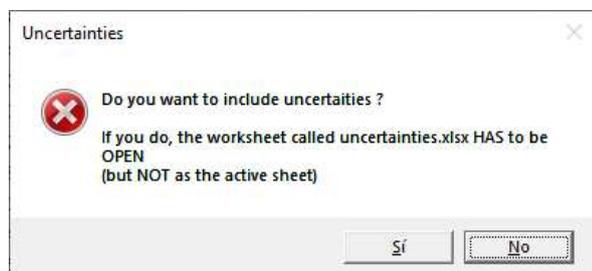
Figure 21. Screenshot of the 'uncertainties' question when running the Macro in the CSV converter file.

Now the macro will create two files, in the same folder where you have stored the CSV converter (see Figure 22):

- 'CSV_for_import_into_SP.CSV': this is the actual CSV file containing the LCIs. Click 'OK'.
- 'Control_file.txt': Click 'OK'. This file shows a summary of the conversion process. It can be deleted.
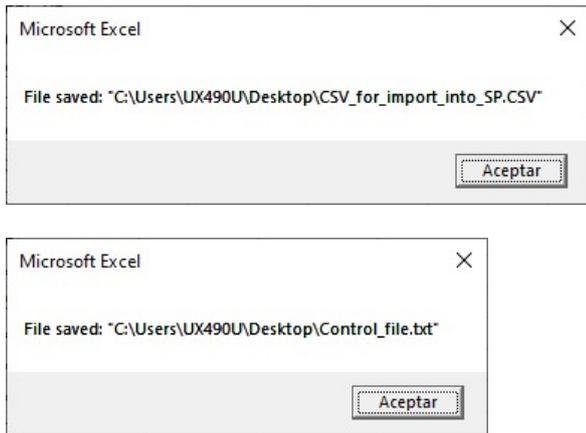
Figure 22. Screenshots of the Macro windows showing the location of the files produced.

4.1.2 Exporting LCIs in CSV format, including uncertainty factors

In order to export LCIs to SimaPro including uncertainty factors, the procedure is essentially the same as described in the previous section, up to the point where the macro asks the question 'Do you want to include uncertainties?' (Figure 21). At this point, the procedure is as follows:

- Open a new Excel workbook, and save it with the name 'uncertainties.xlsx'. If the workbook is not configured with English language, make sure the active sheet is named 'Sheet1'.

- Copy from range A1:BD801 in WW LCI's sheet 'Uncert'.

- In this 'uncertainties' workbook, paste in cell A1 the content, as values, from range A1:BD801 in WW LCI's sheet 'Uncert'. If data cleaning operations have been conducted in the LCI in its ready to CSV format, such as removing rows or columns, the same must be done in the 'uncertainties' workbook, since both matrices must have the same number of rows and columns i.e. one uncertainty factor for each man value.

- Now return to the CSV converter, making it the active one. Go to the menu Tools\Macro\Macros…, and run the 'MakeFileCSV' macro.

- This time, when asked the question 'Do you want to include uncertainties?', click 'Yes'.

This will create the same two files described in section 4.1.1: CSV_for_import_into_SP.CSV, containing the LCIs with uncertainty factors, and Control_file.txt, which can be safely deleted.

4.1.3 Importing LCIs in CSV format into SimaPro

In order to perform the iumport operation, it is necessary to have ecoinvent v3.6 in SimaPro. The data set names currently used by WW LCI refer to this ecoinvent version.

The procedure is as follows:

- Open SimaPro and the database where the inventories are going to be imported.

- Make sure the 'Ecoinvent 3 – consequential – unit' library is activated. Do this by going to the 'Libraries' section in the SimaPro explorer, and tick in the previously mentioned library if needed (Figure 23).
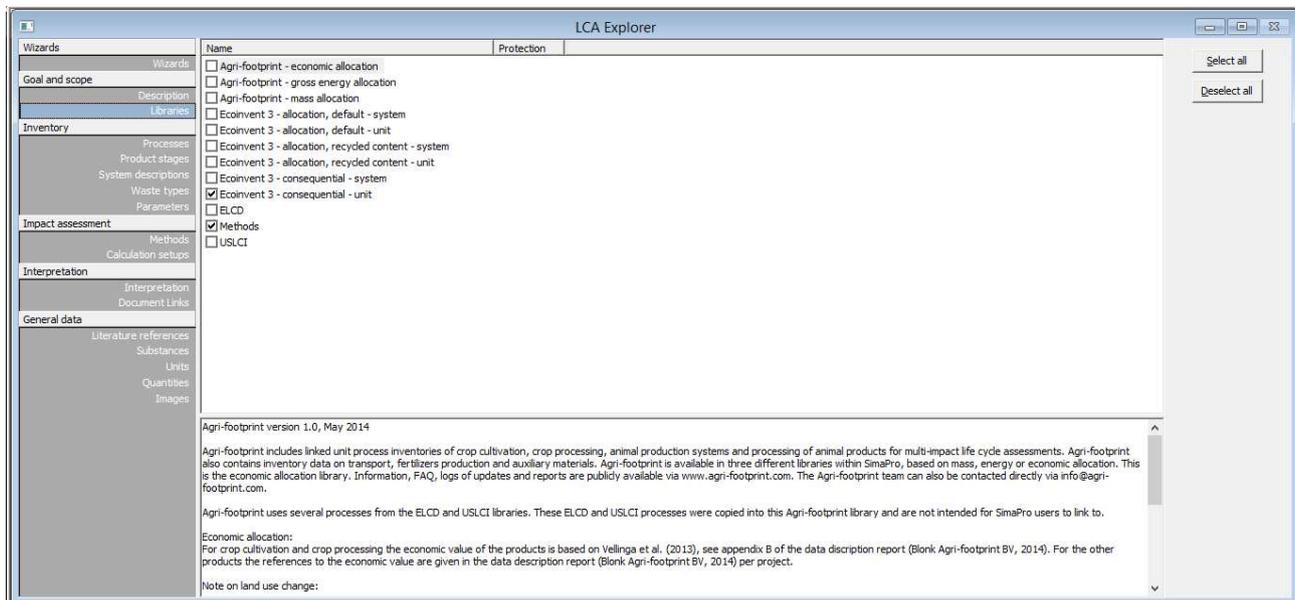
Figure 23. Screenshot of the 'Libraries' section in SimaPro.

