Ecoinvent web-based tool for wastewater treatment inventories (WWinvent)

Lluís Corominas, George Ekama, Yves Comeau, Peter A. Vanrolleghem, Pascal Lesage

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CONTENTS

1 Introduction

1.1 Objective of the ecoinvent wastewater tool

Wastewater treatment is an activity that is often encountered in LCA: many activities generate wastewater, and, unless this wastewater is discharged without treatment to the environment or is treated onsite, a complete LCA needs to account for the burdens of transporting this wastewater in a sewer system and treating it in a wastewater treatment plant (WWTP). The ecoinvent database has multiple datasets covering the treatment of wastewater. However, these datasets are often insufficient for three reasons. First, the burdens of wastewater treatment depend directly on the composition of the wastewater. Second, the technologies used for wastewater treatment will also affect both the impacts of the treatment itself and the amount of pollutants that are not removed by the WWTP and ultimately discharged to the environment. Third, the datasets do not account for the fraction of wastewater that is discharged to the sewer system but is not connected to a WWTP, and hence is directly discharged in the environment.

The “ecoinvent wastewater tool” (in this report, “tool” for short) aims to cover this gap:

- It can generate wastewater-specific wastewater treatment inventories: the user needs only to inform the tool about the composition of the wastewater.
- It generates inventories for the treatment of this wastewater in a number of WWTP configurations that can be adapted to represent the WWTP actually found in a region where the wastewater is discharged.
- It accounts for wastewater that is discharged to the sewer system but is not connected to a WWTP.

Of specific interest to ecoinvent data providers, it also generates ecoSpold files for these inventories, allowing the datasets to be submitted, via the ecoEditor, to ecoinvent. This allows data providers who are submitting data on an activity to jointly submit the datasets for the treatment of the wastewater their activity generates.

1.2 Scope of the tool

The tool focuses on wastewater that is sent to the sewer system. It therefore excludes wastewater that is directly discharged to the environment by a transforming activity, which should be accounted for in the elementary flows of this activity. It also excludes the onsite treatment of wastewater, whose burdens should be included within the scope of the transforming activity.

The tool typically generates two datasets (see Figure 1). The first is a “no treatment” dataset, that accounts for the fraction of wastewater discharged to the sewer system but not treated in a WWTP (section 4.1), and for Combined Sewer Overflow (CSO) (section 4.2), which are discharges of wastewater to the environment due to episodes of overflow in the sewer system. The second is a treatment dataset that accounts for the treatment of the fraction of the wastewater that ultimately reaches the WWTP.

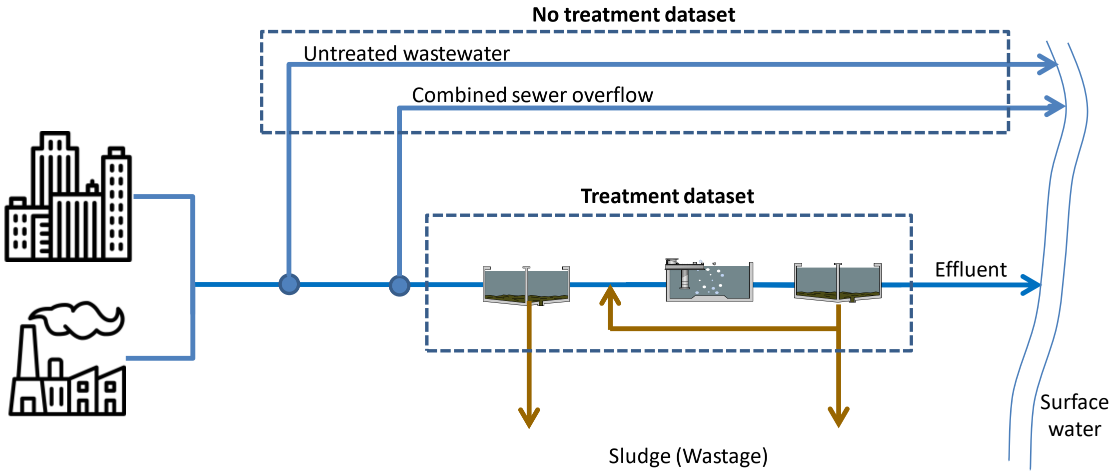


Figure 1: Scope of the tool and the two datasets generally generated

The system boundary of this tool includes the construction and the operation of the WWTP. With regards to operation, it accounts for elementary flows of untreated wastewater, combined sewer overflows and treated flows at the WWTP. In addition, it accounts for energy consumption for pumping, aeration and sludge thickening at a centrifuge. It also accounts for the consumption of most common chemicals used in WWTPs. Sludge treatment is out of the scope of this tool. Sludge from primary treatment and sludge from secondary treatment is quantified and well characterized, but their treatment is handled outside of this tool.

The tool can be used in four different contexts (Table 1), which differ on two aspects:

- Specific vs. average WWTP: If the user of the tool has knowledge on wastewater treatment technologies and also knows in which WWTP the wastewater will be treated, it is possible, via user-modifiable parameters, to model a specific WWTP. Most users, however, will not have this type of information, and will hence generate an average dataset, based on the installed wastewater treatment capacity in a region.

- Municipal vs. “specific activity” wastewater: The tool can generate datasets for both the treatment of average municipal wastewater and for the treatment of wastewater from a specific activity (henceforth “activity wastewater”) cotreated in a WWTP that is treating municipal wastewater. In both cases, the tool estimates the burdens of treating 1m^3 of the wastewater within the WWTP.

Table 1: Four uses of the tool

	Wastewater from a specific activity	**Average municipal wastewater**
Average WWT	Generate datasets that describe how a wastewater generated from	Generate datasets on the treatment of average municipal

	an activity will be treated on average. User supplies wastewater characteristics but does not need to supply any information on how the wastewater will be treated.	wastewater. User supplies wastewater characteristics but does not need to supply any information on how the wastewater will be treated.
Specific WWT	Generate datasets that describe how a wastewater generated from an activity will be treated in a specific WWTP. User supplies wastewater characteristics and information on the WWTP.	Generate datasets that describe the treatment of wastewater in a specific WWTP. User supplies wastewater characteristics and information on the WWTP.

1.3 Wastewater treatment modelling

The model behind the tool is based on internationally recognized process design guidelines rather than sampled data from a restricted number of WWTP (see Section 2). It therefore models plausible, but not actual, WWTP.

WWTP is a multifunctional process: it cotreats wastewater from multiple sources. The approach taken to allocate WWTP inputs and outputs to the wastewater of interest is ISO 14044's "step 2" approach: the partition reflects the way in which these inputs and outputs are changed by a quantitative change in the amount of treatment of the wastewater of interest. To achieve this, the model is run twice (Figure 2): once with just the municipal wastewater (Q_{ref}), and once with the municipal wastewater and 1 m3 of the activity wastewater ($Q_{ref+act}$). Both runs generate a number of results (amount of sludge generated, electricity consumed, etc.), and the difference is calculated for all of these. For some modelled input or output X, the ratio $(X_{ref+act} – X_{ref})/(Q_{ref+act} – Q_{ref})$ reflects the way X is changed by the cotreatment of each m^3 of activity wastewater. While this approach is based on subdivision it is also coherent with a consequential approach (it reflects the consequence of cotreating the wastewater of interest). The tool output is therefore consistent with both an attributional and a consequential database.

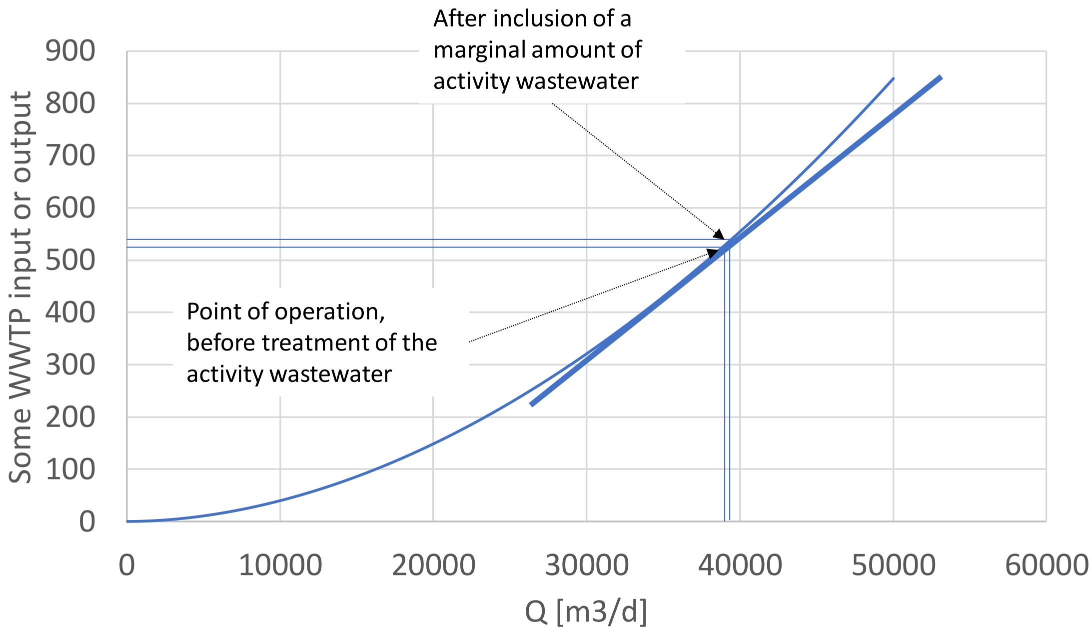


Figure 2: Graphical representation of the allocation approach

For the treatment of municipal wastewater, where the composition of the reference wastewater and the wastewater of interest are the same, the same approach is used: the calculated $(X_{ref+act} - X_{ref})/(Q_{ref+act} - Q_{ref})$ reflects the burdens of treating one additional m^3 of wastewater, which is taken to be representative of treating any m^3 of the wastewater. This is a simplification that may yield results different to those that a simple X_{total}/Q_{total} approach would yield.

1.4 Using the tool

The procedure for using the tool is described in detail in section 8. The main steps are as follows:

- The user must provide data on the wastewater to treat: its source (e.g. from steel production, average municipal), its properties (COD, temperature, etc.), the region where the water is discharged to the sewer system and the volume of water to treat.
- The user then specifies whether the dataset to generate should reflect a specific WWTP or an average for the selected region.
- If the user selects "specific WWTP", then he must adapt the design parameters of the WWTP: included technologies, composition of the wastewater and design parameters
- If the user selects "average", then a table with results per included WWTP is generated. The user can have an in-depth look at each WWTP model individually.
- The user then downloads ecoSpold files.
- These ecoSpold files are to be opened in the ecoEditor, and fields needing adaptation should be revised (e.g. comment fields, uncertainty fields). Once the datasets are ready, they are simply submitted via the ecoEditor. Typically, these would be submitted at the same time as the datasets modelling the activity that generates the activity wastewater.

2 Description of the model

The model behind the tool is based on the activated sludge process guideline typically known as Metcalf and Eddy (Tchobanoglous et al., 2014). This is one of the most widely accepted guidelines for the wastewater treatment community. Activated sludge process design guidelines comprise a set of equations that computed in a sequential manner are used to quantify a number of design outputs as a function of design inputs. The design inputs include influent characteristics (e.g. flow rate, concentration of pollutants), operational settings (e.g. oxygen concentration in the biological reactor), safety factors, process kinetics and stoichiometric parameters and effluent requirements (e.g. target ammonia concentration in the effluent of the WWTP). The design outputs comprise aerobic, anoxic, anaerobic volumes, oxygen demand; internal and external recycle flow rates, settling areas and dosage of chemicals (external carbon source, metal salts, and alkalinity). This guideline follows a mechanistic approach which can be considered a reduced/modified/simplified version of the International Water Association (IWA) Activated Sludge Models (ASM) (Henze et al., 2000). The values of the design outputs have a direct link to the design inputs. For example, in some guidelines the biodegradable fraction is important for evaluating oxygen demand, process sludge production and aeration volume requirements. Also, the stricter effluent requirements and the higher level of safety will increase aerobic/anoxic volumes requirements, external/internal recycle rates and the oxygen demand. After all, design outputs will somehow determine characteristics (reactor configuration, blowers' capacity, pumping stations' size, storage tank volume) of the plant.

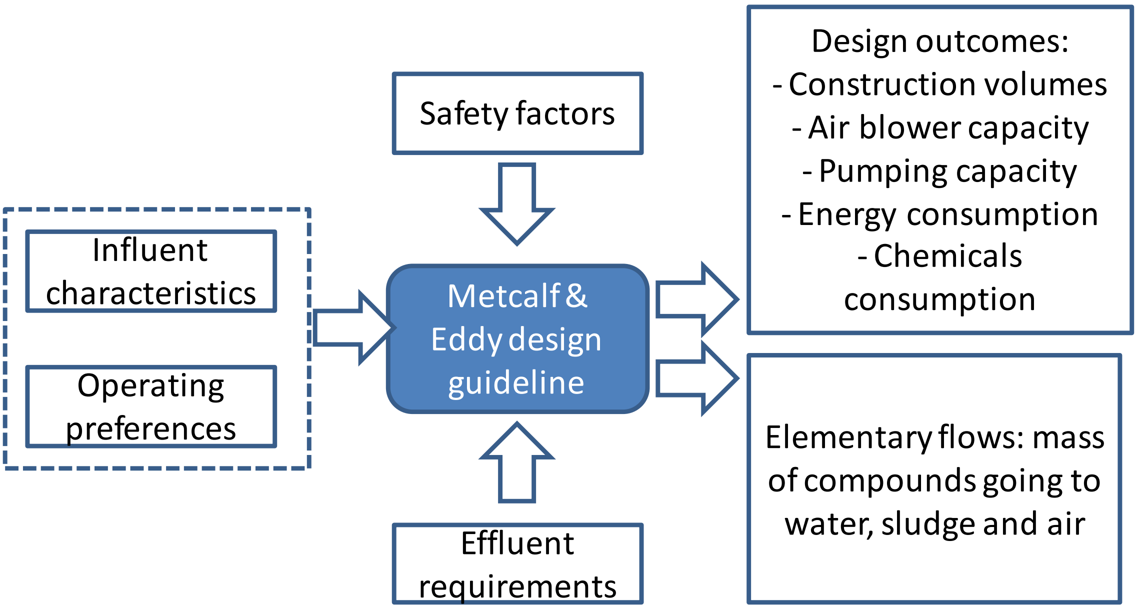


Figure 3. Activated sludge modeling approach (after Corominas et al., 2010)

The following technologies are modelled according to the Metcalf and Eddy design equations. The correspondence with the latest version of the 2014 edition is provided in the following table.

Table 2. Technologies included and their exact reference in Tchobanoglous et al. (2014).

	Metcalf and Eddy chapter	Example (initial page)
BOD removal only	Chapter 8-6	756
BOD and nitrification	Chapter 8-6	762
BOD and N removal	Chapter 8-7	810
Biological P removal	Chapter 8-8	880
Chemical P removal	chapter 6-4	484*

* The example of Metcalf and Eddy is for pre-precipitation, but here it is applied for co-precipitation.

The proposed modelling approach is sensitive to the choice of technology, temperature, pollutants loads, design practice in the selected country and the legal requirements for the pollutant loads in the effluent of the WWTP. In this report we explain how we extract the design equations from Tchobanoglous et al. (2014) and integrate them into a tool which allows estimating inventories for LCA studies. For a deeper understanding of the design equations the reader is referred to Tchobanoglous et al. (2014). The tool is transparent in the sense that the user can have access to the actual implementation of the equations.

2.1 Influent fractionation

All measurements used as inputs to the model have to be translated into model variables and some model outputs need to be converted into variables, which can be compared with measurements of the real system. The wastewater influent needs to be characterized following a model-specific fractionation procedure to convert measurements into model state-variables.

Metcalf and Eddy design guidelines work with the following model state-variables: sCOD (soluble or filtered COD), bCOD (biodegradable COD), rbCOD (readily biodegradable COD), BOD (Total 5d biochemical oxygen demand), sBOD (soluble BOD), VFA (Volatile Fatty Acids), VSS (volatile suspended solids), TSS (total suspended solids), NH4 (ammonium), PO4 (phosphate), and Alkalinity.

In order to convert measurements into these Metcalf and Eddy variables we will first conduct the detailed influent fractionation typical from the ASM-family models; then, the fractions obtained from these detailed fractionation will be combined to obtain the Metcalf and Eddy variables.

2.1.1 COD Influent fractionation

COD					
bCOD				nbCOD	
bsCOD (readily biodg)		bpCOD (slow biodg)		nbsCOD (=sCODe)	nbpCOD
Complex	VFA	Colloidal	Particulate		

COD					
sCOD			pCOD		
bsCOD (readily biodg)		nbsCOD (=sCODe)	bpCOD (slow biodg)		nbpCOD
Complex	VFA		Colloidal	Particulate	

Figure 4. COD fractionation. b:biodegradable; nb: non-biodegradable; s:soluble; p:particulate;

A) Detailed fractionation

The fractionation proposed according to most recent literature subdivides total COD fractions as CSU (non-biodegradable organic matter), SB (Soluble (rapidly) biodegradable matter), CB (Slowly biodegradable colloidal matter), XB (Particulate biodegradable organics), XH (organisms) and XU (Particulate unbiodegradable organics). Average typical ratios provided for raw municipal wastewater are provided below (taken from BioWin simulation platform).

