

# A second-generation life cycle inventory model for chemicals discharged in wastewater

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## 1. Introduction

We present a new model and tool to calculate life cycle inventories (LCIs) of chemicals discharged in urban wastewater, WW LCI v2, resulting from the integration and further development of two existing models, namely WW LCI v1 (Muñoz et al. 2016) and SewageLCI (Birkved and Dijkman 2012).

## 2. Materials and methods

**Error! Reference source not found.** shows an overview of the model's concept. A chemical substance's properties are used to predict its fate in a municipal wastewater treatment plant (WWTP), as well as in the environment. Based on the predicted fate factors, the model calculates an LCI including the operation of the WWTP and sludge disposal processes, as well as emissions from degradation in the environment of any fraction of the chemical directly released to the environment.

WW LCI v2 integrates the approach of SewageLCI, i.e. fate modelling of chemicals released to the sewer, with that of WW LCI, i.e. a complete life cycle inventory, including infrastructure requirements, energy consumption and auxiliary materials used for the treatment of wastewater and disposal of sludge, as well as emissions resulting from direct discharges. In addition, WW LCI v2 has been expanded to account for different wastewater treatment levels, i.e. primary treatment, secondary (biological) treatment, tertiary treatment (sand filtration) and independent treatment by means of septic tanks. As for sludge disposal, composting of sludge has been added as a management option in WW LCI v2, adding to the existing options of reuse in agriculture, landfilling and incineration in WW LCI v1. In order to reflect current wastewater treatment scenarios, the model includes a database with statistics on wastewater treatment levels and sludge disposal practices in 56 countries. The model is programmed in an Excel spreadsheet, which accommodates simultaneous calculations for 30 chemicals, either individually or as a mixture.

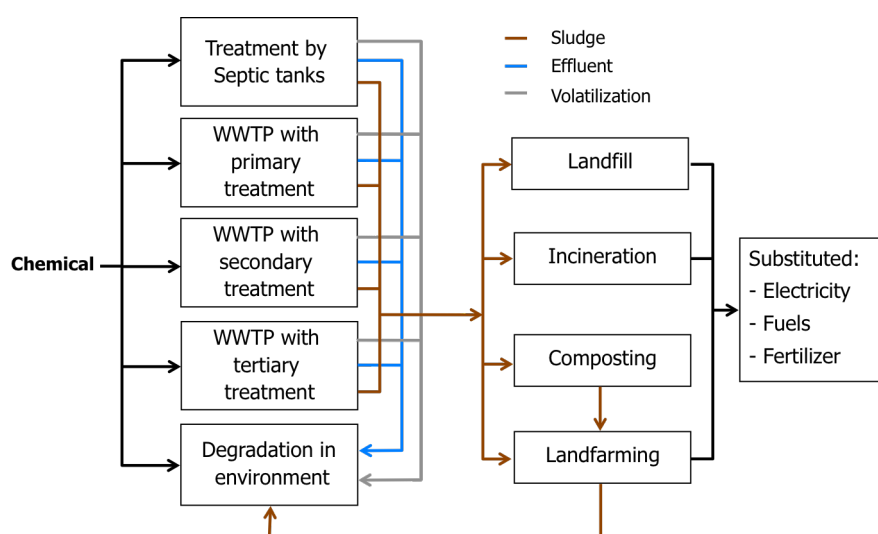


Figure 1. Conceptual diagram of WW LCI v2.

The model covers the treatment of organic as well as inorganic chemicals. Input variables by the user include chemical-specific data such as elemental composition, anaerobic degradability, generic physical-chemical properties, half-lives in the environment and fate factors in a conventional WWTP with activated sludge.

WW LCI 2.0 provides a database on the current status of wastewater treatment levels and sludge disposal practices in 56 countries, based on a wide variety of public sources

such as Eurostat, OECD data as well as country-specific statistics. These statistics are automatically loaded as input data to the model, thus providing a basis for country-specific LCIs.

### 3. Results and discussion

The output of WW LCI v2 is a comprehensive inventory (Figure 2) linked toecoinvent v3 data sets, that can be imported to LCA software in order to complement a life cycle assessment study of a particular chemical or a chemical mixture associated to a product or service. Impact assessment calculations are then easy to perform for different impact categories.