- Go to 'File\Import\' and the import window will pop up. Click on 'Add' and browse to find the CSV file previously created with the CSV converter 'CSV_for_import_into_SP.CSV'.

- The settings for the import operation should be as shown in Figure 24 below.
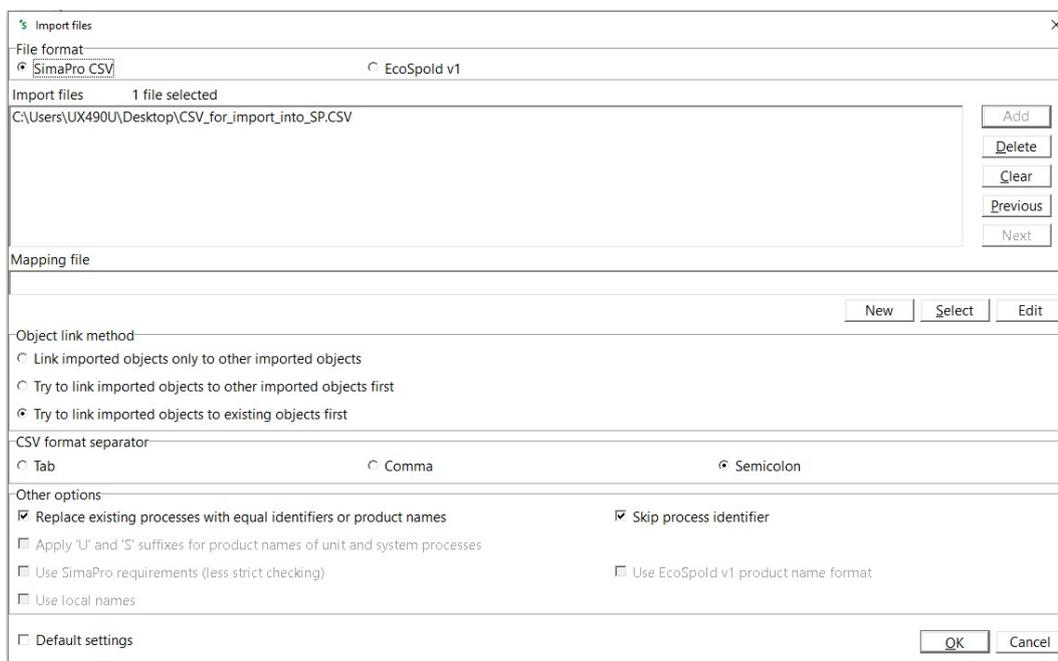
Figure 24. Screenshot of the import window in SimaPro, with the settings to perform the import.

- Click 'OK' and the import operation will start. After a few seconds, the Import overview window will appear, as shown in Figure 25 below. The number of data sets to be added or replaced are shown in the summary screen. This screen is for information only. Click 'OK' and the actual import will start.
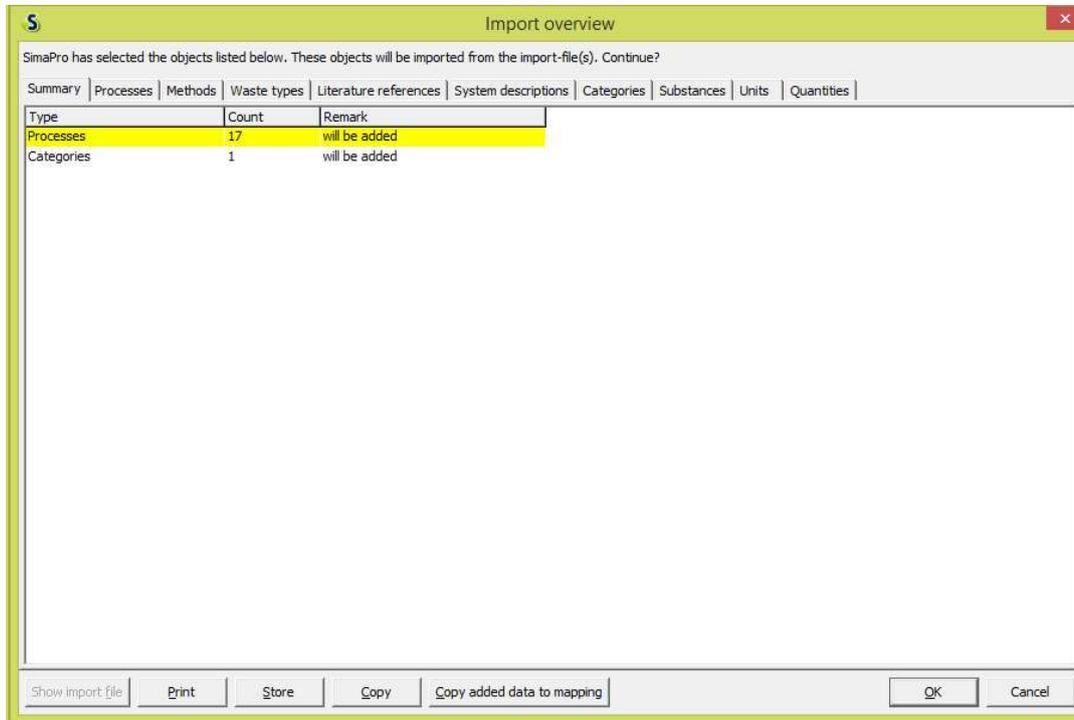
Figure 25. Screenshot of the import overview window in SimaPro.