According to Influent Specifier (BioWin)

Raw municipal WW

Avg ratios

				Total COD fractions				
				Avg typical ratios		**Detail 1**	**Detail 2**	**Detail 3**
			CS_U	**0,05**	**0,38**		**0,05**	**0,05**
0,15		**S_{VFA}**	**S_B**	**0,16**			**0,16**	**0,024**
0,85		**S_F**						**0,136**
	0,25		**C_B**		**0,64**	**0,17**	**0,17**	**0,17**
	0,75	**$X_{B,H}$**	**X_B**			**0,47**	**0,47**	**0,47**
			X_H	**0,02**			**0,02**	**0,02**
			X_U	**0,13**			**0,13**	**0,13**
							1,00	**1,00**

Hence, during the detailed fractionation the following variables are calculated:

```
CS_U  = f_CSU_COD*COD;
S_VFA = f_SB_COD* f_VFA_SB* COD;
S_F   = f_SB_COD * COD - S_VFA;
C_B   = (1-f_XB_XCB) *f_XCB_COD*COD;
X_B   = f_XB_XCB*f_XCB_COD*COD;
X_H   = f_XH_XCOD*COD;
X_U   = f_XU_COD*COD;
X_COD = X_B + X_H + X_U;
CS_B  = C_B + S_VFA + S_F;
X_BH  = X_B + X_H;
```

B) Metcalf and Eddy inputs

The following equations are needed to convert the detailed fractionation into Metcalf and eddy inputs. The factors in green are obtained as well from Biowin default fractionation.

```
sCOD       = CS_U + S_VFA + S_F + C_B;
bCOD       = COD - X_U - CS_U;
rbCOD      = S_VFA + S_F;
BOD        = COD/fCOD_cBOD5;
sBOD       = sCOD/fCOD_cBOD5;
VFA        = S_VFA;
VSS        = X_COD/fXCOD_VSS;
TSS        = XIg + VSS;
NH4        = fSNH4_TKN*TKN;
PO4        = fSPO4_TP*TP;
Alkalinity = SAlk;
```

Table 3. Typical values for raw municipal wastewater

Symbol	Description	Units	Range	Avg
f_{COD_cBOD5}	COD to BOD5 ratio	g COD/g BOD5	1.9-2.2	2.04
f_{SB_COD}	Rapidly biodegradable COD fraction	g COD/g COD	0.12-0.25	0.16
f_{VFA_SB}	VFA fraction of the rapidly biodegrad. COD	g COD/g COD	0.0-0.3	0.15
f_{XCB_COD}	Slowly biodegradable COD fraction	g COD/g COD	-	0.64
f_{XB_XCB}	Particulate fraction of the slowly biodegradable COD	g COD/g COD	-	0.73
f_{XCOD_VSS}	Particulate COD to VSS ratio	g COD/g VSS	1.5-1.7	1.6
f_{XU_COD}	Unbiodegradable particulate COD fraction	g COD/g COD	-	0.13
X_{Ig}	Inorganic suspended solids	mg ISS/L	15-45	45
f_{XH_XCOD}	Heterotrophic biomass fraction of the XCOD	g COD/g COD	-	0.02
f_{CSU_COD}	Unbiodegradable filterable COD fraction	g COD/g COD	0.03-0.08	0.05
f_{SNH4_TKN}	NH4 to NTK fraction	g N/g N	0.5-0.8	0.66
f_{SPO4_TP}	o-PO4 over total P fraction	g P/g P	0.3-0.6	0.5
S_{Alk}	Alkalinity	meq/L	100	300

Table 4. COD influent fractionation (in red what is an input; in green what is calculated)

Symbol	Description	Equation/Value
COD	Total chemical oxygen demand	Input
sCOD	soluble chemical oxygen demand	= CS_U + S_VFA + S_F + C_B;
BOD	Five day carbonaceous biochemical oxygen demand	= COD/f_{COD_cBOD5};
sBOD	Soluble five day carbonaceous biochemical oxygen demand	= sCOD/f_{COD_cBOD5};
bCOD	Biodegradable COD	= COD - X_U - CS_U;
rbCOD	Readily biodegradable COD	= S_VFA + S_F;
VFA	Volatile fatty acids	= S_VFA;

Other fractions are needed to close the mass balances around the WWTP.

Table 5. COD influent fractionation (continuation)

Symbol	Description	Equation/Value

nbCOD	Non-biodegradable COD	= COD - bCOD
nbsCODe	Non-biodegradable soluble COD	= sCOD - (bCOD/BOD) x sBOD
nbpCOD	Non-biodegradable particulate COD	= COD - bCOD - nbsCODe

2.1.2 Nitrogen influent fractionation (in red what is an input; in green what is calculated)

<table>
<tr><th colspan="5">TKN</th></tr>
<tr><td>NH_4</td><td colspan="4">ON</td></tr>
<tr><td rowspan="2"></td><td colspan="2">bON</td><td colspan="2">nbON</td></tr>
<tr><td>bsON</td><td>bpON</td><td>nbsON</td><td>nbpON</td></tr>
</table>

Figure 5. TKN fractionation. b:biodegradable; nb: non-biodegradable; s:soluble; p:particulate; ON: organic nitrogen;

Table 6. N influent fractionation

Symbol		Equation/Value	Source/Comments
TKN	Nitrogen Kjeldahl	Input	
NH4	Ammonia	Input	
ON	Organic nitrogen	TKN-NH4	
nbpON	Nonbiodegradable particulate organic nitrogen	nbpON = fN(nbVSS) ; fN=0.064 ;	0.064 taken from Tchobanoglous et al. (2014)
nbsON	Nonbiodegradable soluble organic nitrogen	= 0.3 g/m3 ;	0.3 taken from ASM2d (Henze et al., 2000)
TKN_N2O	Nitrogen that is ultimately converted into N2O, expressed as a percentage of the influent TKN	TKN_N2O = fN2O x TKN; fN2O = 0.001 gN-N2O/gN-TKN	The range can be between 0.0001 and 0.112 according to Foley et al. (2015). Our default is 0.001;
bTKN	Biodegradable TKN available for nitrification	bTKN = TKN - nbpON – nbsON – TKN_N2O	This is the fraction of N used for nitrification. We assume 100% of bTKN is hydrolyzed to Ammonia.

2.1.3 Phosphorus influent fractionation

TP				
PO_4	OP			
	bOP		nbOP	
	bsOP	bpOP	nbsOP	nbpOP

Figure 6. P fractionation. b: biodegradable; nb: non-biodegradable; s:soluble; p:particulate; OP: Organic Phosphorus

Table 7. Influent P fractionation (in red what is an input; in green what is calculated)

Symbol	Description	Equation/Value	Source/Comments
TP	Total phosphorus	Input	
PO4	Phosphate	Input	
OP	Organic phosphorus	TP-PO4	
nbpOP		nbpP = fP·(nbVSS) ; fP = 0.015 gP/gnbpVSS;	fP value taken from Tchobanoglous et al. (2014).
nbsOP		= 0 gP/m3	value provided by Ekama
nbOP		= nbsOP + nbpOP	
aP		aP = TP-nbOP	

2.1.4 Suspended solids

TSS		
VSS		iTSS
nbVSS	bVSS	

Figure 7. Suspended solids fractionation. b: biodegradable; nb: non-biodegradable; i: inorganic

Table 8. Suspended solids fractionation equations

Symbol	Description	Equation/Value
TSS	Total suspended solids	input
VSS	Volatile suspended solids	input
iTSS	Inorganics	iTSS = TSS – VSS
VSSCOD	Volatile suspended solids ratio	=(TCOD-sCOD)/VSS

nbVSS	Non-biodegradable volatile suspended solids	= nbpCOD / VSSCOD x VSS

2.1.5 Default fractionation factors for industrial wastewater

There is limited information in the literature on the fractionation of industrial wastewater. As a preliminary approach the authors of this report have provided default fractions for four types of industrial wastewater:

- Type 1: Highly soluble - high degradability (Beverages industry wastewater)
- Type 2: Highly particulate - high degradability (pig manure)
- Type 3: Highly soluble - low degradability (tanning wastewater)
- Type 4: Highly particulate - low degradability (thermomechanical pulp and paper wastewater)

Table 9. Default fractionation factors for different types of wastewater; BOD* is the BOD5

Symbol	Description	Units	Type 1	Type 2	Type 3	Type 4
f_{COD_cBOD5}	COD to BOD* ratio	g COD/g BOD5	1,71	3,0	2,2	2,50
f_{SB_COD}	Rapidly biodegradable COD fraction	g COD/g COD	0,61	0,20	0,28	0,28
f_{VFA_SB}	VFA fraction of the rapidly biodegradable COD	g COD/g COD	0,55	0,30	0,00	0,00
f_{XCB_COD}	Slowly biodegradable COD fraction	g COD/g COD	0,26	0,70	0,34	0,39
f_{XB_XCB}	Particulate fraction of the slowly biodegradable COD	g COD/g COD	0,71	0,75	0,88	0,60
f_{XCOD_VSS}	Particulate COD to VSS ratio	g COD/g VSS	1,51	1,48	1,37	2,18
f_{XU_COD}	Unbiodegradable particulate COD fraction	g COD/g COD	0,09	0,05	0,05	0,29
X_{Ig}	Inorganic suspended solids	mg iTSS/L	100	6500	135	1315
f_{XH_XCOD}	Heterotrophic biomass fraction of the XCOD	g COD/g COD	0,11	0,02	0,00	0,00
f_{CSU_COD}	Unbiodegradable filterable COD fraction	g COD/g COD	0,04	0,05	0,33	0,04
f_{SNH4_TKN}	NH4 to NTK fraction	g N/g N	0,10	0,55	0,0	0,57
f_{SPO4_TP}	o-PO4 over total P fraction	g P/g P	0,93	0,18	0,0	0,00
S_{Alk}	Alkalinity	meq/L	60	2,0	2,0	22

2.2 Operating preferences (design choices)

Operating preferences are to be established before executing the design. Table 12 provides a list of the operating preferences and their correspondence to the different modeled elements is.

2.2.1 Elementary flows (COD, N, P)

The inputs of the tool determine the mass of compounds (in kg/d) that enter the studied wastewater treatment system. Then, different equations are used to estimate how much of these compounds are discharged to the effluent water (Fj,water), to the air (Fj,air) and as sludge (Fj,sludge), where j is the element balanced (COD, N or P).

COD balance: For organic matter we provide the elementary flows based on COD (chemical oxygen demand). The following terms are needed to close the balance:

- Carbonaceous oxygen demand
- Load that is discharged into the effluent because (i) it has not been degraded in the system (non-biodegradable soluble compounds that leave the system as they enter), (ii) it is biodegradable but has not been degraded, or (iii) the COD content of the solids that do not settle
- COD that goes into sludge because of sludge production or because it is the nonbiodegradable particulate fraction (nbpCOD).

N balance:

- TKN and NO_3 loads that are discharged into the effluent because (i) they have not been removed and (ii) the N content of the solids that do not settle
- N that goes into sludge (i) because of sludge production or (ii) because it is the nonbiodegradable particulate fraction (nbpON).

P balance:

- PO_4^{3-} load that is discharged into the effluent because (i) it has not been degraded and (ii) the P content of the solids that do not settle
- P that goes into sludge because of sludge production or because it is the nonbiodegradable particulate fraction (nbpP).

Additionally, we provide equations to estimate the amount of CO_2, N_2 and N_2O emitted. We provide the users a verification that the mass balances close with an error smaller than 1%. This is provided in the results section of the tool.

2.2.2 Primary settling

Primary settlers are designed to allow particulate compounds in the wastewater to settle. They are the first stage of treatment after the removal of rags and grit in the inlet works. The settled sludge is removed by pump or gravity feed to a sludge treatment process. The most common situation is that primary settlers remove 2/3rd of the raw wastewater organic nitrogen (TKN minus ammonia) and 2/3rd of the raw wastewater organic phosphorus (TP minus OP) (Personal consultation with George Ekama). The primary settler removes as well part of the inorganics from the raw wastewater. Soluble compounds leave the primary settler as they enter. Still, the user of this tool can modify these removal efficiencies in the design parameters tab.

Table 10. Primary settling parameters

Wastewater fraction	Description	Value	Unit
removal_bpCOD	Removal efficiency of biodegradable particulate COD	40	%
removal_nbpCOD	Removal of non-biodegradable particulate COD	60	%
removal_ON	Removal efficiency of organic nitrogen	66.6	%
removal_OP	Removal efficiency of organic phosphorus	66.6	%
removal_iTSS	Removal efficiency of inorganics	70	%

2.2.3 BOD removal only

A typical complete-mix activated sludge process for BOD removal is shown on Figure 8. Effluent from the primary settler and the recycled return activated sludge are introduced in the aerobic biological reactor. In the aerobic reactor oxygen is supplied to the system, and organic substrates are oxidized to provide energy and a carbon source for the growth of heterotrophic bacteria.

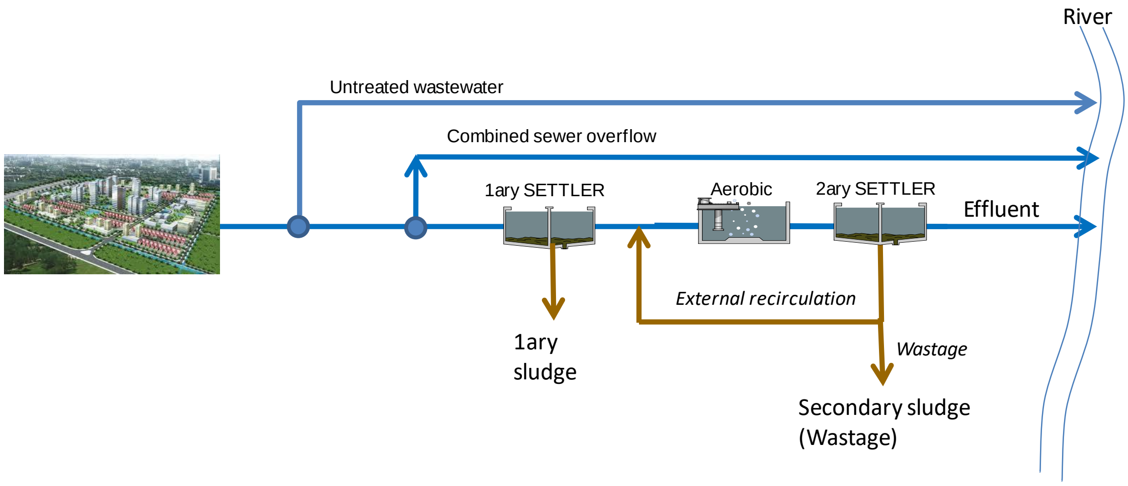


Figure 8. BOD removal only technology scheme

Notes:

- For organic matter we provide the elementary flow based on COD; just one C balance based on COD. The BOD is included within the balance, but will not have a separate balance. In order to estimate the C content of COD we use as a default value of 3 g COD/g TOC; still, the user can change that factor in the tool.
- The CO_2 balance includes the CO_2 from BOD oxidation (includes COD removal under aerobic and under anoxic conditions, with the assumption that the yield in aerobic conditions is the same as in anoxic conditions) plus CO_2 from endogenous decay minus the CO_2 consumed by nitrifiers
- 1.42 is the conversion g COD/g VSS (The conversion factor 1.42 is required to express the mass of microbial VSS in COD units, assuming the generally acknowledged empirical formula C_5H_7NO2 for bacterial biomass (Tchobanoglous et al., 2014).
- COD air is the carbonaceous oxygen demand. It is needed for the COD mass balance, but is actually not an outcome for ecoinvent. The emission to air is expressed in terms of CO_2 (COD plus oxygen is converted into CO_2 by the organisms). There is no real emission of COD to air, we just estimate it to close the mass balance.
- 3.6% of the CO_2 is assumed to be of non-biogenic origin (Law et al., 2013). This value is relevant for estimation of greenhouse gas (GHG) emissions. The user can change this value if better estimates are available.

2.2.4 BOD removal and nitrification

The treatment goal is to remove organic matter and convert influent ammonia into nitrate. Besides heterotrophic bacteria in charge of removing organic substrates, in a BOD removal and nitrification system, sufficient sludge retention time is needed to ensure the growth of autotrophic bacteria. These can grow by obtaining energy from ammonia and nitrite oxidation using bicarbonate as the carbon source. This process is called nitrification and occurs in two steps: i) the aerobic oxidation of ammonium to nitrite by the ammonium oxidizer bacteria (AOB) and ii) the aerobic oxidation of nitrite into nitrate by the nitrite oxidizer bacteria (NOB).

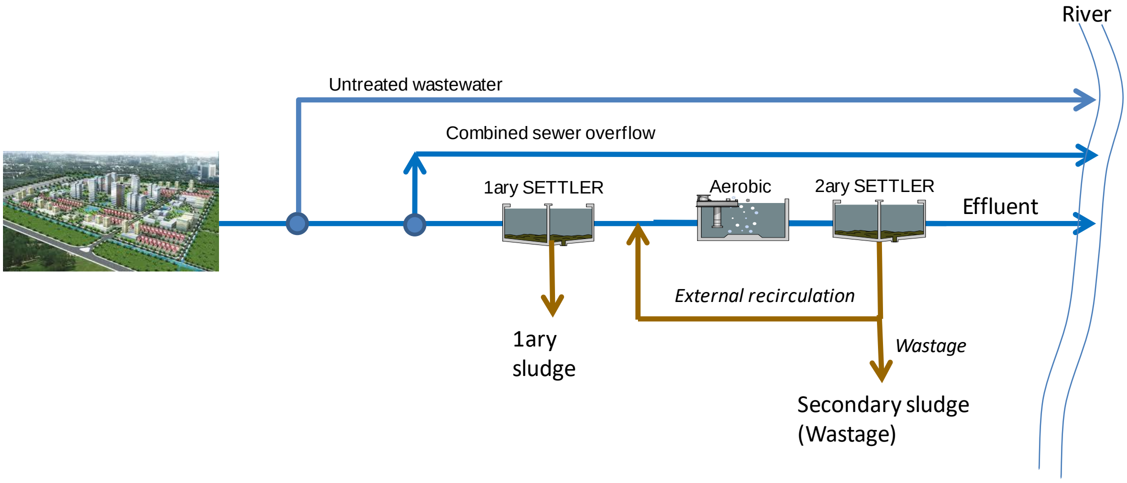


Figure 9. BOD removal and nitrification technology scheme

2.2.5 BOD and N removal

The treatment goal is to remove organic matter and nitrogen. The selected configuration is a Modified Ludzack-Ettinger process (MLE). In MLE configurations, the initial contact of the influent wastewater and return activated sludge occurs in an anoxic zone (ANOX), which is followed by an aerobic zone (AER) (see process layout in Fig. 8). The process relies on the nitrate formed in the aerobic zone being returned via an internal recycle to the anoxic zone to be denitrified.