- Once the import is finished, in the LCA Explorer in SimaPro, under 'Processes\Material\' a new folder will appear, named '_WW LCI' as shown in Figure 26 below. This folder includes the imported LCIs, ready to be used.
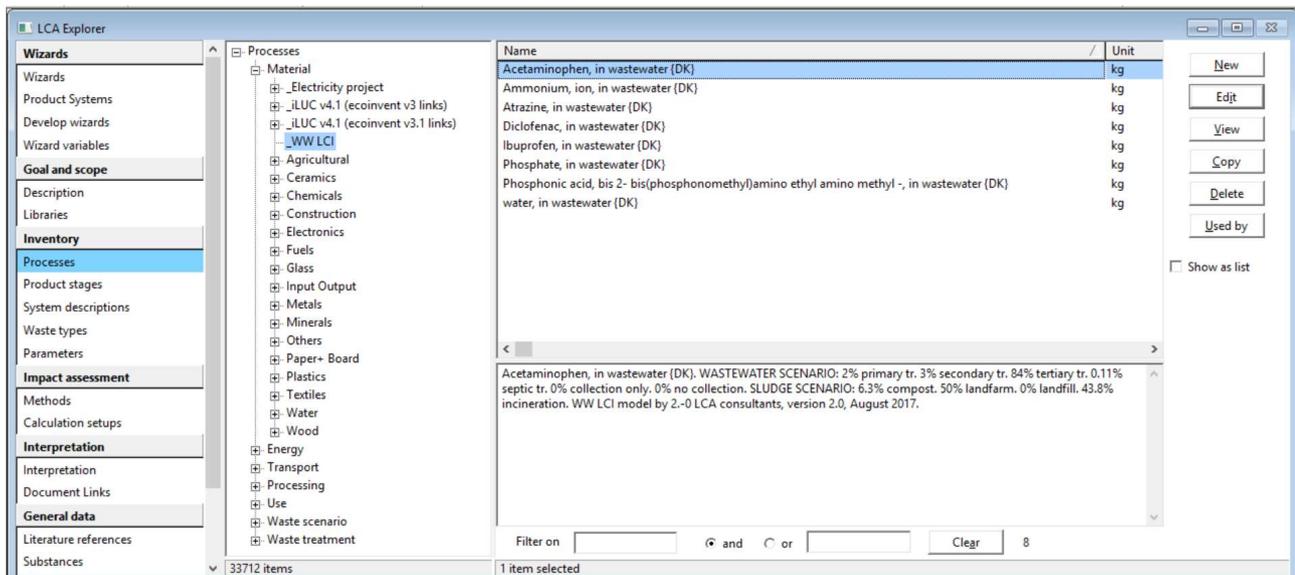
Figure 26. Screenshot of the LCA explorer in SimaPro, showing the list of imported data sets.

4.1.4 Linking WW LCI to other ecoinvent system models

WW LCI is designed to link by default to the ecoinvent consequential system model. However, it is possible and relatively easy to link the LCIs to any of the other existing ecoinvent system models. The link to ecoinvent in WW LCI is done in the sheet 'Ready to CSV output' in WW LCI, where in column B, the ecoinvent data set names are shown. In order to link to an alternative system model, for example the 'Allocation at the point of substitution' (APOS) system model, the following steps must be followed:

- Select the entire B column in the 'Ready to CSV output' sheet,

- Open the 'Find and Replace' box in Excel. In the 'Replace' ribbon, type 'Conseq' in the 'Find what:' line and type 'APOS' in the 'Replace with:' line, as seen in Figure 27 below.

- Finally click on 'Replace All'.
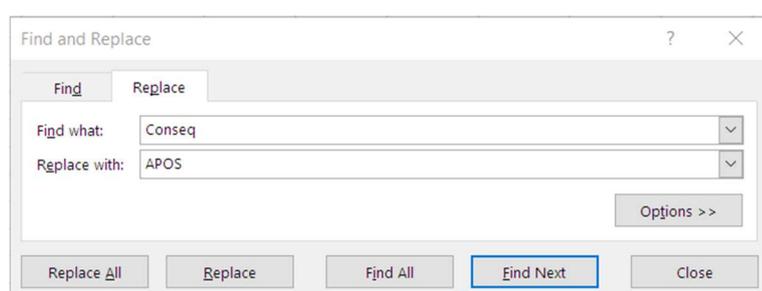
Figure 27. Screenshot of the Find and Replace dialog box in Excel.

With this operation, all ecoinvent data set names will be changed according to the APOS system model, to which they will be linked when data sets are imported to SimaPro. The only additional remark concerning the import operation is that the targeted system model (APOS in our example) must be active in the SimaPro database before importing (see Figure 23).

It must be highlighted, though, that WW LCI applies substitution, leading to credits related to co-products (substituted energy, fertilizers, etc). These credits might be inconsistent with other (attributional) LCI modelling approaches. The user must decide how to deal with these co-products when a different ecoinvent system model is used.