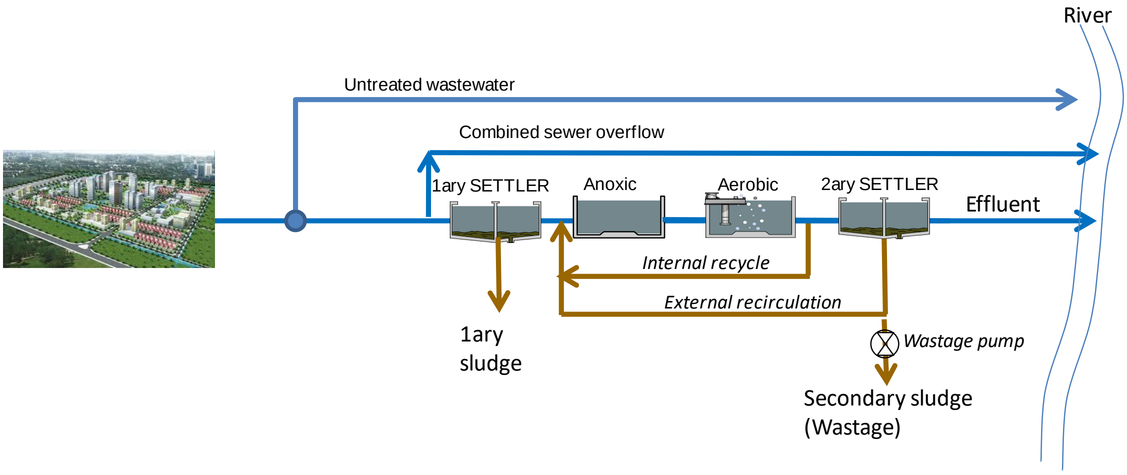


Figure 10. BOD removal and N removal technology scheme

2.2.6 Biological P removal

In the biological removal of phosphorus, the phosphorus in the influent wastewater is incorporated into cell biomass, which subsequently is removed from the process as a result of sludge wasting. Phosphorus accumulating organisms (PAOs) are encouraged to grow and consume phosphorus in systems that use a reactor configuration that provides PAOs with a competitive advantage over other bacteria. An anaerobic tank is then needed, that is placed ahead of the activated sludge anoxic tank.

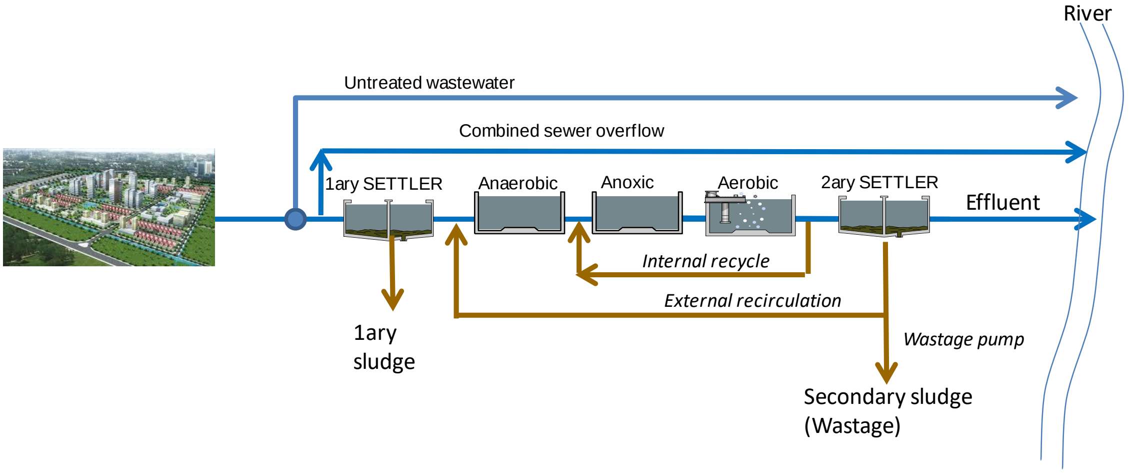


Figure 11. Biological P removal technology scheme

2.2.7 Chemical P removal

The chemical precipitation of phosphorus is brought about by the addition of the salts of multivalent metal ions that form precipitates of sparingly soluble phosphates. The multivalent metal ions used most commonly are calcium [Ca(2)], aluminium [Al(3)] and iron [Fe(3)]. In this tool co-precipitation is so far implemented, i.e. the addition of chemicals to form precipitates that are removed along with waste biological sludge are added to (1) the effluent from primary sedimentation, (2) the mixed liquor (in the activated sludge process), or (3) the effluent from a biological treatment process before secondary sedimentation.

Table 11. Calculations needed before starting the design

Id	Description	Equation/Value	Source/notes
VSSe	WWTP Effluent volatile suspended solids (g/m3)	= TSSef · 0.85	TSSef: Average effluent TSS concentration (from 5 to 35 mg/L); 35 mg/L is the limit established by the directive 91/271 EU. This will be imposed in the design exercise; and from this one VSSe is estimated. But to be on the safe side, the design is made for 25 mg TSS/L.
Qwas	Wastage flow rate (m3/d	$Qw\ (\frac{m3}{d}) = \frac{\frac{V_{reactor} \times MLSS}{SRT} - TSS_{eff} \times Q_{in}}{-1 \times TSS_{eff} + TSS_{was}}$ V in m3, MLSS in g/m3, SRT in days, TSS in g/m3, Q in m3/d	Typical equation of SRT calculation (see Tchobanoglous et al., 2014) $V_{reactor}$ is the total volume of biological reactor. SRT is different depending on the technology. For BOD removal only, the SRT is an input (e.g. 5 days). For technologies involving nitrification, the SRT is estimated during the design process.
Qin	Influent flow (m3/d)		
Qe	Effluent flow (m3/d)	Qe=Qin-Qwas	

Table 12. Design choices (columns indicate whether that particular input is required for a particular technology).

Symbol	Description	unit	CSO	1ary settl	BOD only	BOD + NH4	BOD + N	ChemP or BioP
NH4eff	Effluent ammonia target	g N/m^3				X	X	
NO3eff	Effluent nitrate target	g N/m^3					X	
PO4eff	Effluent phosphate target	g P/m^3						X
CSO_particulate	Fraction of particulates that are discharged with the combined sewer overflows	%	X					
CSO_soluble	Fraction of solubles that are discharged with the combined sewer overflows	%	X					
removal_bpCOD	Percentage removal of bpCOD during primary settling	%		X				
removal_nbpCOD	Percentage removal of nbpCOD during primary settling	%		X				
removal_ON	Percentage removal of ON during primary settling	%		X				
removal_OP	Percentage removal of OP during primary settling	%		X				
removal_iTSS	Percentage removal of iTSS during primary settling	%		X				
MLSS_X_TSS	Design mixed liquor suspended solids	g/m^3			X	X	X	
DO	Dissolved oxygen concentration in biological aerobic reactor	g/m^3 as O_2			X	X	X	
clarifiers	Number of clarifiers	clarifiers			X	X	X	
sBODe	soluble BOD in the effluent	g/m^3 as O_2			X	X	X	
TSSe	Total suspended solids in the effluent	g/m^3			X	X	X	
zb	Site elevation above sea level	m			X	X	X	
Pressure	Pressure at site elevation	Pa			X	X	X	
Df	Liquid depth above diffusers in biological reactor	m			X	X	X	
h_settler	Height of settler	m			X	X	X	
X_R	Return sludge mass concentration	g/m^3			X	X	X	
SRT	Sludge Retention Time	d			X			
SOR	Hydraulic application rate for secondary settler	$m^3\ m^{-2} \cdot d^{-1}$			X	X	X	
SF	Peak to average TKN load	Ø			X	X	X	
Anoxic_mixing_energy	Mixing energy for anoxic reactor	kW/1000 m^3					X	
FeCl3_solution	Ferric chloride solution	%						X
FeCl3_unit_weight	Ferric chloride unit weight	kg/L						X
days	Time of storage of the ferric chloride	d						X
influent_H	Influent pumping water lift height	m			X	X	X	

Table 13. List of model parameters with their default values

Symbol	Description	Value	Units
Elementary composition of sludge			
	COD content of biological sludge	1.42	g COD/g VSS
	N content of biological sludge	0.12	g N /g VSS
	P content of biological sludge	0.015	g P/g VSS
Physics (universal)			
Pa	standard pressure at sea level	10.33	m
R	ideal gases constant	8314	kg*m^2/s^2*kmol*K*1000
g	gravity	9.81	m/s^2
M	air molecular weight	28.97	g/mol
M_Fe	Fe molecular weight	55.845	g/mol
M_P	P molecular weight	30.974	g/mol
Kinetic coefficients heterotrophs	*Table 8-14, page 755 of Tchobanoglous et al. (2014)*		
K_S	half saturation constant of heterotrophic growth on COD	8	g_bCOD/m^3
Y_H	heterotrophic growth yield	0.45	g_VSS/g_bCOD
b_H	heterotrophic organisms decay rate	0.12	1/d
f_d	fraction of biomass contributing to biomass debris	0.15	-
Kinetic coefficients nitrifiers	*Table 8-14, page 755 of Tchobanoglous et al. (2014)*		
$\mu_{n,AOB,max}$	maximum growth rate of AOB organisms	0.9	1/d
K_{NH4}	half saturation constant of AOB growth on ammonia	0.5	g NH_4-N/m^3
Y_N	AOB growth yield	0.15	g VSS/g NH_4-N
b_{AOB}	autotrophic organisms decay rate	0.17	1/d
$K_{O,AOB}$	half saturation constant of AOB growth on oxygen	0.50	g O_2/m^3
Aeration-related			
C_s_20	saturation DO at sea level at 20ºC	9.09	g/m^3
F	fouling factor	0.90	-
de	mid-depth correction factor	0.40	(range: 0.25 - 0.45)
E	oxygen transfer efficiency	0.35	

Table 14. Calculation of sludge production (the excess sludge calculation with chemical addition is explained in the chemical P removal section); In the case of the BOD removal technology only, the SRT is an input; Px,bio is Px, bio, OHO for the BOD removal technology only, and is $Px, bio, OHO\&AOB$ for the technologies that involve nitrification.

Symbol	Description	Equation
$b_{H,T}$	heterotrophic organisms decay rate corrected for temperature	$b_{H,T} = b_H \times \theta^{T-20}$
$b_{AOB,T}$	autotrophic organisms decay rate corrected for temperature	$b_{AOB,T} = b_{AOB} \times \theta^{T-20}$
$\mu_{n,AOB}$	specific growth rate of nitrifiers	$\mu_{n,AOB} = \left(\frac{\mu_{n,AOB,max}}{K_{NH4} + NH4eff}\right)\left(\frac{DO}{K_{O,AOB} + DO}\right)$
$\mu_{n,AOB,T}$	specific growth rate of nitrifiers corrected for temperature	$\mu_{n,AOB,T} = \mu_{n,AOB} \times \theta^{T-20}$
SRT	sludge retention time	$SRT = \frac{1}{\mu_{n,AOB,T}}$
Px,bio_OHO (kg/d)	biomass sludge production in VSS units (heterotrophic organisms growth)	$Px, bio, OHO\ (VSS) = \frac{Q_{in}Y_H(S_0 - S)}{1 + b_{H,T}(SRT)} + \frac{(f_d)(b_{H,T})Q_{in}(S_0 - S)SRT}{1 + b_{H,T}(SRT)}$
Px,bio_OHO&AOB (kg/d)	biomass sludge production in VSS units (heterotrophic and nitrifier organisms growth)	$Px, bio, OHO\&AOB\ (VSS) = \frac{Q_{in}Y_H(S_0 - S)}{1 + b_{H,T}(SRT)} + \frac{(f_d)(b_{H,T})Q_{in}(S_0 - S)SRT}{1 + b_{H,T}(SRT)} + \frac{Q_{in}Y_N(NOx)}{1 + b_{AOB,T}(SRT)}$
Px,VSS (kg/d)	Sludge production in VSS units (biomass and non-biodegradable VSS)	$Px, VSS = Px, bio + Q_{in} \times nbVSS$
Px,TSS (kg/d)	Total sludge production in TSS units (inorganics from the influent included as well)	$P_{x,TSS} = \frac{Px, bio}{0.85} + Q_{in}(nbVSS) + Q_{in}(iTSS)$

Table 15. Water, air and sludge composition for the "BOD removal only" technology; NOx is assumed to be NO_3. [Comment 1]: The first term summed in is the direct oxidation of influent bCOD, while the second term is the endogenous respiration of microbial biomass. 3.6% of the CO_2 is assumed to be of non-biogenic origin (Law et al., 2013), and is accounted in the GHG emissions. aP is the available phosphorus as explained in Table 7.

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
COD	$F_{COD,water}\left(\frac{g}{d}\right) = Q_{in} \times sCODe + Q_e \times VSSe \times 1.42$ $sCODe\left(\frac{g}{m^3}\right) = nbsCOD + \frac{K_S(1 + b_{H,T} \times SRT)}{SRT(Y_H - b_{H,T}) - 1}$	$F_{COD,O2demand}\left(\frac{g}{d}\right) = Q_{in} \times (S_0 - S) - 1.42 \times Px,bio,OHO \times 1000\ (g/kg)$	$F_{COD,sludge}\left(\frac{g}{d}\right) = A + B - C$ $A = Px,bio,OHO \times 1.42 \times 1000\ (g/kg)$ $B = Q_{in} \times nbpCOD$ $C = Q_e \times VSSe \times 1.42$
CO_2	-	$F_{CO2,air}\left(\frac{g}{d}\right) = k_{CO2/COD} \times Q_{in} \times (1 - Y_H) \times (S_0 - S) + k_{CO2/biomass} \times \frac{(1-f_d)(b_{H,T})Q_{in}(S_0-S)SRT}{1+b_{H,T}(SRT)}$ [Comment 1]	-
TKN	$F_{TKN,water}\left(\frac{g}{d}\right) = Q_{in} \times (TKN_{in} - nbpON) + Q_e \times VSSe \times 0.12 - (0.12 \times Px,bio,OHO \times 1000)$	-	$F_{TKN,sludge} = A + B - C$ $A = 0.12 \times Px,bio \times 1000\ (g/kg);$ $B = Q_{in} \times nbpON$ $C = Q_e \times VSSe \times 0.12$
NOx	-	-	-
N_2	-	-	-
N_2O	-	-	-
TP	$F_{TP,water}\left(\frac{g}{d}\right) = (Q_{in} \times PO4_e) + (Q_e \times VSSe \times 0.015)$ $PO4_e\left(\frac{g}{m^3}\right) = aP - Psynthesis$ $P_{synthesis} = 0.015 \times Px,bio,OHO \times 1000\ (g/kg)$	-	$F_{TP,sludge} = A + B - C$ $A = 0.015 \times P_{x,bio} \times 1000\ (g/kg)$ $B = Q_{in} \times nbpP$ $C = Q_e \times VSSe \times 0.015$

Table 16. Water, air and sludge composition for the "BOD removal and nitrification" technology

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
COD	$F_{COD,water}\left(\frac{g}{d}\right) = Q_{in} \times sCODe + Q_e \times VSSe \times 1.42$ $sCODe\left(\frac{g}{m^3}\right) = nbsCOD + \frac{K_S(1 + b_{H,T} \times SRT)}{SRT(Y_H - b_{H,T}) - 1}$	$F_{COD,O2demand}\left(\frac{g}{d}\right) = Q_{in} \times (S_0 - S) - 1.42 \times Px, bio, OHO\&AOB \times 1000 \left(\frac{g}{kg}\right) + 4.57 \times \frac{F_{NOx,water}}{Q_e}$	$F_{COD,sludge}\left(\frac{g}{d}\right) = A + B - C$ $A = Px, bio, OHO\&AOB \times 1.42 \times 1000\ (g/kg)$ $B = Q_{in} \times nbpCOD$ $C = Q_e \times VSSe \times 1.42$
CO_2	-	$F_{CO2,air}\left(\frac{g}{d}\right) = k_{CO2/COD} \times Q_{in} \times (1 - Y_H) \times (S_0 - S) + k_{CO2/biomass} \times \frac{(1-f_d)(b_{H,T})Q_{in}(S_0-S)SRT}{1+b_{H,T}(SRT)} - 4.49 \frac{gCO2}{gN\ nitrified} \times F_{NOx,water}$	
TKN	$F_{TKN,water}\left(\frac{g}{d}\right) = Q_e \times (NH4_e + VSSe \times 0.12) + Q_{in} \times (nbsON)$	-	$F_{TKN,sludge} = A + B - C$ $A = 0.12 \times Px, bio \times 1000\ (g/kg);$ $B = Q_{in} \times nbpON$ $C = Q_e \times VSSe \times 0.12$
NOx	$F_{NOx,water}\left(\frac{g}{d}\right) = Q_{in} \times bTKN - Qe \times NH4_{eff} - 0.12 \times Px, bio, OHO\&AOB \times 1000\ (g/kg)$	-	$Q_{was} \times \frac{F_{NOx,water}}{Q_e}$
N_2	-	-	-
N_2O	-	$F_{N2O,air} = Qin \times TKN\_N2O$	-
TP	$F_{TP,water}\left(\frac{g}{d}\right) = (Q_{in} \times PO4_e) + (Q_e \times VSSe \times 0.015)$ $PO4_e\left(\frac{g}{m^3}\right) = aP - Psynthesis$ $P_{synthesis} = 0.015 \times Px, bio, OHO\&AOB \times 1000\ (g/kg)$	-	$F_{TP,sludge} = A + B - C$ $A = 0.015 \times P_{x,bio} \times 1000\ (g/kg)$ $B = Q_{in} \times nbpP$ $C = Q_e \times VSSe \times 0.015$

Table 17. Water, air and sludge composition for the "BOD and N removal" technology. NOx,e is imposed by design input. NOx_{nitri} is the nitrate concentration in the effluent obtained from the nitrification design exercise (prior to denitrification).