4.2 GaBi

As opposed to the export-import operation in CSV format for SimaPro, exporting data to the GaBi software can be performed directly from the WW LCI file in Excel. It must be highlighted that when preparing this manual, the actual export-import procedure for GaBi, as described in its user manual (p. 144 in PE 2012), does not work. However, we describe below a workaround to overcome this limitation.

The LCI data in a compatible format for GaBi are located in the sheet 'Ready to GaBi'. This sheet contains two LCIs:

- The first LCI, starting in column A, corresponds to the discharge of a wastewater mixture, as defined by the user. As opposed to the export operation in CSV format for SimaPro, WW LCI currently does

not support the export of the LCIs associated with the individual wastewater components, but only to the mixture they contribute to.

- The second LCI, starting in column K, corresponds to the global marginal market for N fertilizers, used to account for substituted fertilizer through agricultural reuse of sludge, compost and wastewater (see the model documentation for details). Using this LCI instead of the corresponding ecoinvent dataset is strongly recommended.

Figure 28. Screenshot of 'Ready to GaBi' sheet in WW LCI.

4.2.1   Exporting and importing the wastewater mixture LCI

Exporting the LCI for a wastewater mixture requires, first of all, filtering out any flows with the name '0'. This is done with the filter in cell B128 with the heading 'Flows' (see Figure 29). This will avoid the import of such unnecessary flows to GaBi. As an optional additional step, the same can be done with flows that have a zero value in columns D or E, thus ensuring that the exported LCI includes only flows with actual values.

Figure 29. Deselecting flows with a name zero in the 'Ready to GaBi' sheet.

At this point, the procedure to import this LCI to GaBi is the following:

- Select the 'Inputs' data range, from column A to J, containing the rows with the filtered values for input flows, and copy this range.

- In GaBi, create a new process in an existing project by right-clicking on 'Processes' in the GaBi explorer and again clicking on 'New' (Figure 30).
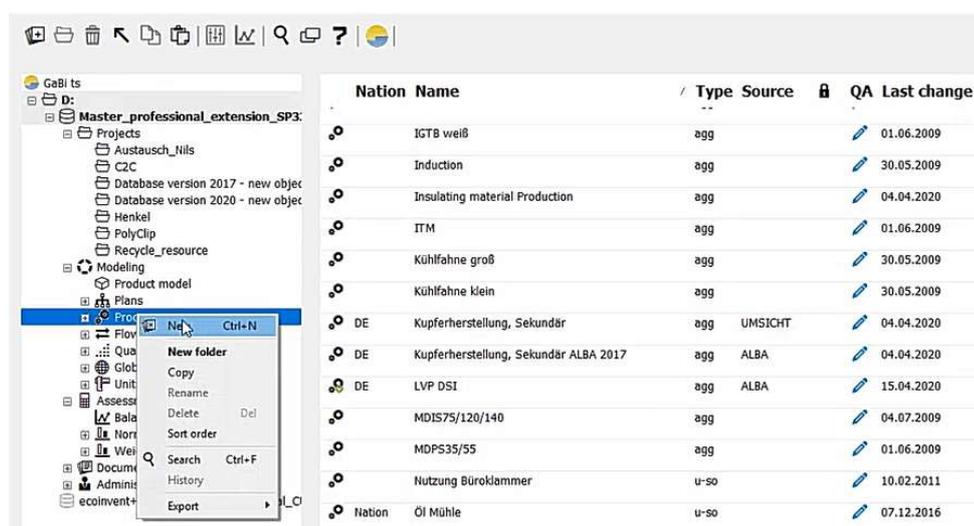
Figure 30. Creating a new empty process in GaBi.

- In the new process, place the cursor in the 'Inputs' empty area and right-click on 'Paste'. This will paste all the inputs flow from excel.

- Repeat the same operation with the 'Outputs' data range in WW LCI.

- It is very likely that some flows are not recognized by GaBi, such as certain flows specific to WW LCI. In such cases, a 'Question' box will pop up, asking to either create this new flow or search for it in the Gabi flow library. In this case, the right course of action is to click on 'Create new object' and define each new flow with its right units (mass, volume, etc.), which are shown in the WW LCI inventory. Once these new flows are created, the 'Question' box will no longer pop up in subsequent import operations as the flows are already registered in GaBi.