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
COD	$F_{COD,water}\left(\frac{g}{d}\right) = Q_{in} \times sCODe + Q_e \times VSSe \times 1.42$ $sCODe\left(\frac{g}{m^3}\right) = nbsCOD + \frac{k_S(1 + b_{H,T} \times SRT)}{SRT(Y_H - b_{H,T}) - 1}$	$F_{COD,O2demand}\left(\frac{g}{d}\right) = Q_{in} \times (S_0 - S) - 1.42 \times Px, bio, OHO\&AOB \times 1000 \left(\frac{g}{1kg}\right) + 4.57 \times \frac{F_{NOx,water}}{Q_e} - 2.86 \times Q_e \times (NOx, nitri - NOx, e)$	$F_{COD,sludge}\left(\frac{g}{d}\right) = A + B - C$ $A = Px, bio, OHO\&AOB \times 1.42 \times 1000\ (g/kg)$ $B = Q_{in} \times nbpCOD$ $C = Q_e \times VSSe \times 1.42$
CO_2	-	$F_{CO2,air}\left(\frac{g}{d}\right) = k_{CO2/COD} \times Q_{in} \times (1 - Y_H) \times (S_0 - S) + k_{CO2/biomass} \times \frac{(1-f_d)(b_{H,T})Q_{in}(S_0-S)SRT}{1+b_{H,T}(SRT)} - 4.49 \frac{gCO2}{gN\ nitrified} \times F_{NOx,water}$	
TKN	$F_{TKN,water}\left(\frac{g}{d}\right) = Q_e \times (NH4_e + VSSe \times 0.12) + Q_{in} \times (nbsON)$	-	$F_{TKN,sludge} = A + B - C$ $A = 0.12 \times Px, bio \times 1000\ (g/kg);$ $B = Q_{in} \times nbpON$ $C = Q_e \times VSSe \times 0.12$
NOx	$F_{NOx,water}\left(\frac{g}{d}\right) = Q_e \times NOx, e$	-	$Q_{was} \times NOx, e$
N_2	-	$F_{N2,air}\left(\frac{g}{d}\right) = Q_{in} \times (NOx_{nitri} - NOx, e)$	-
N_2O	-	$F_{N2O,air} = Qin \times TKN\_N2O$	-
TP	$F_{TP,water}\left(\frac{g}{d}\right) = (Q_{in} \times PO4_e) + (Q_e \times VSSe \times 0.015)$ $PO4_e\left(\frac{g}{m^3}\right) = aP - Psynthesis$ $P_{synthesis} = 0.015 \times Px, bio, OHO\&AOB \times 1000\ (g/kg)$	-	$F_{TP,sludge} = A + B - C$ $A = 0.015 \times P_{x,bio} \times 1000\ (g/kg)$ $B = Q_{in} \times nbpP$ $C = Q_e \times VSSe \times 0.015$

Table 18. Water, air and sludge composition for the "Biological P removal" technology. $f_{rbCOD/P}$ is is obtained from the implementation of Figure 8-38 of Metcalf and Eddy. Px, biorefers either to Px, bio, OHO or $Px, bio, OHO\&AOB$ depending if BioP removal is coupled to a BOD removal only system or to a BOD and nitrification or to a BOD and N removal system. $f_{rbCOD/P}$ defines the required readily biodegradable COD to remove P biologically. This approach does not impose a PO4 concentration in the effluent, but imposes an accumulation of the available phosphate, limited by the availability of rbCOD.

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
TP	$F_{TP,water}\left(\frac{g}{d}\right) = (Q_e \times PO4_e) + (Q_e \times VSSe \times (\frac{(PO4_{in} - PO4_e)}{Px, vss}))$ $PO4_e = PO4in - P_{EBPR} - P_{synthesis}$ $P_{EBPR} = \frac{\frac{rbCOD}{Qin}}{f_{rbCOD/P}}$ $P_{synthesis} = 0.015 \times Px, bio \times 1000\ (g/kg)$	-	$F_{TP,sludge} = A + B - C$ $A = P_{synthesis} + P_{EBPR}$ $B = Q_{in} \times nbpP$ $C = Q_e \times VSSe \times (\frac{(PO4_{in} - PO4_e)}{Px, vss})$

Table 19. Water, air and sludge composition for the "Chem P removal" technology.

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
TP	$F_{TP,water}\left(\frac{g}{d}\right) = (Q_e \times PO4_e) + (Q_e \times VSSe \times (\frac{(PO4_{in} - PO4_e)}{Px, vss}))$ PO4e is imposed through the design inputs		$F_{TP,sludge} = A + B - C$ $A = P_{synthesis} + (aPchem - PO4e) \times Qin$ $\boldsymbol{B} = Q_{in} \times nbpP$ $\boldsymbol{C} = Q_e \times VSSe \times (\frac{(PO4_{in} - PO4_e)}{Px, vss})$ $aPchem = aP - Psynthesis$ $P_{synthesis} = 0.015 \times Px, bio \times 1000\ (g/kg)$

2.3 Other pollutants

The same metals (and other elements) and transfer functions to water, air and sludge applied in the tool developed previously by Ecoinvent (Doka 2007) have been applied in this tool.

Table 20. Transfer coefficients of metals and other elements

Element	Influent WW concentration (mg/L)	Transfer to air (%)	Transfer to fresh sludge (%)	Transfer to effluent water (%)
B	0	0,0%	50,0%	50,0%
Cl	0,03003122	0,0%	0,0%	100,0%
Br	0	0,0%	0,0%	100,0%
F	3,2769E-05	0,0%	0,0%	100,0%
I	0	0,0%	0,0%	100,0%
Ag	0	0,0%	75,0%	25,0%
As	0,0000009	0,0%	22,0%	78,0%
Ba	0	0,0%	95,0%	5,0%
Cd	2,8063E-07	0,0%	50,0%	50,0%
Co	1,6177E-06	0,0%	50,0%	50,0%
Cr	1,2232E-05	0,0%	50,0%	50,0%
Cu	3,7443E-05	0,0%	75,0%	25,0%
Hg	2,0004E-07	0,0%	70,0%	30,0%
Mn	0,000053	0,0%	50,0%	50,0%
Mo	9,5744E-07	0,0%	50,0%	50,0%
Ni	6,5891E-06	0,0%	40,0%	60,0%
Pb	8,6314E-06	0,0%	90,0%	10,0%
Sb	0	0,0%	50,0%	50,0%
Se	0	0,0%	50,0%	50,0%
Sn	0,0000034	0,0%	59,0%	41,0%
V	0	0,0%	50,0%	50,0%
Zn	0,00010935	0,0%	70,0%	30,0%
Be	0	0,0%	50,0%	50,0%
Sc	0	0,0%	50,0%	50,0%
Sr	0	0,0%	50,0%	50,0%
Ti	0	0,0%	50,0%	50,0%
Tl	0	0,0%	50,0%	50,0%
W	0	0,0%	50,0%	50,0%
Si	0,0031263	0,0%	95,0%	5,0%
Fe	0,00709277	0,0%	50,0%	50,0%
Ca	0,05083371	0,0%	10,0%	90,0%
Al	0,00103784	0,0%	95,0%	5,0%
K	0,0003989	0,0%	0,0%	100,0%
Mg	0,00570707	0,0%	10,0%	90,0%
Na	0,00218597	0,0%	0,0%	100,0%

2.4 Sludge composition

2.4.1 Primary sludge composition

The composition of primary sludge depends on the removal of the different fractions during primary settling. The following equations allow for the estimation of the composition of primary sludge.

<u>Factors:</u>

f_CV_nbp	= VSS_COD,	(g_pCOD/g_VSS)
f_CV_bp	= bpCOD_bVSS	(g_bpCOD/g_bVSS)
f_C	= 0.51	(g_C /g_VSS)
f_N_nbp	= 0.12	(g_N /g_VSS)
f_N_bp	= 0.06	(g_N /g_VSS)
f_P_nbp	= 0.015	(g_P /g_VSS)
f_P_bp	= 0.010	(g_P /g_VSS)
f_O_nbp	= 16/18*(1 - f_CV_nbp/8 - 8/12*f_C - 17/14*f_N_nbp - 26/31*f_P_nbp)	(g_O/g_VSS)
f_O_bp	= 16/18*(1 - f_CV_bp/8 - 8/12*f_C - 17/14*f_N_bp - 26/31*.f_P_bp)	(g_O/g_VSS)
f_H_nbp	= 2/18*(1 + f_CV_nbp - 44/12*f_C + 10/14*f_N_nbp - 71/31*f_P_nbp)	(g_H/g_VSS)
f_H_bp	= 2/18*(1 + f_CV_bp - 44/12*f_C + 10/14*f_N_bp - 71/31*f_P_bp)	(g_H/g_VSS)

<u>Sludge composition:</u>

C_content	=	f_C	*	VSS_removed		(kg/d)
H_content	=	nbVSS_removed*f_H_nbp	+	bVSS_removed*f_H_bp		(kg/d)
O_content	=	nbVSS_removed*f_O_nbp	+	bVSS_removed*f_O_bp		(kg/d)
N_content	=	nbVSS_removed*f_N_nbp	+	bVSS_removed*f_N_bp		(kg/d)
P_content	=	nbVSS_removed*f_P_nbp	+	bVSS_removed*f_P_bp		(kg/d)

VSS_removed and bVSS_removed correspond to the sludge that is formed during primary settling.

Water content estimation. It is assumed that after the centrifuges a total dry solids percentage of 25% is achieved. This means that 75% is water (by weight relations). Hence, if 786 kg TSS/d is produced as primary sludge, then the water content (WC) is = 786/25*75 = 2358 kg water/d. This water is assumed to be recycled back to the influent of the WWTP.

2.4.2 Secondary sludge composition

Sludge production is estimated through the Metcalf & Eddy equations (see Px,VSS calculated in section 2.3.1). Assuming the COD_VSS ratio of 1.42, the composition in terms of C, H, O, N and P is calculated as follows:

If the COD/VSS (f_CV=1.42), C/VSS (f_C=0.51), N/VSS (f_N=0.12) and P/VSS (f_P=0.015) are known then the O/VSS (F_O) and H/VSS (f_H) can be calculated with the following equations:

f_O = 16/18 (1- f_CV/8 - 8/12 f_C – 17/14 f_N – 26/31 f_P)

f_H = 2/18 (1+ f_CV - 44/12 f_C + 10/14 f_N – 71/31 f_P)

So for f_CV = 1.42; f_C = 0.51 , f_N=0.12 and f_P = 0.015, then f_O=0.288 and f_H=0.067.

f_C + f_H + f_O + f_N + f_P must be = to 1.000.

Overall:

C_content = P_X_VSS * 0.51 (kg/d)

H_content = P_X_VSS * 0.067 (kg/d)

O_content = P_X_VSS * 0.288 (kg/d)

N_content= P_X_VSS * 0.12; 0.12 is the value provided by Metcalf & Eddy on the N content in sludge (kg/d)

P_content = P_X_VSS * 0.015; 0.015 is the value provided by Metcalf & Eddy on the P content in sludge (kg/d)

Water content estimation. It is assumed that after the centrifuges a total dry solids percentage of 25% is obtained. This means that 75% is water (by weight relations). Hence, if 786 kg TSS/d is produced as primary sludge, then the water content (WC) is = 786/25*75 = 2358 kg water/d.

2.4.3 Sludge composition of precipitate from chemical P removal

Chemical P removal promotes the formation of extra sludge. The composition of that extra sludge depends on the amount of iron chloride added, and is estimated as follows.

<u>Chemical P removal process variables needed:</u>
- extra_iSS (kg/d)
- Fe_P_mole_ratio (mole Fe/mole P)

<u>Molecular weights of Fe and P</u>
- M_Fe = 55.845; //g/mol (Fe molecular weight)
-M_P = 30.974; //g/mol (P molecular weight)

<u>Fractions:</u>
Fe_content = extra_iSS * M_Fe*Fe_P_mole_ratio/(106.8*Fe_P_mole_ratio + 80);
H_content = extra_iSS * (3*Fe_P_mole_ratio + 1)/(106.8*Fe_P_mole_ratio + 80);
P_content = extra_iSS * M_P/(106.8*Fe_P_mole_ratio + 80);
O_content = extra_iSS * 48*(Fe_P_mole_ratio + 1)/(106.8*Fe_P_mole_ratio + 80);

Notes: 106.8 is the molecular weight of iron chloride; 48 is the molecular weight of 3 oxygens

2.5 Energy consumption

Only electricity consumption for aeration, pumping, mixing, dewatering and other overhead uses are included. No other sources of energy (e.g. natural gas boiler) are considered. Other than energy for sludge dewatering, energy consumed or produced during the treatment of sludge is also excluded.

2.5.1 Aeration energy consumption

Metcalf & Eddy provides equations to design the aeration capacity. Any text after // are comments to the equations.

R0 = (Q*(S0-S)/1000 -1.42*P_X_bio)/24 + 0; // kg_O2/h

note:

C_T = air_solubility_of_oxygen(T,0); //mg_O2/L -> elevation=0 TableE-1, Appendix E, implemented in "utils.js"

Pb = Pa*Math.exp(-g*M*(zb-0)/(R*(273.15+T))); //Pa -> pressure at plant site

C_inf_20 = C_s_20 * (1+de*Df/Pa); //mg_O2/L

OTRf = R0; //kgO2/h; OTRf is calculated separately per each technology; as denitrification implies less consumption of Oxygen because part of the COD is removed anoxically by using NO_3^- as electron acceptor.

SOTR = (OTRf/(alpha*F))*(C_inf_20/(beta*C_T/C_s_20*Pb/Pa*C_inf_20-C_L))*(Math.pow(1.024,20-T)); //kg/h

kg_O2_per_m3_air = density_of_air(T,Pressure)*0.2318 //oxygen in air by weight is 23.18%, by volume is 20.99%

air_flowrate = SOTR/(E*60*kg_O2_per_m3_air) ||0; //m3/min

However, Metcalf & Eddy does not provide energy consumption calculations. A simplified approach is suggested that uses SOTR calculated from Metcalf & Eddy, and uses typical ranges of Standard Aeration Energy (SAE). For fine bubble systems SAE ranges between 3.6 and 4.8 kgO2/kWh, and 4 kgO_2/kWh is taken as a default value.

$$AE\ (kW) = \frac{SOTR\ \left(\frac{kgO2}{h}\right)}{SAE\ \left(\frac{kgO2}{kWh}\right)}$$

kW can be converted into kWh consumed per day (kWh/d) by multiplying AE*24.

Overall, this approach results in a low energy consumption in the biological reactors of about 0.2 $kWh{\cdot}m^{-3}$ of treated wastewater. This is at the lower end of typical ranges, which are between 0.13 and 5.5 $kWh{\cdot}m^{-3}$ (Enerwater, 2015). Hence, the designed WWTPs are assumed to be well designed in terms of energy equipment)

2.5.2 Pumping energy consumption and mixing energy consumption

Pumping flows are calculated with the Metcalf and Eddy equations. Then, energy consumption factors (PE_Qx) (obtained from Gernaey et al., 2014) are used per each type of pump including internal recirculation, external recirculation, wastage and mixing.

Table 21. Pumping energy consumption

Element	Equation	Factors
Internal recirculation	Qint * PE_Q_{int}	PE_Q_{int}: 0.004 kWh.m^{-3} (Gernaey et al., 2014
External recirculation	Qr * PE_Q_r	PE_Q_r: 0.008 kWh.m^{-3} (Gernaey et al., 2014
Wastage	Qwas * PE_Q_w	PE_Q_w: 0.050 kWh.m^{-3} (Gernaey et al., 2014)
Mixing	PEmix * Vanoxic	PEmix is assumed to be 5 kWh m^{-3} d^{-1}. Vanoxic (m^3) is the volume of the anoxic reactor obtained during the design of the BOD and N removal technology
Influent pumping	P (Watts)= rho.g.Q.H, where: rho is density of water = 1000 kg/m^3 g = gravitation constant = 9.81 m/s^2 Q is flow in m^3/s H is water lift height and friction head in m.	A standard lift height of 10 m is used. The user can change it if they have a better estimation. P excludes losses in gear box and electrical inefficiency. So, for electrical power consumption these losses increase the power consumption.

2.5.3 Dewatering

The multiplication factor 20 kWh/tDM sludge is used (Corominas et al., 2013).

Hence, DewE (kWh) = 20 * P_X_TSS/1000;

2.5.4 Other

Table 22 shows the data taken from different WWTPs (Stillwell et al., 2010) to generate linear relationships between wastewater flow treated and other energy consumption.