- Finally, a name is given to the created process (see Figure 31) and it is saved in an appropriate folder.
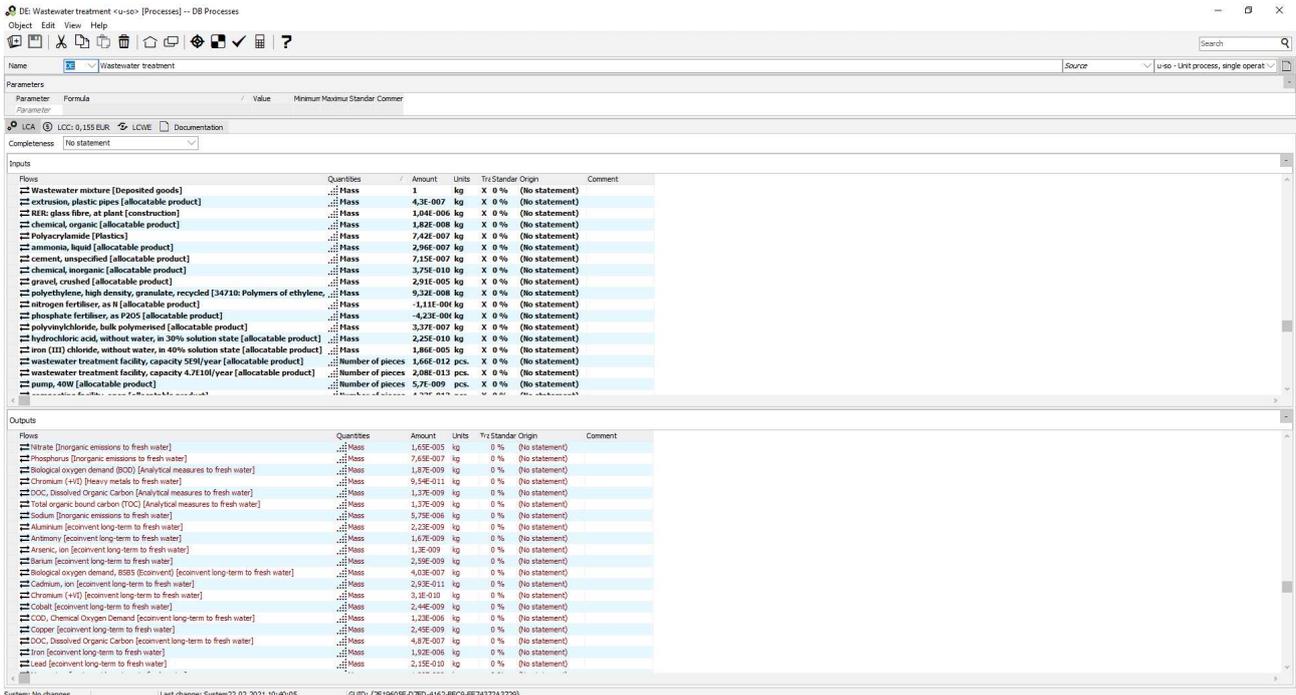
Figure 31. An imported wastewater mixture process in GaBi.

At this point, the imported process can be used in a GaBi plan, just like any other process. The last step in order to be able to calculate a balance with GaBi is to link the technosphere inputs in the imported process to the right ecoinvent supplying processes, in either their unit process format or aggregated format. The latter is suggested as the quickest option for linking. Also, as opposed to SimaPro, the imported LCI does not automatically link to the required suppliers, such as, for example, electricity production in Denmark, leaving the choice of geography and supplier to the user.

4.2.2 Exporting and importing the N fertilizer market LCI

This LCI is intended to be linked, in a GaBi plan, to the wastewater mixture LCI, in particular to the flow 'nitrogen fertiliser, as N' in the latter. The procedure to import this market mix is the same as explained in the previous section, with the advantage that it only needs to be imported once, given that this LCI is static (it does not change with different user-specific wastewater compositions). Another difference is all input and output flows should be automatically recognized by GaBi, as they all use the nomenclature of ecoinvent v3.6. Therefore, the 'Question' box will not pop up when the content from WW LCI is pasted in the new process. Last but not least, the following specific linking instructions must be followed for certain flows:

- The flow 'Nitrogen fertiliser, as N' must be linked by the user to the aggregated ecoinvent process for the production of urea ammonium nitrate, as N, with the RoW geography.

- The flow 'phosphate fertiliser, as P2O5' must be linked by the user to two simultaneous supplying ecoinvent aggregated processes: -0.9 kg P2O5 must be linked to the RoW market for monoammonium phosphate production, as P2O5, and -0.21 kg must be linked to the global market for phosphate fertiliser, as P2O5.

- The flow 'Potassium fertiliser, as K2O' must be linked by the user to two simultaneous supplying ecoinvent aggregated processes: -0.095 kg must be linked to the global data set for potassium nitrate production, as K2O, and -0.21 kg must be linked to the global market for potassium fertiliser, as K2O.

The suggested name for this process is 'Market for nitrogen fertiliser, as N (2.-0 LCA consultants)', although this is optional. Once the process is saved and properly connected to its supplying ecoinvent processes in a GaBi plan, it can be used for linking to all wastewater mixture LCIs.
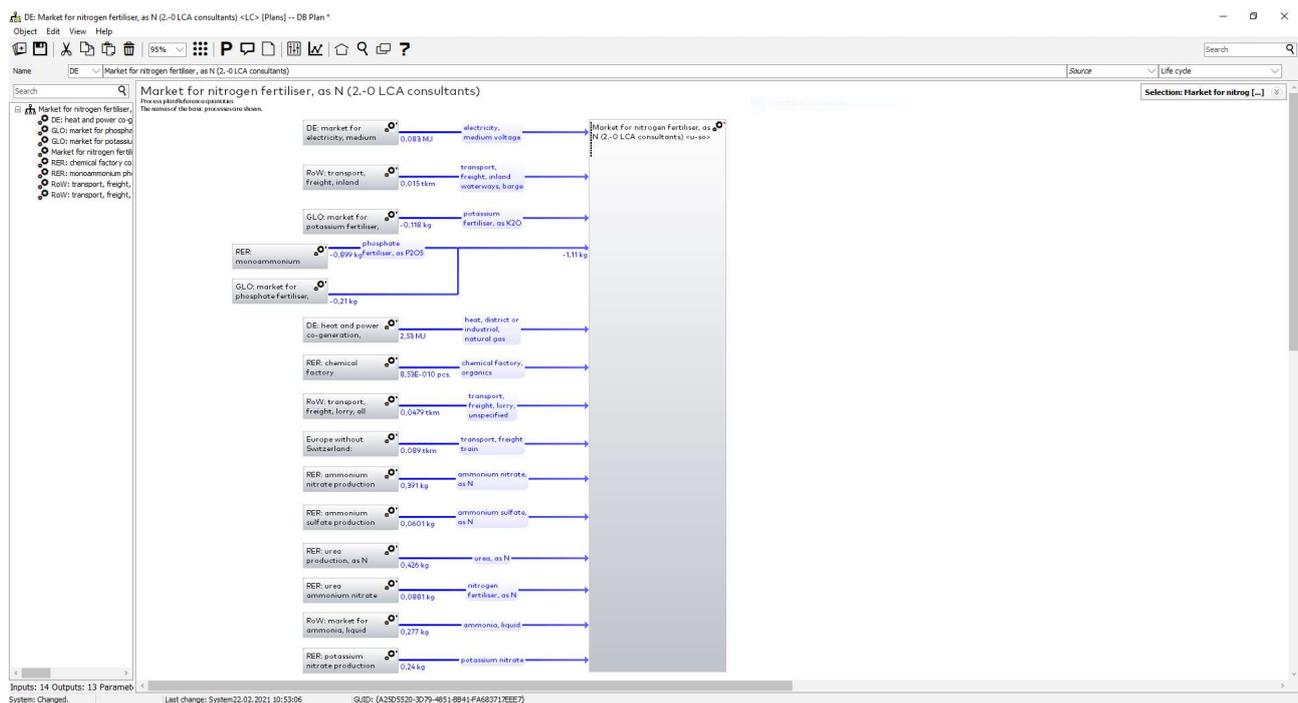
Figure 32. A GaBi plan with the global marginal mix for N fertilizer.