Table 22. Reference energy consumption data (Stillwell et al., 2010)

Volume of treated wastewater (m^3/d)	3785	18927	37854	75708	189271
Lighting and buildings (kWh/d)	200	400	800	1200	2000
Pumping (kWh/d)	171	716	1402	2559	6030
Pre-treatment (kWh/d)	51	89	136	253	606
Primary (kWh/d)	15	78	155	310	776
Biological (kWh/d)	947	4718	9429	18637	46264
Sludge treatment (kWh/d)	6	243	4204	7194	16268
Total	1390	6244	16126	30153	71944

2.5.4.1 Without primary treatment:

otherE (kWh/d) = 0.0124 * Flow + 337.77

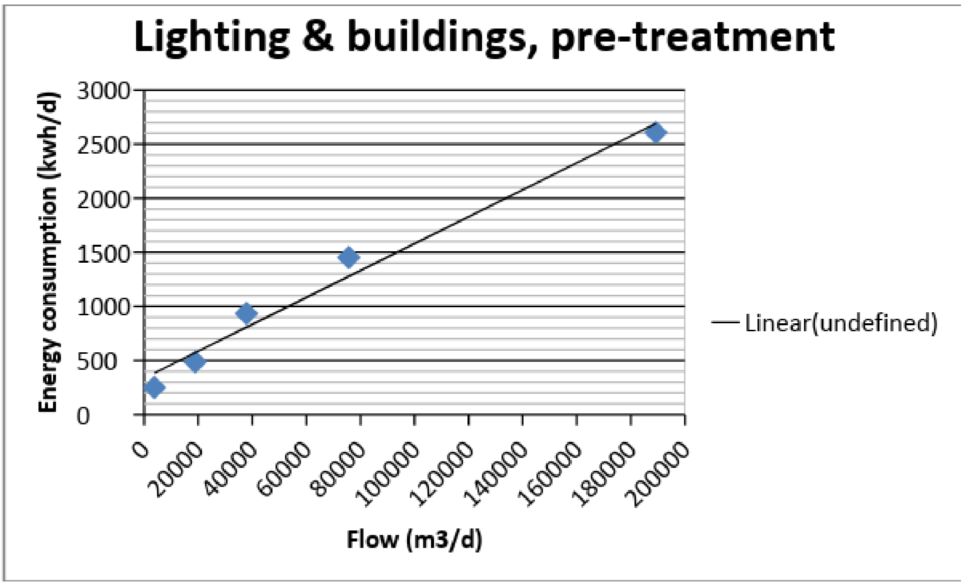


Figure 12. Energy consumption of WWTPs of different sizes, excluding primary treatment

2.5.4.2 With primary treatment:

otherE (kWh/d) = 0.0165 * Flow + 337.59

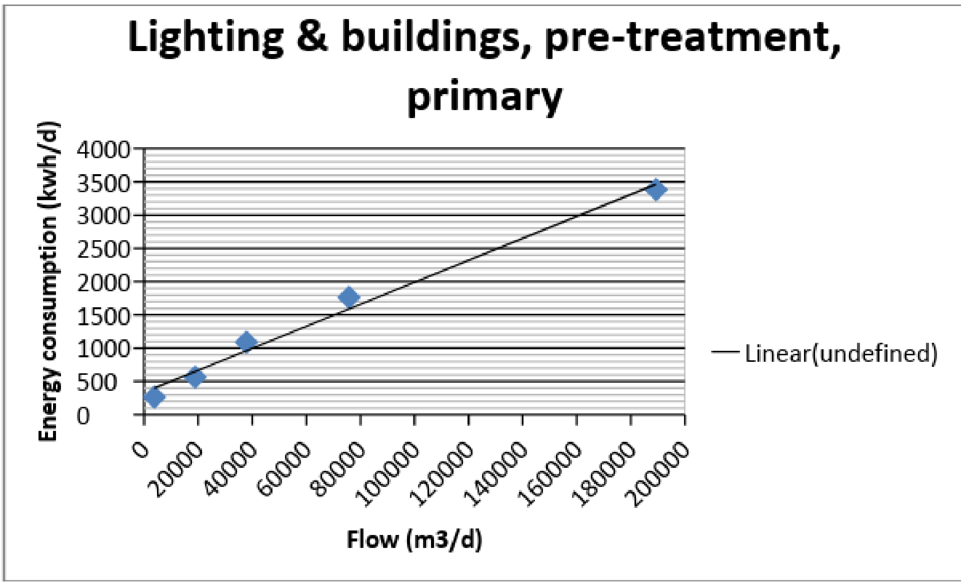


Figure 13. Energy consumption of WWTPs of different sizes, including primary treatment

2.6 Chemicals consumption

This work does not include a comprehensive list of chemicals that might be consumed in WWTPs, but it provides empirical factors for the three most widely used ones: lime to maintain the pH, iron chloride for chemical P removal and polyelectrolyte for thickening sludge.

2.6.1 Chemicals for alkalinity control

Nitrification is pH-sensitive and removal rates decline significantly at pH values below 6.8. A pH of 7.0 to 7.2 is normally used to maintain reasonable nitrification rates, and for locations with low-alkalinity waters, alkalinity is added at the WWTP to maintain acceptable pH values. The amount of alkalinity added depends on the initial alkalinity concentration and amount of ammonia to be oxidized. Alkalinity may be added in the form of lime, soda ash, sodium bicarbonate, sodium carbonate, or magnesium hydroxide. In this tool we assume that the added chemical is sodium carbonate ($NaHCO_3$) as this is the chemical available in the Ecoinvent database and is easy to handle in WWTPs.

alkalinity_used_for_nitrification (g $CaCO_3/m^3$) = 7.14 (g $CaCO_3$/gN) *NOx (gN)

where 7.14 (g $CaCO_3$/gNH_4-N nitrified) is obtained from the following stoichiometric equation:
$NH_4^+ + 2HCO_3^- + 2O_2 \rightarrow NO_3^- + 2CO_2 + 3H_2O$

It is assumed that 70 g $CaCO_3$/m3 is the residual alkalinity needed to maintain pH in the range 6.8-7.0. Hence, 70 equals the influent alkalinity minus the used alkalinity + the alkalinity added.

alkalinity_added (kg CaCO3/d)=(70-Alkalinity+alkalinity_used_for_nitrification)*Q/1000; where Q is the flow rate in m^3/d.

In order to convert the alkalinity from $CaCO_3$ to $NaHCO_3$ the following equation is used:

alkalinity_added_$NaHCO_3$ (kg $NaHCO_3$/d)= alkalinity_added * (84 g $NaHCO_3$/100 g $CaCO_3$)

2.6.2 Iron chloride for chemical P removal

In this tool phosphate precipitation with iron was implemented. In the case of iron, 1 mole will precipitate 1 mole of phosphate; however, these reactions are competing with other reactions and dosages are established on the basis of bench-scale tests. Metcalf and Eddy includes in Figure 6-13 the Fe/P molar ratio required to achieve different effluent phosphate concentrations. It is assumed that the precipitant is iron chloride 40%, which is available in the Ecoinvent database.

Table 23. Parameters for the chemical P model

Parameter	Default value
Fe_P_mole_ratio	look-up table (Figure 6-13, pag 484 Tchobanoglous et al., 2014)
Raw_sludge_specific_gravity	1.03
Raw_sludge_moisture_content	94
Chemical_sludge_specific_gravity	1.05
Chemical_sludge_moisture_content	92.5

Table 24. Model inputs for chem P removal.

	Default values
FeCl3_solution	40%
FeCl3_unit_weight	1.35 kg/L

The dosage of iron chloride to remove the available PO_4^{3-} (PO4 in the following equations, obtained after subtracting the influent PO_4^{3-} minus the PO_4^{3-} used for the growth of organisms) is calculated as follows. The user can select the target PO_4^{3-} concentration in the effluent (PO4_eff).

Fe_III_dose = Fe_P_mole_ratio*(PO4-P-PO4-Peff)*M_Fe/M_P; (mg/L)
Fe_dose = Q*Fe_III_dose/1000; (kg/d)
percent_Fe_in_FeCl3 = 100*M_Fe/162.3; (%)
amount_FeCl3_solution = Fe_dose/percent_Fe_in_FeCl3*100; (kg/d)
FeCl3_volume = amount_FeCl3_solution/(FeCl3_solution/100*FeCl3_unit_weight) ||0; (L/d)

The storage volume of FeCl3 is calculated as follows:
storage_req_15_d = FeCl3_volume/1000*days; (m3)

There is an increase in the sludge production when adding iron chloride. This is as well calculated as follows.

Fe_dose_M = Fe_III_dose/1000/M_Fe; (M (mol/L))
P_removed = (PO4 - PO4_eff)/1000/M_P; (M(mol/L))
Fe1.6H2PO4OH_sludge = P_removed*251*1000; //mg/L (251 is $Fe_{1.6}H_2PO_4OH$ molecular weight)
Excess_Fe_added = Fe_dose_M - 1.6*P_removed; (M (mol/L))
FeOH3_sludge = Excess_Fe_added*(106.8)*1000; (mg/L (106.8 is $FeCl_3$ molecular weight))
Excess_sludge = FeH2PO4OH_sludge + FeOH3_sludge; (mg/L)
Excess_sludge_kg = Q*Excess_sludge/1000; (kg/d)

(see the composition of excess sludge in section 2.5.3)

2.6.3 Polyelectrolyte for thickening (dewatering polymer)

The polyelectrolyte dosage per Ton of dry matter of sludge was taken from Morera et al. (2017) for the WWTP of Girona, which is 10 kg polyelectrolyte/Tn DM. It is assumed that the polyelectrolyte proxy in the Ecoinvent database is acrylamide.

3 Construction inventories

In this tool we propose to use the following range of WWTP sizes, based on population equivalents:

Table 25. Main characteristics of the WWTPs included in the construction inventories

Class	Class 4	Class 3b	Class 3a	Class 2	Class 1
PE range	2,000-10,000	10,000-20,000	20,000-50,000	50,000-100,000	over 100,000
PE reference WWTP	8,750	18,750	44,153	100,000	206,250
Name reference WWTP	Navàs	Balaguer	Manlleu	L'Escala	Girona

A PE range of WWTPs smaller than 2000 PE was not included as it would be better represented with a soft technology (wetlands or ponds) rather than a conventional activated sludge technology. In the following sections it is explained how the construction inventories for the 5 reference WWTPs (1 large and 4 small to medium) were obtained.

3.1 Large WWTP

3.1.1 Procedure followed to obtain a detailed construction inventory

Detailed inventories for civil works includes the following steps (Figure 14): (1) Obtain the construction budget for the WWTP. In the budget, all elements needed for civil works (e.g., excavations, handrails, concrete, etc.) are listed, along with the price and the amount of each one. (2) Then, all these elements in the budget are identified and grouped in a simplified list (e.g., excavation of a representative type of soil, a representative type of concrete, etc.). (3) Once all elements of the budget are identified and grouped, it is necessary to search for equivalent elements in a specialized constructive database of reference (in this case the local database Banc BEDEC, which is used by constructors to make their budgets). This database provides all the necessary information about materials and energy consumed to build a unit of each element. (4) Finally, the material and energy inventories are calculated by relating the elements obtained from the construction budget to the equivalent elements of the reference database.

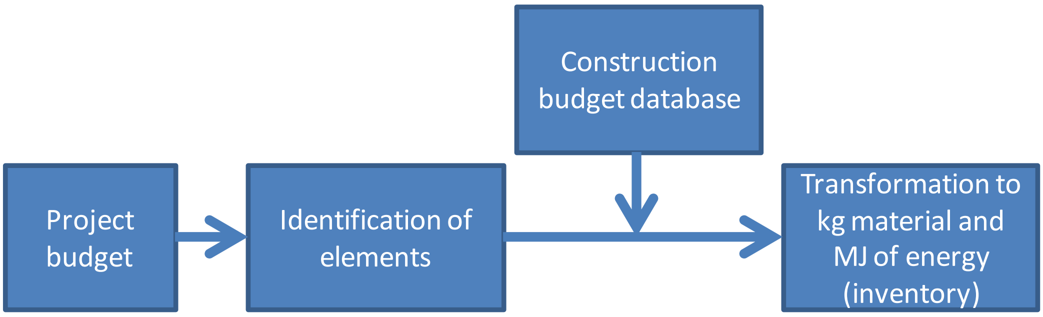


Figure 14. Procedure followed to obtain the detailed inventory of the WWTP construction. Equipment is not included in this inventory.

Five WWTP units were considered in the case study: (1) pumping + pretreatment, (2) primary treatment, (3) secondary treatment, (4) sludge line and deposition, and (5) buildings and services. Table 26 provides a description of the elementary processes considered for each operational unit considered in this work. The procedure was applied to obtain detailed inventories for each these units of the WWTP.

Table 26. Description of all unit processes included in each operation unit studied.

Operational unit	Elementary processes included
Pumping+pretreatment	Wastewater well reception, pumping station, pretreatment building, part of the connections and part of the unit to dose chemicals
Primary treatment	Primary settlers, units to mix water and chemicals, chamber to measure the flow and part of the connections
Secondary treatment	Biological reactors, secondary settlers, chamber to measure the sludge sent to the sludge line, chamber to measure and pump the sludge sent back to the biological reactor, part of the unit to dose chemicals and part of the connections
Sludge line and deposition	Thickening tanks and buildings for the thickening tanks, chamber to pump the sludge, dewatering building, zone for the dewatered sludge, anaerobic digestion unit and part of connections, final sludge treatment in a composting plant
Others	Chemicals storage, control building, adaptation of the land and sidewalks

3.1.2 Goal and scope definition

The goal was to perform an LCA of the Girona WWTP, considering the construction of the plant (civil works), the operation and dismantling, and making an individual analysis for the five WWTP units. The functional unit of the study is 1 m^3 of treated wastewater assuming that the WWTP is working at full capacity. In fact, WWTPs are designed and constructed to serve a specific capacity. However, the treated flow does not always match the design flow. The lifetime of the WWTP was assumed to be 30 years. The sensitivity of the LCA assessment on the lifetime of the WWTP is addressed in a sensitivity analysis. Salvage values for the equipment are considered when the life spans of the WWTP and of the equipment do not match.

The studied WWTP is located in Girona (Catalonia, NE of Spain). It treats the wastewater from the main city and different nearby towns located around the WWTP before the effluent is discharged into the Ter River. The plant has a capacity of 206,250 population equivalents (PE), which corresponds to a design flow rate of 55,000 $m^3 \cdot d^{-1}$. However, in the year 2013 the WWTP of Girona treated on average 42,000 $m^3 \cdot d^{-1}$. The water line consists of a Modified Ludzack-Ettinger (MLE) configuration with biological removal of organic matter and nitrogen and chemical removal of phosphorus. The sludge line consists of thickening, anaerobic sludge digestion with electricity production from the biogas, and sludge dewatering. The dewatered sludge is sent to a nearby composting plant. The composting plant is a private installation located 20 km away from the WWTP, and it treats not only the sludge from the WWTP but also other organic residues from other facilities. Figure 15 shows a scheme of the WWTP with a separation of each analyzed operational unit and an indication of the operational data used to perform the LCA of the operation.

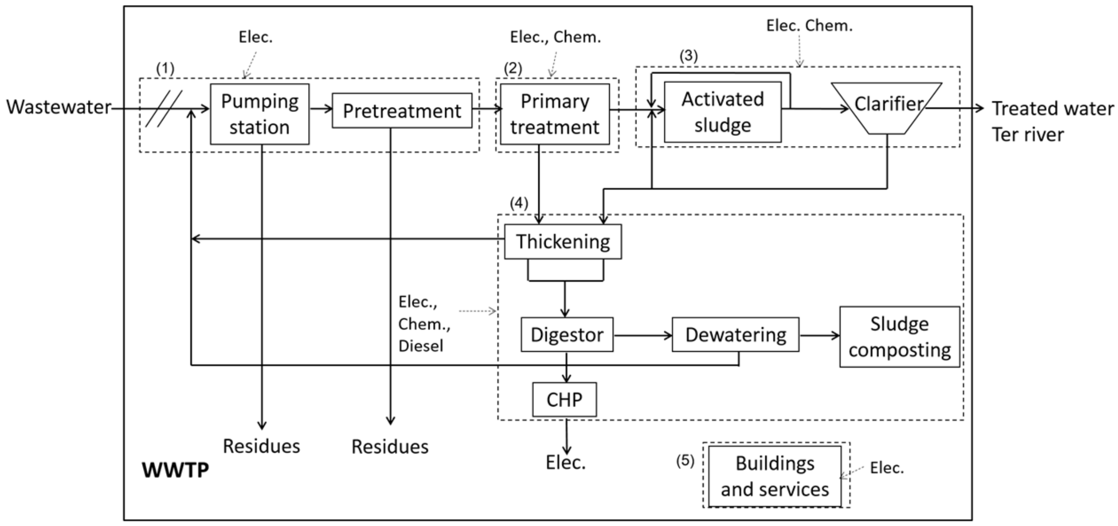


Figure 15. Layout of the WWTP of Girona.

Pumping and pretreatment includes five pumps, two channels that are 16 meters long, two sieves, screening and grease separation. Primary treatment has three primary settlers, each with a total capacity of 412 m^3. Secondary treatment consists of three different reactors with a total capacity of 29,620 m^3 and three settlers, each with a capacity of 5,027 m^3. The sludge line includes two thickeners with 16 m of diameter, two primary digesters with a 3,432 m^3 volume, two secondary digesters with an 814 m^3 volume, two dewatering devices and a cogeneration device.

The system boundaries (Figure 16) consider the WWTP's construction, operation and dismantling. The production of all materials (and their transport) and energy used to build the WWTP (civil works + equipment) are accounted for. The dismantling is considered in this study for the most abundant materials for both civil works and equipment, assuming that concrete and reinforced concrete are disposed at a landfill for inert waste, 91% of metals are recycled (Sansom and Avery, 2014) and 25% of plastics are recycled, 34% of plastics are incinerated with electricity recovery and the rest disposed in a landfill (Plastics Europe, 2012). The construction of the composting plant is not within the system boundaries.

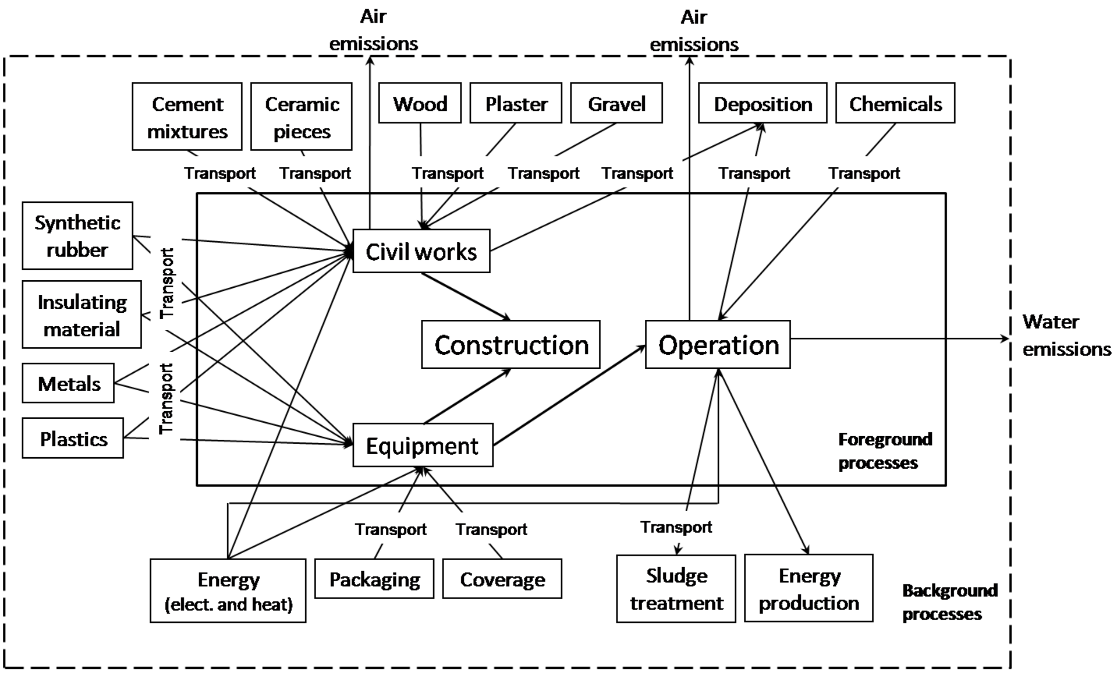


Figure 16. Elements included in the inventory. Equipment is available in the inventory of Morera et al. (2017) but has not been included in the inventory of this ecoinvent tool.

3.1.3 Inventory analysis

The procedure described in section 3.1.1 has been applied to obtain the construction inventories of each of the five WWTP units in terms of materials and energy. Hence, for all WWTP stages (pre-treatment, primary treatment, secondary treatment, sludge line, buildings and services) materials and energy were accounted for. A summary of the construction inventory can be found in Table 30. 45 different types of materials have been used in the construction of the WWTP of Girona (see Table S-1 from supporting information of Morera et al. (2017) for a complete material inventory). Even though Morera et al. (2017) included inventory of equipment materials, such inventory has not been included in this ecoinvent inventory analysis. Hence, equipment has not been accounted for in the inventories for these 4 WWTPs. Transports have been estimated considering the weight of the materials and assuming an average distance of 40 km.

3.1.4 Small-medium WWTPs

3.1.4.1 Unit processes classification

The functional unit of the study is the construction of a WWTP. Four WWTPs with capacities ranging from 1,500 to 21,000 $m^3 \cdot d^{-1}$ (Table 27) were chosen for inventory development. The WWTPs have similar configurations, employing an oxidation ditch to remove carbon and nitrogen and simple sludge treatment via thickening and dewatering. The lifetime of the WWTP was assumed to be 30 years.

Table 27. Location, capacity and operation scheme of the studied WWTPs. Dark grey represents the pretreatment, black the biological reactor, light grey the secondary settler and light grey with lines in diagonal represents the sludge treatment.

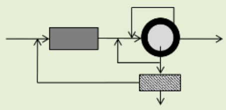
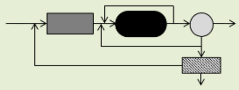
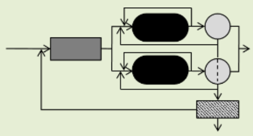
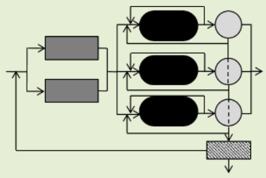
Location (Region)	Capacity ($m^3 \cdot d^{-1}$)	Configuration
Navàs (Bagès)	1,500	
Balaguer (La Noguera)	3,750	
Manlleu (Osona)	14,400	
L'Escala (Alt Empordà)	21,000	

Table 28. Specifications of the different WWTPs

WWTP name	Navàs	Balaguer	Manlleu	L'Escala	Girona	Navàs
Capacity (m^3/d)	1500	3750	14400	21000	55000	1500
Capacity (PE)	8750	18750	44153	100000	206250	8750
Entrance load (kgBOD_5/d)	525	1125	5328	6300	12375	525
Entrance load TN (kg N/d)	112,5	356,25	576	1260	3190	112,5
Concrete volume in biological reactor (m^3)	542,366	859,468	2256,391	5002,596	7983,07	542,366

The construction inventories for the four plants were created by first obtaining the constructive budget of each plant. Next, the constructive budget database, Banc BEDEC (Barcelona, Spain), was used to estimate the materials and energy use associated with each budget item. The budget items and associated materials and energy use were categorized based on WWTP treatment elements including: pre-treatment, secondary treatment, sludge line, buildings, urbanization, tube connections and power station (Table 30). More information on this inventory development methodology can be found in Morera et al. (2017).

Table 29. Elements considered in the budget that were included in the construction inventory.

Elements	Sub-elements
Pre-Treatment	- Receiving waters well - Pumping station - Screening

	- Grit removal - Degreasing operations
Secondary Treatment	- Biological reactor - Secondary settler
Sludge Line	- Thickener - Dewatering
Buildings	- Control and Services Buildings - Buildings that hold key elements
Urbanization	- Process of asphalting inside the WWTP - Sidewalks construction - Construction of green zones - Placement of metal fences around the WWTP
Tube connections	- Tube connections
Power connections	- Buildings that hold the electricity transformer

An assumption made is that reactors were all partially buried leaving a height of 1.5 meters above ground. The soil that was excavated was assumed to be compact soil in all cases. Gravity thickening was assumed for all WWTPs.

3.1.5 Materials classification and grouping

A grouping of materials was applied to compare the mass of materials between inventories of this study and of Ecoinvent, selecting one material representative and summing up all masses of materials belonging to the same group. No grouping was applied though when calculating the environmental impacts out of the inventories, and hence all materials with their own characterization factors were applied.

3.1.6 Other assumptions

- The excavation process was calculated from the consumption of diesel needed for the machines to excavate the needed volume of soil.

- The electricity is generated on site by an electrical generator (current practice on-site, after personal communication with the construction company Voltes S.L.U).

- These inventories account for transport of the excess excavated soil to the landfill or the transport from the manufacturer to the workplace with a distance of 40 km each, assuming also the internal transports.

- The concrete category applied in the inventories is concrete with non-special requirements. Construction companies (e.g. Voltes S.L.U) advised that the concrete used for the construction of WWTPs does not need any special requirements.

Table 30. Inventory for the 5 WWTPs.

name	ByProduct	unit	class 1	class 2	class 3a	class 3b	class 4
wastewater treatment facility, capacity class X, between Y and Z PE	ReferenceProduct	unit	1	1	1	1	1
waste reinforced concrete	ByProduct	kg	5.31E+07	3.16E+07	1.75E+07	5.51E+06	2.60E+06
waste polyvinylchloride product	ByProduct	kg	1.22E+08	1.30E+04	9.23E+07	8.49E+08	6.80E+08
waste polyethylene/polypropylene product	ByProduct	kg	4.87E+08	5.82E+04	4.27E+08	2.88E+08	1.54E+08
waste glass sheet	ByProduct	kg	1.27E+06	1.03E+03	2.60E+08	6.04E+04	1.26E+08
waste mineral wool	ByProduct	kg	8.45E+05	2.36E+06	-	3.09E+08	2.91E+05
waste brick	ByProduct	kg	1.17E+06	1.29E+06	2.75E+05	4.13E+08	2.20E+08
aluminium scrap, post-consumer	ByProduct	kg	7.88E+06	6.95E+06	6.50E+07	8.98E+08	3.65E+08
iron scrap, unsorted	ByProduct	kg	4.75E+08	2.19E+04	5.01E+08	7.33E+08	1.22E+08
inert waste	ByProduct	kg	1.29E+08	7.51E+07	7.03E+07	1.14E+07	6.49E+06
diesel, burned in building machine	FromTechnosphere	MJ	1.24E+07	9.30E+06	6.87E+06	1.78E+06	1.06E+06
concrete, normal	FromTechnosphere	m^3	2.15E+08	1.28E+04	7.13E+08	2.28E+07	1.07E+08
reinforcing steel	FromTechnosphere	kg	1.97E+06	1.13E+06	5.61E+08	7.83E+08	5.06E+07
steel, low-alloyed	FromTechnosphere	kg	5.45E+08	3.22E+04	5.00E+08	8.00E+08	1.11E+07
wire drawing, steel	FromTechnosphere	kg	2.80E+08	1.63E+04	8.01E+07	1.01E+08	7.53E+08
aluminium, primary, ingot	FromTechnosphere	kg	7.88E+06	6.95E+06	6.50E+07	8.98E+08	3.65E+08
anodising, aluminium sheet	FromTechnosphere	m^2	3.94E+06	3.47E+06	3.25E+07	4.49E+08	1.83E+08
zinc coat, pieces	FromTechnosphere	m^2	5.79E+08	9.92E+06	1.77E+08	2.59E+08	2.98E+08
steel, chromium steel 18/8	FromTechnospher	kg	1.02E+07	2.25E+06	8.12E+08	3.41E+08	8.85E+08

	e						
bronze	FromTechnosphere	kg	-	8.67E+06	-	1.97E+08	8.50E-01
copper	FromTechnosphere	kg	5.40E-01	4.13E+06	-	1.25E+08	5.47E+08
wire drawing, copper	FromTechnosphere	kg	5.40E-01	3.60E+06	-	6.29E+08	4.22E+08
brass	FromTechnosphere	kg	-	4.41E+06	3.62E+08	1.08E+08	4.02E+04
cast iron	FromTechnosphere	kg	1.08E+08	3.67E+03	-	-	9.92E+02
enamelling	FromTechnosphere	m^2	5.38E+08	1.83E+03	-	-	4.96E+02
polyvinylchloride, bulk polymerised	FromTechnosphere	kg	1.10E+08	1.17E+04	8.30E+08	7.64E+08	6.12E+08
polyvinylchloride, emulsion polymerised	FromTechnosphere	kg	1.22E+08	1.30E+06	9.23E+07	8.49E+08	6.80E+08
polypropylene, granulate	FromTechnosphere	kg	1.79E+06	7.21E+06	-	7.15E+04	-
polyurethane, rigid foam	FromTechnosphere	kg	1.07E+07	5.31E+06	2.33E+08	3.30E+08	1.29E+08
silicone product	FromTechnosphere	kg	4.22E+05	1.10E+05	6.39E+08	9.15E+08	2.83E+08
synthetic rubber	FromTechnosphere	kg	1.29E+08	6.59E+06	3.48E+08	1.79E+07	1.22E+07
polystyrene, expandable	FromTechnosphere	kg	-	3.10E+06	-	-	-
polyethylene terephthalate, granulate, amorphous	FromTechnosphere	kg	-	2.65E+06	-	3.39E-01	9.76E-01
polystyrene, extruded	FromTechnosphere	kg	1.30E+07	2.17E+06	-	1.81E+05	6.38E+03
polyethylene, high density, granulate	FromTechnosphere	kg	1.24E+08	1.96E+06	7.62E+07	3.44E+05	3.44E+05

nylon 6-6	FromTechnosphere	kg	5.45E+04	2.99E+06	-	7.64E-01	7.64E-01
glass fibre reinforced plastic, polyester resin, hand lay-up	FromTechnosphere	kg	4.60E+08	5.20E+04	-	7.92E+02	7.52E+08
polystyrene, general purpose	FromTechnosphere	kg	-	1.23E+06	-	1.37E+08	3.95E+08
glued laminated timber, for outdoor use	FromTechnosphere	m^3	2.66E+08	8.77E+05	5.05E+08	1.47E+08	5.44E-01
particle board, for outdoor use	FromTechnosphere	m^3	4.45E+08	7.78E+06	5.81E+08	1.68E+08	1.34E+08
lime mortar	FromTechnosphere	Kg	2.25E+05	3.60E+05	8.58E+08	5.05E+07	3.46E+08
cement mortar	FromTechnosphere	Kg	3.28E+08	1.12E+05	1.98E+08	3.29E+08	3.86E+08
adhesive mortar	FromTechnosphere	Kg	1.20E+08	7.09E+04	1.01E+08	5.98E+08	5.53E+08
concrete, high exacting requirements	FromTechnosphere	m^3	2.63E+08	6.61E-02	-	-	-
gypsum plasterboard	FromTechnosphere	kg	-	5.05E+06	-	1.18E+07	3.36E+06
cover plaster, mineral	FromTechnosphere	kg	2.05E+00	3.12E+04	7.03E+02	2.45E+08	4.51E+08
concrete block	FromTechnosphere	kg	7.74E+08	5.64E+05	2.43E+08	3.07E+05	1.56E+08
lightweight concrete block, polystyrene	FromTechnosphere	kg	1.13E+08	1.29E+05	-	2.21E+07	1.81E+02
light clay brick	FromTechnosphere	kg	2.87E+08	5.88E+05	3.15E+07	8.30E+08	6.26E+08
sand	FromTechnosphere	kg	-	1.07E+08	4.60E+07	1.89E+06	1.04E+06
gravel, crushed	FromTechnosphere	kg	5.34E+06	6.85E+05	6.30E+06	1.76E+06	2.27E+05
diesel	FromTechnosphere	kg	2.66E+08	1.70E+06	6.85E+08	2.92E+08	8.04E+06

flat glass, coated	FromTechnosphere	kg	1.27E+06	1.03E+03	2.60E+08	6.04E+04	1.26E+08
alkyd paint, white, without water, in 60% solution state	FromTechnosphere	kg	5.18E+04	2.75E+04	2.04E+02	2.21E+05	1.17E+02
bitumen adhesive compound, hot	FromTechnosphere	kg	1.55E+06	5.21E+04	9.78E+08	2.00E+08	1.17E+07
alkyd resin, long oil, without solvent, in 70% white spirit solution state	FromTechnosphere	kg	5.09E+07	2.36E+06	-	-	-
solvent, organic	FromTechnosphere	kg	-	1.82E+02	-	2.88E+01	-
mastic asphalt	FromTechnosphere	kg	1.50E+06	7.57E+02	8.53E+05	1.15E+02	-
stone wool	FromTechnosphere	kg	8.45E+05	2.36E+06	-	3.09E+08	2.91E+05
sanitary ceramics	FromTechnosphere	kg	-	2.56E+02	-	6.06E+01	6.71E+01
acrylic varnish, without water, in 87.5% solution state	FromTechnosphere	kg	-	6.48E+06	-	-	2.62E+04
acrylic filler	FromTechnosphere	kg	-	1.78E+05	-	4.84E+04	-
adhesive, for metal	FromTechnosphere	kg	2.01E+05	7.15E-02	-	-	2.15E+04
printed paper	FromTechnosphere	kg	8.41E-01	3.02E+06	-	1.69E+05	-
natural stone plate, polished	FromTechnosphere	kg	-	9.15E+04	2.36E+08	2.30E+08	-
polycarbonate	FromTechnosphere	kg	-	1.28E-02	-	-	-
compost	FromTechnosphere	kg	-	1.80E+04	-	-	2.35E+07
expanded clay	FromTechnosphere	kg	-	3.32E+04	-	-	-
acrylonitrile-butadiene-styrene copolymer	FromTechnosphere	kg	-	9.94E+06	-	-	-

diesel, burned in diesel-electric generating set, 18.5kW	FromTechnosphere	MJ	7.49E+08	1.81E+05	5.02E+08	1.31E+08	2.15E+08
transport, freight, lorry >32 metric ton, EURO4	FromTechnosphere	metric ton*km	8.67E+06	8.29E+06	5.75E+06	8.93E+08	4.06E+08
sheet rolling, steel	FromTechnosphere	kg	3.09E+08	-	2.10E+08	8.57E+08	4.74E+08
impact extrusion of steel, cold, 5 strokes	FromTechnosphere	kg	2.69E+08	-	4.86E+08	7.60E+08	1.22E+07
injection moulding	FromTechnosphere	kg	6.48E+08	-	3.60E+08	2.34E+08	5.67E+08
extrusion, plastic pipes	FromTechnosphere	kg	4.84E+08	-	7.64E+07	1.89E+08	2.73E+07
Water, unspecified natural origin	FromEnvironment	m^3	3.79E+08	-	3.25E+08	5.95E+08	8.66E+07
Transformation, from grassland, natural (non-use)	FromEnvironment	m^2	4.97E+04	-	1.67E+04	1.17E+04	1.93E+03
Occupation, construction site	FromEnvironment	m^2*year	4.97E+04	-	1.67E+04	-	1.93E+03
Transformation, to industrial area	FromEnvironment	m^2	4.52E+04	-	1.06E+04	-	-
Transformation, to urban/industrial fallow (non-use)	FromEnvironment	m^2	4.50E+03	-	6.11E+03	-	-
Occupation, industrial area	FromEnvironment	m^2*year	1.35E+06	-	3.17E+05	-	-
Occupation, urban/industrial fallow (non-use)	FromEnvironment	m^2*year	1.35E+05	-	1.83E+05	-	-
wastewater treatment facility, capacity class 3a, between 20,000 and 50,000 PE	ReferenceProduct	unit	-	-	1.00E+00	-	-
butyl acrylate	FromTechnosphere	kg	8.06E-01	-	6.15E-01	-	2.02E-01
epoxy resin, liquid	FromTechnosphere	kg	8.13E+06	-	8.93E-01	4.29E+08	4.78E+05
wastewater treatment facility, capacity class 1, greater than	ReferenceProduct	unit	1.00E+00	-	-	-	-

100,000 PE								
polystyrene foam slab	FromTechnosphere	kg	5.57E+04	-	-	2.99E+08	-
switch, toggle type	FromTechnosphere	kg	2.14E+00	-	-	6.44E+07	1.85E+08
cement, unspecified	FromTechnosphere	kg	1.52E+04	-	-	1.07E+08	-
wastewater treatment facility, capacity class 3b, between 10,000 and 20,000 PE	ReferenceProduct	unit	-	-	-	1.00E+00	-
polyester-complexed starch biopolymer	FromTechnosphere	kg	-	-	-	3.94E+08	-
wastewater treatment facility, capacity class 4, between 2,000 and 10,000 PE	ReferenceProduct	unit	-	-	-	-	1.00E+00
polysulfide, sealing compound	FromTechnosphere	kg	-	-	-	-	1.27E+04
ethylene vinyl acetate copolymer	FromTechnosphere	kg	-	-	-	-	3.76E+05

3.2 Sewer system

The modelling of the sewer system is taken from Doka (2009) and represents a rough estimate at best. Doka (2009) provided Swiss data on meters per capita of sewers per capacity. This value is converted to m^3 of transported wastewater using the capacity and treated volume amounts from the Spanish wastewater treatment plants discussed in the previous section. The same relations are assumed to hold whether the water sent to the sewer is ultimately discharged to the environment or treated.

4 "Direct discharge of wastewater" dataset

Not all wastewater generated by the population is collected in sewer systems, not all sewer systems are connected to a WWTP, and some sewer systems may be associated with losses before reaching the WWTP. This tool specifically accounts for the latter two of these aspects in a specific dataset, "direct discharge of wastewater".