5 Some tips for optimal use of the LCIs in LCA software

5.1 Substance names in a Tier 2 assessment

The Tier-2 LCIs generated by WW LCI may include emissions to air and/or water of the actual wastewater components being assessed. For example, a volatile chemical being released to air by the WWTP, or a persistent chemical that escapes the treatment and is discharged with the treated effluent, or if there is a percentage of the population that is not connected to a WWTP. In these cases, there is a possibility that these emissions may contribute to one or more impact categories, for example ecotoxicity.

In order for the assessed wastewater components to be captured by the life impact assessment (LCIA) methods either in SimaPro or in GaBi, there are two options:

- In WW LCI, the chemical substance can be named with the same name as used in the substances' library in SimaPro, or under 'Flows' in GaBi's database explorer. In this way, any emissions will be automatically classified into any LCIA methods containing that flow name. In any case, even if an existing name is used, it is always recommended to check LCIA methods to know with certainty whether or not the assessed chemical substances are classified or not, and if appropriate, to provide characterization factors for them.

- If a different name is preferred which currently does not exist in the software's library, then, to make sure the LCIA methods capture the assessed chemical substance, it has to be manually classified with that name under any relevant impact categories, with the appropriate characterization factors.

5.2 Global warming potential of 'CO₂, stored, biogenic'

One of the most relevant impact categories in LCA is climate change/global warming, which typically uses the global warming potential (GWP) as characterization factor. In this context it is common practice to consider carbon dioxide emissions from biogenic origin as having a net GWP of zero, given that these emissions are counterbalanced by the carbon dioxide recently sequestered by the growing biomass, through photosynthesis.

As explained by Muñoz et al. (2013), a consistent carbon accounting requires, that if, as explained above, biogenic carbon dioxide emissions are considered neutral, then any biogenic carbon storage needs to be attributed a GWP of -1 when measured as carbon dioxide equivalents. In WW LCI this kind of biogenic carbon storage occurs in several instances:

- When a substance (containing biogenic carbon) is landfilled and part of the carbon remains stored due to incomplete degradation.

- When a substance (containing biogenic carbon) is discharged to the environment and it is buried in sediments, where again part of the carbon remains stored due to incomplete degradation.

This storage is captured in WW LCI by means of the inventory flow 'Carbon dioxide, biogenic, stored'. In order to consistently account for this carbon storage when using the LCIs in calculations involving climate

change, it is required to go to the software's LCIA method of choice and add the above-mentioned flow with a characterization factor of -1 kg CO_2/kg CO_2, biogenic, stored.

It must be stressed that this adjustment is only needed:

- For the flow 'Carbon dioxide, biogenic, stored'. The flow 'Carbon dioxide, stored fossil' does not require any adjustment.

- If biogenic carbon dioxide is considered neutral. In case there is no distinction in the LCIA method between carbon dioxide emissions from biogenic and fossil origin, i.e. CO_2 biogenic = CO_2 fossil = 1, then the flow 'Carbon dioxide, biogenic, stored' does not require any adjustment, i.e. its GWP remains zero.

For further details on consistent carbon accounting, see Muñoz et al. (2013) including section 1 in its online-available appendix.

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Appendix. WWTP fate factor estimates from SimpleTreat

The content in this appendix, namely the text in the following paragraphs and all tables, is directly reproduced from the Technical Guidance Document on Risk Assessment (EC 2003), in its appendix 2: 'Fate of chemicals in a wastewater treatment plant based on the SimpleTreat model'. These data can be used to derive WWTP fate factors for use in WW LCI.

The tables in this appendix provide values for the fate of substances that enter the sewage treatment plant, estimated according to the SimpleTreat 3.0 model (Struijs et al., 1996). The tables provide information on how much of a substance that enters the sewage treatment plant goes to air, surface water and to sewage sludge and how much is degraded. Separate tables are given depending on the categorization of a substance according to the results of screening biodegradation tests (see Table 6).