4.1 Collected wastewater not connected to a WWTP

Wastewater collected but not connected to a WWTP is modelled as a direct emission to the environment. The dataset converts all the pollutants in the wastewater (e.g. mass concentration of Total Kjeldahl Nitrogen, mass concentration of a metal) into emissions to water (Nitrogen, organic bound to surface water, metal ion to surface water). The actual water is also emitted to the environment (Water to surface water). The reference flow is 1 m^3 of wastewater directly discharged to the environment from the sewer.

The fraction of wastewater that is discharged to the environment from sewer systems without treatment is accounted for in the production volume of the dataset. During linking, ecoinvent will calculate the relative shares of water being treated and that directly discharged based on the relative production volumes of the direct discharge and treatment datasets. The production volume is calculated using data from the report on the WHO/UNICEF joint monitoring program of 2017, which includes sanitation data for most countries of the world. The data is available through https://washdata.org/data.

From the data obtained for 2015 the following ratio is estimated:

$$\frac{\text{\% population whose wastewater is collected in sewers but discharged to rivers without treatment}}{\text{percentage of population connected to sewers}}$$

This percentage per country is applied to the production volume of water discharged to the sewer system, which is a user input and is calculated by the production volume of the unit process generating the wastewater and the amount of wastewater generated per unit of its reference flow.

Geographies in the ecoinvent database are mapped to those in the WHO data. In cases where ecoinvent geographies did not have a direct match in the WHO data, a best match was manually found.

4.2 Combined sewer overflow wastewater

Combined sewer systems (CSS) collect rainwater runoff, municipal sewage, and industrial wastewater in the same pipe. Normally, these systems will transport the total volume of sewage to a WWTP for treatment. However, some very intense rain episodes result in volumes of runoff that, when mixed with municipal and industrial waste, can exceed the capacities of a CSS. When capacity is exceeded, a combined sewer overflow (CSO) occurs, which is the discharge of untreated sewage (mixed with urban runoff) from a CSO structure directly into surface water. Because CSOs contain untreated municipal and industrial waste, toxic materials, and debris, they impact the physicochemical, biological, hydraulic, and aesthetic status of receiving water bodies.

These emissions are accounted for in the "untreated wastewater" dataset. They are calculated in a three-step process:

- A fraction of wastewater pollutants reported in the wastewater properties are assumed discharged due to the CSO episodes. This fraction is country-specific, and depends on the share of sewer systems that are combined (rather than separate), on rainfall, snowmelt, etc. In the tool, the default values used are taken from Doka (2009): 1% of the particulate compounds of the wastewater and 2% of the soluble compounds. The tools' thorough influent wastewater fractionation allows differentiating amongst soluble and particulate compounds. These represent Swiss data, and may not apply to other situations. The data provider can change these values directly in the tool.
- The calculated amounts of compounds lost due to CSO episodes are then converted to emissions to water using the same approach as outlined for direct discharge of water.
- Finally, these emissions are scaled to account only for collected wastewater that is actually connected to a WWTP (to avoid double counting), and then scaled again to the reference flow of the direct discharge dataset, where CSO is reported. The resulting equation is:

$$\frac{\text{kg emission}}{\text{m}^3\text{directly discharge water}} =$$

$$\frac{\text{compounds lost due to CSO}}{\text{m}^3\text{treated water}} \times \frac{\text{m}^3\text{treated water}}{\text{m}^3\text{total water}}$$

$$\times \frac{\text{m}^3\text{total water}}{\text{m}^3\text{directly discharged water}}$$

Note that in regions where the fraction of directly discharged water is 0, CSO is not accounted for. Indeed, in these cases, the ratio (m^3 total water/m^3 directly discharged water) has a division by 0 problem, and the production volume of the "no treatment" dataset would be 0. This is a limitation of the model. Future versions should consider including CSO in the treatment dataset instead, or including them in the market dataset, where sewers could also eventually be included.

4.2.1 Sewer system

The water that is discharged directly to the environment still uses the sewer system. Hence, it is necessary to include the sewer infrastructure input. This is done using the same sewer system proportions as for the wastewater treatment dataset, where it was based on the capacity of existing WWTPs. This is a rough approximation, which can be corrected by the data provider if more specific information is available.

For countries where there are no WWTPs, the sewer estimation uses the default market shares of WWTPs, based on the South African situation for now (see Section 7).

5 Uncertainty assessment

The uncertainty of all quantified data in the ecoSpold datasets is estimated using the Pedigree matrix approach:

- A basic uncertainty factor is identified for all types of exchanges, ranging from 0.0006 for inputs of electricity to 0.65 for emissions of metals to water.
- Pedigree scores, which cover different aspects of data quality, are also given, which will result in “additional” uncertainty.

The approach assumes that all parameters are lognormally distributed.

The tool needs to provide basic uncertainty factors and pedigree scores in a very general way, without any information on the quality of the data that the data provider will input into the model. It therefore behoves the user to check these values directly in the ecoEditor tool and make adjustments where appropriate. All uncertainty fields are documented to inform the user on how the default uncertainty factors were selected. Here are some of the assumptions that were made when selecting the default basic uncertainty and pedigree scores:

- Production volumes of direct discharge and treatment datasets: The uncertainty of these production volumes is based on the uncertainty of the WHO data used to identify how much wastewater sent to the sewer system is actually treated. It therefore neglects the uncertainty in the actual amount of wastewater generated upstream.
- Emissions to water of direct discharge:
    - The basic uncertainty of emissions associated with direct discharge of wastewater is approximated as the uncertainty of an emission to water. For example, the uncertainty for the emission of metals associated with the direct discharge of wastewater containing a metal pollutant is approximated as 0.65, the basic uncertainty of a heavy metal emission to water. This will overestimate the uncertainty for wastewaters that were well characterized.
    - The pedigree scores depend on whether the CSO (scores = [5, 5, 4, 5, 1]) or the directly discharged (scores = [1, 1, 1, 1, 1]) amounts are greater.
- Except for infrastructure inputs, technosphere exchange amounts calculated by the model are all given a basic uncertainty of 0.0006 and pedigree scores of [3, 5, 1, 5, 4].
- Infrastructure and sewer inputs are given basic uncertainty factors of 0.3. The pedigree scores for sewer amounts is [5, 5, 5, 5, 5], and for infrastructure, [5, 5, 1, 5, 5].

6 Calculation engine

The main goal of the tool is to estimate the inputs and outputs of treating 1 m^3 of a particular activity wastewater in a reference (or a set of reference) WWTP/s that already treats a (much larger) volume of water. For this estimation, the model runs twice, once with just the reference wastewater and once with the reference wastewater and a marginal amount (1m^3/d) of activity wastewater. The difference is taken to be a reflection of how inputs and outputs (elementary flows, energy consumption, chemicals consumption, sludge production, etc.) change with an additional amount of the activity wastewater, and hence the approach follows the ISO14044 Step 2 approach. Because it uses a marginal difference in influent at the WWTP point of operation, the approach is sometimes referred to in this text as the "marginal" approach. This work does not provide a design for a WWTP for an activity wastewater.

In the case there is only one reference WWTP:

1) The WWTP model is run only accounting for the "municipal" wastewater characteristics of the inhabitants connected to the WWTP. Design outcomes and elementary flows are obtained.
2) A mass balance is conducted on the "municipal" wastewater characteristics plus the activity wastewater characteristics. A second set of design outcomes and elementary flows is obtained.
3) The difference between the results obtained in step 2 minus step 1 is the burden associated to the activity wastewater.

In the case there is a mix of reference WWTPs (WWTP mixes):

1) The approach explained for just one reference WWTP is repeated for as many reference WWTPs are available.
2) The results of each iteration are weighted based on the percentage of treated load (measured as population equivalents) per each reference WWTP.

It is worth mentioning that adding activity wastewater to the existing "municipal" wastewater can have positive or negative effects. The simplest example is adding an activity wastewater that has much higher temperature than the "municipal" wastewater. If the temperature at the WWTP is increased, the kinetics are faster and hence there is larger removal of pollutants. This means that adding an activity wastewater does not always results in increases of environmental burdens for all variables. This explains the negative values obtained by the tool (in the inventory of the contributions of the activity wastewater) in some cases.

7 WWTP mixes per region

A WWTP mix is a set of WWTPs where the activity wastewater will be co-treated with other (reference) wastewater. For each WWTP included in a particular mix the following characteristics are to be supplied.

Table 31. List of parameters needed for each element of the mix

Id	Description	unit
% of PE treated	Percentage of entire country PE treated	
Technology	Select type of technology	
Population equivalents	Average PE of plant in mix	PE
COD	Chemical oxygen demand	g COD/m^3
TKN	Kjeldahl nitrogen	g N/m^3
TP	Total Phosphorus	g P/m^3
Temperature		ºC
Q	Flow	m^3/d
NH4eff	Effluent ammonia target	g N/m^3
NO3eff	Effluent nitrate target	g N/m^3
PO4eff	Effluent phosphate target	g P/m^3
Ag	Silver	g/m^3
Al	Aluminum	g/m^3
As	Arsenic	g/m^3
B	Boron	g/m^3
Ba	Barium	g/m^3
Be	Beryllium	g/m^3
Br	Bromine	g/m^3
Ca	Calcium	g/m^3
Cd	Cadmium	g/m^3
Cl	Chlorine	g/m^3
Co	Cobalt	g/m^3
Cr	Chromium	g/m^3
Cu	Copper	g/m^3
F	Fluorine	g/m^3
Fe	Iron	g/m^3
Hg	Mercury	g/m^3
I	Iodine	g/m^3
K	Potassium	g/m^3
Mg	Magnesium	g/m^3
Mn	Manganese	g/m^3
Mo	Molybdenum	g/m^3
Na	Sodium	g/m^3
Ni	Nickel	g/m^3
Pb	Lead	g/m^3
Sb	Antimony	g/m^3
Sc	Scandium	g/m^3
Se	Selenium	g/m^3
Si	Silicon	g/m^3
Sn	Tin	g/m^3
Sr	Strontium	g/m^3
Ti	Titanium	g/m^3
Tl	Thallium	g/m^3
V	Vanadium	g/m^3

W	Tungsten	g/m^3
Zn	Zinc	g/m^3
CSO_particulate	Fraction of particulates that are discharged with the combined sewer overflows	%
CSO_soluble	Fraction of particulates that are discharged with the combined sewer overflows	%
removal_bpCOD	Percentage removal of bpCOD during primary settling	%
removal_nbpCOD	Percentage removal of nbpCOD during primary settling	%
removal_ON	Percentage removal of ON during primary settling	%
removal_OP	Percentage removal of OP during primary settling	%
removal_iTSS	Percentage removal of iTSS during primary settling	%
MLSS_X_TSS	Design mixed liquor suspended solids	g/m^3
DO	Dissolved oxygen concentration in biological aerobic reactor	g/m^3 as O_2
clarifiers	Number of clarifiers	clarifiers
sBODe	Soluble BOD in the effluent	g/m^3 as O_2
TSSe	Total suspended solids in the effluent	g/m^3
zb	Site elevation above sea level	m
Pressure	Pressure at site elevation	Pa
Df	Liquid depth above diffusers in biological reactor	m
h_settler	Height of settler	m
X_R	Return sludge mass concentration	g/m^3
SRT	Sludge Retention Time	d
SOR	Hydraulic application rate for secondary settler	$m^3/m^2 \cdot d$
SF	Peak to average TKN load	Ø
Anoxic_mixing_energy	Mixing energy for anoxic reactor	$kW/1000\ m^3$
FeCl3_solution	Ferric chloride solution	%
FeCl3_unit_weight	Ferric chloride unit weight	kg/L
days	Time of storage of the ferric chloride	d
influent_H	Influent pumping water lift height	m

7.1 Country mixes

The tool is ready to create new country WWTP mixes. As an example the country mix of WWTPs is provided for South-Africa.

Table 32. Example of the South-Africa mix

South Africa	Description	unit	mix 1	mix 2	mix 3	mix 4
% of PE treated	Percentage of entire country PE treated		9,3	13,4	30,1	47,2
Technology	Select type of technology		BOD+ND+BioP	BOD+ND+BioP	BOD+ND+BioP	BOD+ND+BioP
Population equivalents	Average PE of plant in mix	PE	62000	502000	1124000	1765000
COD	Chemical oxygen demand	g COD/m^3	800	800	800	800
TKN	Total Kjeldahl nitrogen	g N/m^3	64	64	64	64
TP	Total phosphorus	g P/m^3	10	10	10	10
Temperature		ºC	14	14	14	14
Q	Flow	m^3/d	7700	62800	140500	220700
NH4eff	Effluent ammonia target	g N/m^3	-	1	-	1
NO3eff	Effluent nitrate target	g N/m^3	-	6	-	6
PO4eff	Effluent phosphate target	g P/m^3	-	1	-	1
Ag	Silver	g/m^3	0	0	0	0
Al	Aluminum	g/m^3	1,0379	1,0379	1,0379	1,0379
As	Arsenic	g/m^3	0,0009	0,0009	0,0009	0,0009
B	Boron	g/m^3	0	0	0	0
Ba	Barium	g/m^3	0	0	0	0
Be	Beryllium	g/m^3	0	0	0	0
Br	Bromine	g/m^3	0	0	0	0
Ca	Calcium	g/m^3	5.08E+04	5.08E+04	5.08E+04	5.08E+04
Cd	Cadmium	g/m^3	3.00E-04	3.00E-04	3.00E-04	3.00E-04
Cl	Chlorine	g/m^3	3.00E+04	3.00E+04	3.00E+04	3.00E+04
Co	Cobalt	g/m^3	1.60E-03	1.60E-03	1.60E-03	1.60E-03
Cr	Chromium	g/m^3	1.22E-02	1.22E-02	1.22E-02	1.22E-02
Cu	Copper	g/m^3	3.74E-02	3.74E-02	3.74E-02	3.74E-02

F	Fluorine	g/m^3	3.28E-02	3.28E-02	3.28E-02	3.28E-02
Fe	Iron	g/m^3	7.09E+04	7.09E+04	7.09E+04	7.09E+04
Hg	Mercury	g/m^3	2.00E-04	2.00E-04	2.00E-04	2.00E-04
I	Iodine	g/m^3	0	0	0	0
K	Potassium	g/m^3	3.99E-01	3.99E-01	3.99E-01	3.99E-01
Mg	Magnesium	g/m^3	5.71E+04	5.71E+04	5.71E+04	5.71E+04
Mn	Manganese	g/m^3	5.30E-02	5.30E-02	5.30E-02	5.30E-02
Mo	Molybdenum	g/m^3	1.00E-03	1.00E-03	1.00E-03	1.00E-03
Na	Sodium	g/m^3	2.19E+03	2.19E+03	2.19E+03	2.19E+03
Ni	Nickel	g/m^3	6.60E-03	6.60E-03	6.60E-03	6.60E-03
Pb	Lead	g/m^3	8.80E-03	8.80E-03	8.80E-03	8.80E-03
Sb	Antimony	g/m^3	0	0	0	0
Sc	Scandium	g/m^3	0	0	0	0
Se	Selenium	g/m^3	0	0	0	0
Si	Silicon	g/m^3	31,263	31,263	31,263	31,263
Sn	Tin	g/m^3	0.0034	0.0034	0.0034	0.0034
Sr	Strontium	g/m^3	0	0	0	0
Ti	Titanium	g/m^3	0	0	0	0
Tl	Thallium	g/m^3	0	0	0	0
V	Vanadium	g/m^3	0	0	0	0
W	Tungsten	g/m^3	0	0	0	0
Zn	Zinc	g/m^3	1.09E-01	1.09E-01	1.09E-01	1.09E-01
CSO_particulate	Fraction of particulates that are discharged with the combined sewer overflows	%	0	0	0	0
CSO_soluble	Fraction of particulates that are discharged with the combined sewer overflows	%	0	0	0	0
removal_bpCOD	Percentage removal of bpCOD during primary settling	%	40	40	40	40
removal_nbpCOD	Percentage removal of nbpCOD during primary settling	%	60	60	60	60

removal_ON	Percentage removal of ON during primary settling	%	66,6	66,6	66,6	66,6
removal_OP	Percentage removal of OP during primary settling	%	66,6	66,6	66,6	66,6
removal_iTSS	Percentage removal of iTSS during primary settling	%	70	70	70	70
MLSS_X_TSS	Design mixed liquor suspended solids	g/m^3	3000	3000	3000	3000
DO	Dissolved oxygen concentration in biological aerobic reactor	g/m^3 as O_2	2	2	2	2
clarifiers	Number of clarifiers	clarifiers	3	3	3	3
sBODe	Soluble BOD in the effluent	g/m^3 as O_2	3	3	3	3
TSSe	Total suspended solids in the effluent	g/m^3	5	5	5	5
zb	Site elevation above sea level	m	500	500	500	500
Pressure	Pressure at site elevation	Pa	95600	95600	95600	95600
Df	Liquid depth above diffusers in biological reactor	m	4,4	4,4	4,4	4,4
h_settler	Height of settler	m	4	4	4	4
X_R	Return sludge mass concentration	g/m^3	8000	8000	8000	8000
SRT	Sludge Retention Time	d	5	-	5	-
SOR	Hydraulic application rate for secondary settler	$m^3/m^2 \cdot d$	24	24	24	24
SF	Peak to average TKN load	Ø	1,5	1,5	1,5	1,5
Anoxic_mixing_energy	Mixing energy for anoxic reactor	$kW/1000\ m^3$	5	5	5	5
FeCl3_solution	Ferric chloride solution	%	40	40	40	40
FeCl3_unit_weight	Ferric chloride unit weight	kg/L	1,35	1,35	1,35	1,35
days	Time of storage of the ferric chloride	d	15	15	15	15
influent_H	Influent pumping water lift height	m	10	10	10	10

7.2 Global mix

The global mix is currently the one belonging to South-Africa. At the time of writing this report, the global average is based on South African data only. Data from other countries will be integrated at a later date.