The data in the tables have been obtained from calculations with the SimpleTreat 3.0 model with the following settings: the volume of wastewater is set at 200 l per capita per day in line with Table 9 (Section 2.3.7.1). Assuming that the total amount of solids in raw sewage produced per inhabitant per day is 0.150 (m^{-3} . d^{-1}) . 0.6 (kg . m^{-3}) = 90 g per inhabitant per day, the concentration of suspended matter in influent has been set to 0.45 (kg . m^{-3}) (see Table 9). In order to maintain the main characteristics of the sludge flow, the steady-state concentration of suspended solids in the primary settler has been set at 150 mg dry weight per l, implying that still 2/3 of the solids in raw sewage is separated by the primary settler. Consequently, settled sewage flowing from the primary settler into the aeration tank contains an oxygen requirement (Ro) of 176 mg BOD per l.

The mode of operation is defined by the input parameter sludge loading rate which specifies the BOD loading of the plant. The operation of the activated sludge reactor is largely specified by thisparameter. This input parameter is in units of kg BOD per kg dry weight per day and is related to the sludge retention time (SRT) or sludge age and the hydraulic retention time (HRT). A medium sludge loading rate of 0.15 kg BOD kg dw^{-1} . d^{-1} is used with a SRT of 9.2 d and an HRT of 7.1 hr.

Compared to previous versions of the model in SimpleTreat 3.0 a correction for stripping chemicals has been included, as the process description is only valid for volatile chemicals (H > 250 Pa . m^3 . mol^{-1}). The overall mass transfer coefficient during surface aeration (ksurf) was assumed proportional to the dissolved oxygen overall transfer rate coefficient (KLaO), estimated from the oxygen requirement (Ro), hydraulic retention time (HRT) and the difference between the oxygen saturation and the actual O$_2$ concentration in the aerator (ΔO$_2$).

In order to account also for the gas phase resistance (H < 250 Pa.m3.mol-1) the proportionality constant Ψ, still having the default value of 0.6, should be multiplied by a factor containing the dimensionless Henry constant (KH) and the ratio of the mass transfer rate coefficients of a chemical in air and water. Munz and Roberts (1987) recommend to apply 40 as a default value for this ratio. As a result the first order rate constant for surface aeration is written as:

$$k_{surf} = \psi \left(\frac{40 \cdot K_H}{40 \cdot K_H + 1} \right) \frac{Ro}{HRT \cdot \Delta O_2}$$

In the following tables H (Henry's law constant) should be used in Pa . m^3 . mol^{-1}.

a) No biodegradability

Fate of chemicals that are not degradable: kbiostp = 0 hr^{-1} in the aqueous phase of activated sludge.

% to air / log Kow	log H -4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	2	15	64	91	95	95
1	0	0	0	0	2	15	64	91	95	95
2	0	0	0	0	2	15	64	91	94	95
3	0	0	0	0	2	14	62	89	92	92
4	0	0	0	0	1	12	52	77	80	80
5	0	0	0	0	1	5	28	48	51	51
6	0	0	0	0	0	1	9	23	27	27

% to water / log Kow	log H -4	-3	-2	-1	0	1	2	3	4	5
0	100	100	100	100	98	85	36	9	5	5
1	100	100	100	100	98	85	36	9	5	5
2	99	99	99	99	97	84	36	9	5	5
3	96	96	96	96	94	82	35	8	5	5
4	79	79	79	79	77	68	30	8	5	4
5	39	39	39	39	39	35	19	6	4	4
6	15	15	15	15	15	14	11	6	4	4

% to sludge / log Kow	log H -4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	0	0	0
3	4	4	4	4	4	4	3	3	3	3
4	21	21	21	21	21	20	18	16	15	15
5	61	61	61	61	60	59	53	46	45	45
6	85	85	85	85	85	85	80	71	69	69

% degraded / log Kow	log H -4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0

% removal / log Kow	log H -4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	2	15	64	91	95	95
1	0	0	0	0	2	15	64	91	95	95
2	1	1	1	1	3	16	64	91	95	95
3	4	4	4	4	6	18	65	92	95	95
4	21	21	21	21	23	32	70	92	95	96
5	61	61	61	61	61	65	81	94	96	96
6	85	85	85	85	85	86	89	94	96	96

b) Inherent biodegradability

Fate of chemicals that are "inherently biodegradable" in an OECD/EU test: kbiostp = 0.1 hr^{-1} in the aqueous phase of activated sludge.

% to air

log Kow	log H −4	−3	−2	−1	0	1	2	3	4	5
0	0	0	0	0	1	10	50	85	91	91
1	0	0	0	0	1	10	50	85	91	91
2	0	0	0	0	1	10	50	85	90	91
3	0	0	0	0	1	9	49	83	88	89
4	0	0	0	0	1	8	41	72	77	77
5	0	0	0	0	0	4	23	45	49	49
6	0	0	0	0	0	1	8	22	26	26

% to water

log Kow	log H −4	−3	−2	−1	0	1	2	3	4	5
0	59	59	59	59	58	52	28	8	5	5
1	59	59	59	59	58	52	28	8	5	5
2	59	59	59	59	58	52	27	8	5	5
3	57	57	57	57	56	50	27	8	5	5
4	48	48	48	48	48	43	24	7	5	4
5	28	28	28	28	27	25	16	5	4	3
6	13	13	13	13	13	13	10	6	4	4

% to sludge

log Kow	log H −4	−3	−2	−1	0	1	2	3	4	5
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	0	0	0
3	4	4	4	4	4	4	3	3	3	3
4	19	19	19	19	19	19	17	16	15	15
5	56	56	56	56	56	55	51	46	45	45
6	83	83	83	83	82	82	78	71	69	68

% degraded

log Kow	log H −4	−3	−2	−1	0	1	2	3	4	5
0	41	41	41	41	41	38	22	7	4	4
1	41	41	41	41	40	38	22	7	4	4
2	41	41	41	41	40	38	22	7	4	4
3	39	39	39	39	39	37	21	6	4	4
4	33	33	33	33	32	31	18	6	4	3
5	17	17	17	17	16	16	10	4	2	2
6	4	4	4	4	4	4	4	2	1	1

% removal

log Kow	log H −4	−3	−2	−1	0	1	2	3	4	5
0	41	41	41	41	42	48	72	92	95	95
1	41	41	41	41	42	48	72	92	95	95
2	41	41	41	41	42	48	73	92	95	95
3	43	43	43	43	44	50	73	92	95	95
4	52	52	52	52	52	57	76	93	95	96
5	72	72	72	72	73	75	84	95	96	97
6	87	87	87	87	87	87	90	94	96	96

c) pass levels within 28 days in a test on "ready biodegradability", 10-day window criterion is not fulfilled

Fate of chemicals that reach the biodegradation pass levels within 28 days in an OECD/EU test on "ready biodegradability but not within the 10 day time window: kbiostp = 0.3 hr^{-1} in the aqueous phase of activated sludge.

% to air

log Kow \ log H	-4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	1	6	36	76	84	85
1	0	0	0	0	1	6	36	76	84	85
2	0	0	0	0	1	6	36	75	83	84
3	0	0	0	0	1	6	35	73	81	82
4	0	0	0	0	1	5	30	64	71	71
5	0	0	0	0	0	3	17	40	45	46
6	0	0	0	0	0	1	7	20	24	25

% to water

log Kow \ log H	-4	-3	-2	-1	0	1	2	3	4	5
0	33	33	33	33	32	29	19	7	5	4
1	33	33	33	33	32	29	19	7	5	4
2	32	32	32	32	32	29	19	7	5	4
3	32	32	32	32	31	29	18	7	5	4
4	27	27	27	27	27	25	16	6	4	4
5	18	18	18	18	17	16	12	5	3	3
6	11	11	11	11	11	10	9	5	4	4

% to sludge

log Kow \ log H	-4	-3	-2	-1	0	1	2	3	4	5
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	0	0	0
3	3	3	3	3	3	3	3	3	3	3
4	17	17	17	17	17	17	16	16	15	15
5	51	51	51	51	51	51	49	46	45	45
6	79	79	79	79	79	78	76	70	68	68

% degraded

log Kow \ log H	-4	-3	-2	-1	0	1	2	3	4	5
0	67	67	67	67	67	64	45	17	12	11
1	67	67	67	67	67	64	45	17	12	11
2	67	67	67	67	67	64	45	17	12	11
3	65	65	65	65	65	62	44	17	11	11
4	55	55	55	55	55	53	38	15	10	9
5	31	31	31	31	31	30	22	9	6	6
6	11	11	11	11	11	10	9	5	3	3

% removal

log Kow \ log H	-4	-3	-2	-1	0	1	2	3	4	5
0	67	67	67	67	68	71	81	93	95	96
1	67	67	67	67	68	71	81	93	95	96
2	68	68	68	68	68	71	81	93	95	96
3	68	68	68	68	69	71	82	93	95	96
4	73	73	73	73	73	75	84	94	96	96
5	82	82	82	82	83	84	88	95	97	97
6	89	89	89	89	89	90	91	95	96	96

d) pass levels within 28 days in a test on "ready biodegradability", 10-day window criterion is fulfilled

Fate of chemicals that are "readily biodegradable" in an OECD/EU test: $kbio_{stp} = 1$ hr^{-1} in the aqueous phase of activated sludge.

	log H									
% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow 0	0	0	0	0	0	3	19	55	66	68
1	0	0	0	0	0	3	19	55	66	68
2	0	0	0	0	0	3	19	54	66	67
3	0	0	0	0	0	3	18	53	64	66
4	0	0	0	0	0	3	16	46	56	57
5	0	0	0	0	0	1	9	29	36	37
6	0	0	0	0	0	1	4	15	20	20

	log H									
% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow 0	13	13	13	13	13	12	9	5	4	3
1	13	13	13	13	13	12	9	5	4	3
2	13	13	13	13	12	12	9	5	4	3
3	12	12	12	12	12	11	9	5	4	3
4	11	11	11	11	11	10	8	4	3	3
5	8	8	8	8	8	7	6	4	3	3
6	7	7	7	7	7	7	6	4	3	3

	log H									
% to sludge	-4	-3	-2	-1	0	1	2	3	4	5
log Kow 0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0
3	3	3	3	3	3	3	3	3	3	3
4	16	16	16	16	16	16	16	15	15	15
5	47	47	47	47	47	47	46	45	45	45
6	72	72	72	72	72	72	71	69	67	67

	log H									
% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow 0	87	87	87	87	87	85	72	41	30	29
1	87	87	87	87	87	85	72	40	30	29
2	87	87	87	87	87	85	72	40	30	29
3	85	85	85	85	84	82	70	39	29	28
4	73	73	73	73	73	71	61	34	26	24
5	45	45	45	45	45	44	38	22	17	16
6	21	21	21	21	21	21	19	12	9	9

	log H									
% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow 0	87	87	87	87	87	88	91	95	96	97
1	87	87	87	87	87	88	91	95	96	97
2	87	87	87	87	88	88	91	95	96	97
3	88	88	88	88	88	89	91	95	96	97
4	89	89	89	89	89	90	92	96	97	97
5	92	92	92	92	92	93	94	96	97	97
6	93	93	93	93	93	93	94	96	97	97