7.3 User own mix

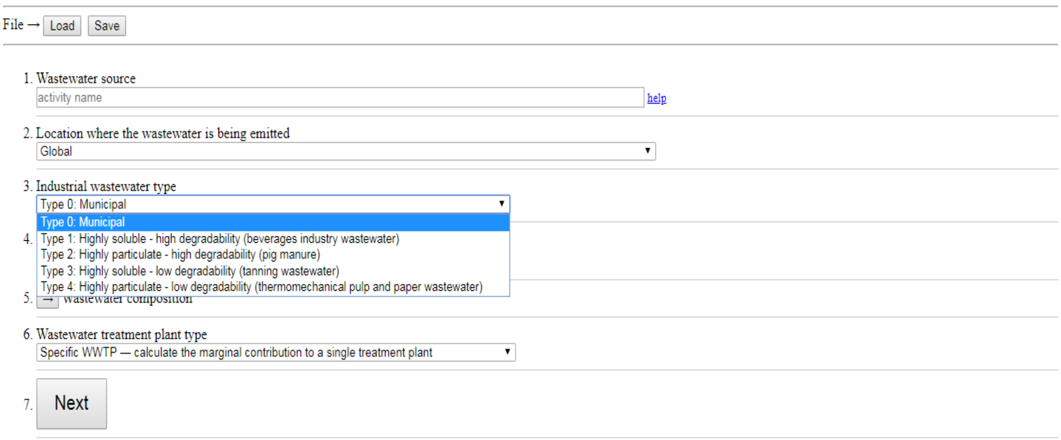
The tool allows for the users to build their own mixes in a user-friendly manner. The mix can be created and then saved as a json file which can be uploaded afterwards.

8 Using the web tool

8.1 Activity data entry page

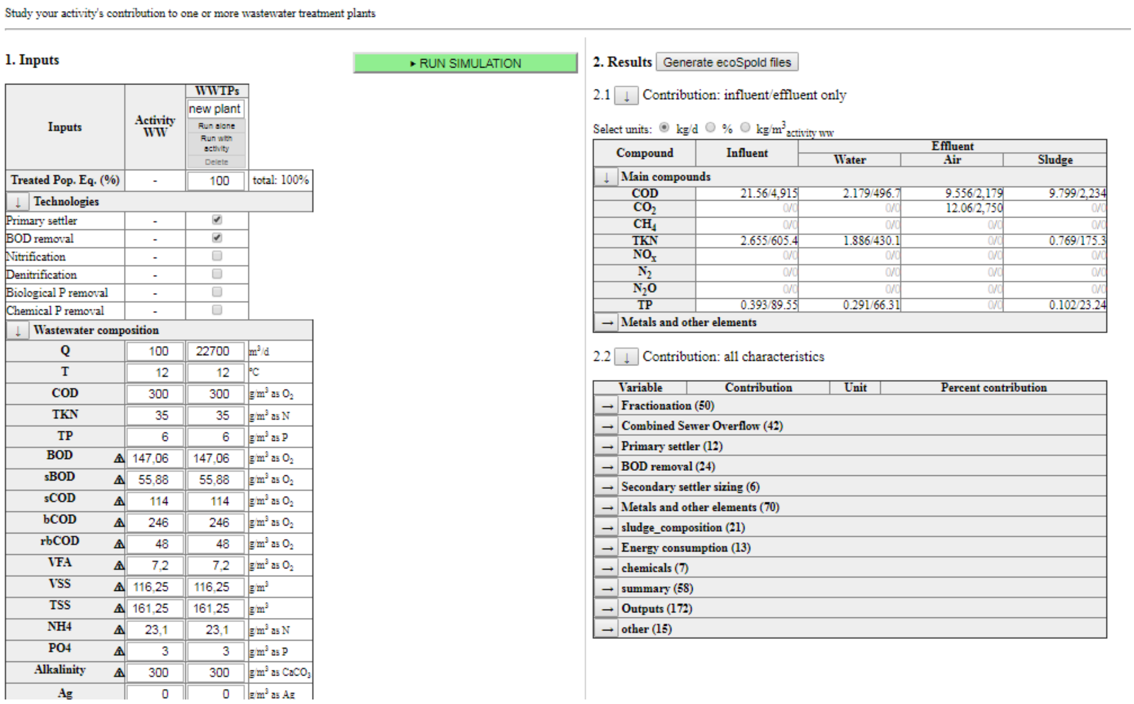
The user enters activity wastewater source, location (select global or a particular country), industrial wastewater type, volume of wastewater discharged, wastewater composition and the wastewater treatment plant type (specific or country average) in the Activity data entry page.

With regards to the industrial wastewater type the user can select amongst the following 5 options: type 0: municipal, type 1: highly soluble and high degradability, type 2: highly particulate and high degradability, type 3: highly soluble and low degradability, and type 4: highly particulate and low degradability. This selection is used to execute the fractionation of the total COD, TKN and TP that has to enter under the wastewater composition tab.



The user selects "Specific WWTP" or "country average WWTP". With the “Specific WWTP” the user will enter the characteristics of a particular user-defined WWTP and run the marginal approach against that one. If the user selects country average WWTP, the default WWTP mix of a given country (selected in the data entry page), with predefined values already available in the tool, is loaded in the following page. The marginal approach is then run n times, one for each element of the WWTP mix.

8.2 Marginal approach calculation page



There are two main sections: Inputs (on the left) and Results (on the right).

A) If the user has selected “specific WWTP” in the activity data entry page there is only one reference WWTP to be defined. Default values are provided but the user can modify them. For the reference WWTPs the type of wastewater is municipal, and hence the “municipal” wastewater fractionation factors are provided. The user selects the technology of the reference WWTP, indicating whether it includes a primary settler, BOD removal, nitrification, denitrification, and/or biological or chemical P removal. With regards to the wastewater composition, the user first enters flow, temperature, COD, TKN and TP. All other wastewater composition fractions can be estimated from the “municipal” fractionation factors by pressing the warning symbol next to each compound. Still, the user can change the values.

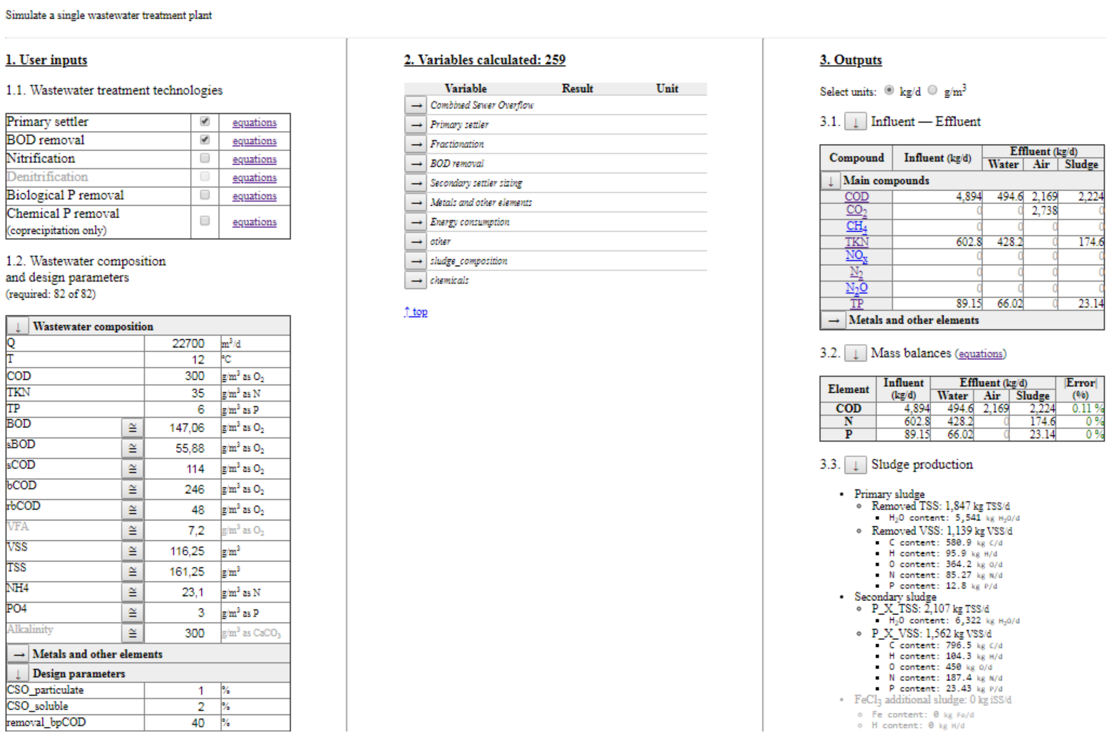
B) If the user has selected “country average WWTP” in the activity data entry page, there are multiple reference WWTPs provided. Default values are provided, and it is recommended not to change them.

When the user is satisfied with the entrance of the inputs the “run simulation” button can be pressed. This button triggers the calculation of the marginal approach. The action is fast to compute, and the user immediately sees the new outcomes in the results section.

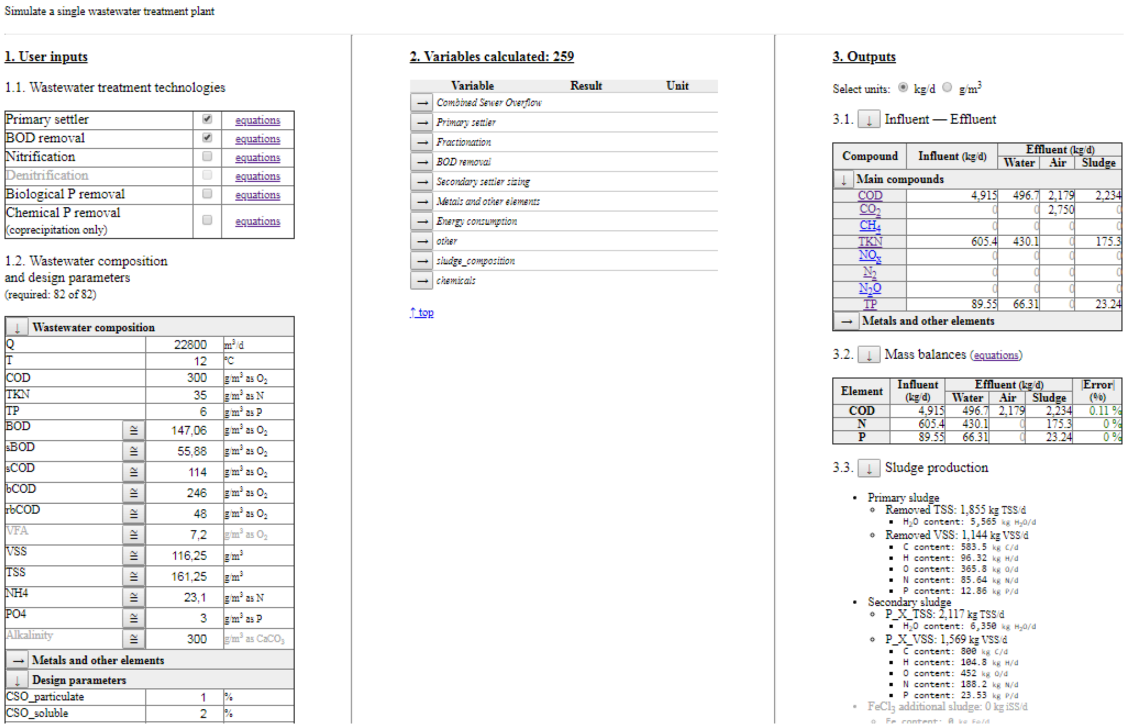
Finally, when results have been computed, the user can press the “Generate Ecospold file” button to generate the Ecospold file.

Advanced users who would like to get more information and understand how these inventories have been generated have two extra options:

1) Run alone: A new web tab opens where the user can run a simulation of the reference WWTP alone, without considering the activity wastewater and not calculating the marginal approach;



2) Run with activity: A new tab opens where the user can execute the modelling approach for the sum of the municipal and the activity wastewater;



The user can have access to the actual implementation of the equations, by clicking the hyperlinks of the calculated variables (section2 of the run with activity webpage).

The user can also access the equations through the information page, where Table 33 is guiding the user.

Table 33. Access to equations implemented in the backend of the tool

Technology	Source	Code
1. Fractionation	M&EA 5th ed (p. 756)	fractionation.js
2. BOD removal	M&EA 5th ed (p. 756)	bod_removal_only.js
3. Nitrification	M&EA 5th ed (p. 762)	nitrification.js
4. Denitrification	M&EA 5th ed (p. 810)	n_removal.js
5. P removal (biologically)	M&EA 5th ed (p. 880)	bio_P_removal.js
6. P removal (chemically)	M&EA 5th ed (p. 484)	chem_P_removal.js
7. SST sizing	M&EA 5th ed (p. 767)	sst_sizing.js
8. Metals and other elements	G. Doka excel tool	metals_doka.js
9. CSO removal	Based on M&EA fractionation	cso_removal.js
10. Primary settler	Ekama	primary_settler.js
11. Sludge composition	Ekama	sludge_composition.js
12. Energy consumption	Ekama, Comeau, Corominas	energy_consumption.js
13. Figures, tables and appendixes	M&EA 5th ed	utils.js
14. Input estimations	BioWin 5.2	estimations.js

15. Construction materials	Morera et al, 2017	construction.js

8.3 Reviewing, modifying and submitting the Spold files

The tool will generate two Spold files. Spold files are files containing LCI data in the ecoSpold2 data format (see https://www.ecoinvent.org/data-provider/data-provider-toolkit/ecospold2/ecospold2.html). While some LCA software can import such files, the most common use of these files is to submit the datasets to ecoinvent so they can integrate them in their database.

To submit the datasets to ecoinvent, the data provider must:

- Open the datasets in the ecoEditor tool;
- Adapt the datasets as required;
- Submit the datasets directly from within the ecoEditor.

The ecoinvent Center will then receive the datasets and proceed to a review. The data provider may be required to make some adaptations to the dataset once they have been reviewed.

8.3.1 Opening the datasets in ecoEditor

When the Spold files are generated by the tool, the data provider will download them. To open them in the ecoEditor, one must:

- Have ecoEditor installed on the computer. The ecoEditor is freeware provided by ecoinvent to "create, edit, review and upload datasets for the future versions of the ecoinvent database" (see https://www.ecoinvent.org/data-provider/data-provider-toolkit/ecoeditor/ecoeditor.html).
- From ecoEditor, click on "Open dataset from file" and select the downloaded files.

That is all there is to it. Learning to use the ecoEditor is not very hard, but in any case the interaction data providers will have with the ecoEditor will be very minimal, given that the web tool already did much of the heavy work to generate the datasets.

8.3.2 Adapting the datasets

The web tool will populate all obligatory fields with data based on the model structure and user inputs. However, given the flexibility of the web tool, it is impossible to predict all specificities of a given use. Therefore, it behoves the data provider to verify the data.

Notably, the fields in the Activity Description and the Modelling and Administrative pages should be checked. The uncertainty fields for wastewater properties and direct discharges should also be revised if the wastewater composition is well known (see Section 5).

8.3.3 Submitting the datasets

The datasets are then submitted directly from within the ecoEditor. Specifically, the datasets need to be submitted to "validation", "external validation" and finally "external review", all options directly available in the ecoEditor tool under the "File" menu item.

9 References

Corominas, L., Flores Alsina, X., Muschalla, D., Neumann, M. et Vanrolleghem, P. A. (2010) Verification of WWTP design guidelines with activated sludge process models. In: Proceedings 83rd Annual WEF Technical Exhibition and Conference (WEFTEC2010). New Orleans, USA, October 2-6 2010. 137-146. https://modeleau.fsg.ulaval.ca/fileadmin/modeleau/documents/Publications/pvr926.pdf

Corominas, L., Larsen, H.F., Flores-Alsina, X., Vanrolleghem, P.A. (2013). Including Life Cycle Assessment for decision-making in controlling wastewater nutrient removal systems. *J Environ Manage*.,128:759-767.

Doka, G. (2007). Life Cycle Inventories of Waste Treatment Services. Ecoinvent report No. 13, Swiss Centre for Life Cycle Inventories, Dübendorf, Switzerland, December 2007.

Enerwater (2015). Standard method and online tool for assessing and improving the energy efficiency of waste water treatment plants. Deliverable 2.1 Study of published energy data. Accessed in https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5a25bfb10&appId=PPGMS.

Foley, J., Yuan, Z., Keller, J., Senante, E., Chandran, K., Willis, J., Shah, A., van Loosdrecht, M.C.M., van Voorthuizen, E. (2015). N2O and CH4 Emission from Wastewater Collection and Treatment Systems: State of the Science Report and Treatment Report. GWRC Report series. IWA Publishing, London, UK. ISBN: 97811780407333.

Gernaey, K.V., Jeppsson, U., Vanrolleghem, P.A., Copp, J.B. (Eds.) (2014). Benchmarking of Control Strategies for Wastewater Treatment Plants. IWA Scientific and Technical Report No. 23. IWA Publishing, London, UK. ISBN: 9781843391463.

Henze, M., Gujer, W., Mino, T., van Loosdrecht, M.C.M. (2000). Activated Sludge Models ASM1, ASM2, ASM2d and ASM3. IWA Scientific and Technical Report No 9. IWA Publishing, London, UK.

Law, Y., Jacobsen, G.E., Smith, A.M., Yuan, Z., Lant, P. (2013). Fossil organic carbon in wastewater and its fate in treatment plants. Water Res.,47(14):5270-5281.

Morera, S., Corominas, L., Rigola, M., Poch, M., Comas, J. (2017). Using a detailed inventory of a large wastewater treatment plant to estimate the relative importance of construction to the overall environmental impacts. *Water Res*.,122:614-623..

Plastics Europe (2012). Plastics e the Facts 2012. An Analysis of European Plastics Production, Demand and Waste Data for 2011. Brussels, Belgium.

Sansom, M., Avery, N. (2014). Reuse and recycling rates of UK steel demolition arisings. Proc. ICE - Eng. Sustain. 167 (3). ISSN 1478-4629

Stillwell, A.S, Hoppock, D.C., and Webber, M.E. (2010). Energy Recovery from Wastewater Treatment Plants in the United States: A Case Study of the Energy-Water Nexus.

Sustainability, 2:945-962.
Tchobanoglous, G., Stensel, H.D., Tsuchihashi, R., Burton, F.L., Abu-Orf, M., Bowden, G., Pfrang W. (2014). Wastewater Engineering: Treatment and Resource Recovery. Fifth edition. McGraw Hill. New York. ISBN: 978-0-07-340118-8.
WHO/UNICEF (2017). Progress on Drinking Water, Sanitation and Hygiene. 2017 update and SDG Baselines.