LCI for WWTP+sludge disposal+environmental degradation				Diufenac	Ibuprofen	Atrazine	Phosphonic acid, bis(2-bis(phosphono methyl)amino ethyl) amino methyl-	Acetaminophen
1			Product in wastewater (kg)	1	1	1	1	1
2			Methanol (kg)	0	0	0.00644332	0	0.014799311
3			FeCl3 (kg)	0	0	0	0	0
4			Electricity (kWh)	0.002019993	0.486023994	0.007761131	0.01648353	0.164846761
5			Heat (MJ)	0.000191969	0.00986485	0.000242184	0.164221902	0.009643918
6			WWTP infrastructure (unit)	5.3177E-13	5.5926E-13	5.31914E-13	5.48243E-13	5.59427E-13
7			Sewer infrastructure (km)	1.10146E-10	1.10146E-10	1.10146E-10	1.10146E-10	1.10146E-10
8			Polyvinylchloride, bulk polymerised (GLO) market for   Conseq, U	0.013205729	0.013205729	0.013205729	0.013205729	0.013205729
9			Polyethylene, high density, granulate (RECI) production   Conseq, U	0.012332031	0.012332031	0.012332031	0.012332031	0.012332031
10			Injection moulding (GLO) market for   Conseq, U	0.02553776	0.02553776	0.02553776	0.02553776	0.02553776
11			Excavation, hydraulic digger (GLO) market for   Conseq, U	0.005113281	0.005113281	0.005113281	0.005113281	0.005113281
12			Sand (GLO) market for   Conseq, U	1.925	1.925	1.925	1.925	1.925
13			Gravel, crushed (GLO) market for   Conseq, U	0.3609375	0.3609375	0.3609375	0.3609375	0.3609375
14			Transformation, from unknown (m2)	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08
15			Transformation, to industrial area, built-up (m2)	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08
16			Occupation, industrial area, built-up (m2y)	5.754E-07	5.754E-07	5.754E-07	5.754E-07	5.754E-07
17			Building, hall, steel construction (m2)	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08	2.3016E-08
18			Sand, at mine (kg)	1.35576E-05	1.35576E-05	1.35576E-05	1.35576E-05	1.35576E-05
19			Sodium hydroxide, 50% in H2O, production mix, at plant (kg)	6.2664E-06	6.2664E-06	6.2664E-06	6.2664E-06	6.2664E-06
20			transport to sludge disposal facilities, lorry (kgkm)	30.89685972	25.49061251	1.030589298	31.04255352	17.1793511
21			Compost plant infrastructure (units)	3.87127E-10	2.67337E-10	1.16716E-11	3.58262E-10	1.62406E-10
22			Electricity (kWh)	0.000102159	7.0547E-05	3.98002E-06	9.45415E-05	4.28571E-05
23			Diesel (MJ)	0.007403811	0.005112823	0.0002322	0.006851767	0.00310601
24			Transport to landfarming (kgkm)	1.932174982	0.980671897	0.054364426	1.79131176	0.448506751
25			process-specific burdens, municipal waste incineration (kg)	0	0	0	0	0
26			process-specific burdens, slag compartment (kg)	0	0	0	0	0
27			process-specific burdens, residual material landfill (kg)	0	0	0	0	0
28			electricity from waste, at municipal waste incineration plant (kWh)	0	0	0	0	0
29			heat from waste, at municipal waste incineration plant (MJ)	0	0	0	0	0
30			iron (III) chloride, 40% in H2O, at plant (kg)	0	0	0	0	0
31			cement, unspecified, at plant (kg)	0	0	0	0	0
32			disposal, cement, hydrated, 0% water, to residual material landfill	0	0	0	0	0
33			transport, freight, rail (km)	0	0	0	0	0
34			transport, lorry 29t (km)	0	0	0	0	0
35			natural gas, burned in industrial furnace low-NOx >100kW (MJ)	0	0	0	0	0
36			electricity, low voltage, at grid (kWh)	0	0	0	0	0
37			light fuel oil, burned in boiler 100kW, non-modulating (MJ)	0	0	0	0	0
38			natural gas, burned in boiler modulating >100kW (MJ)	0	0	0	0	0
39			iron sulphate, at plant (kg)	0	0	0	0	0
40			aluminum sulphate, powder, at plant (kg)	0	0	0	0	0
41				0	0	0	0	0
42				0	0	0	0	0

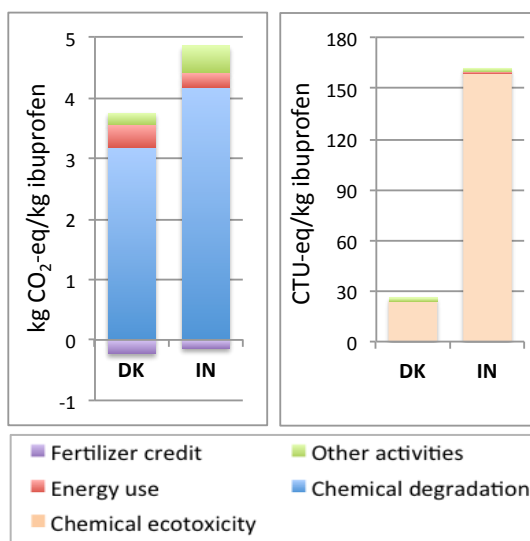
As an example, Figure 3 shows the impact assessment results for greenhouse-gas (GHG) emissions and freshwater ecotoxicity for the pharmaceutical product ibuprofen, considering discharge in Denmark and India, according to the wastewater treatment and sludge disposal scenarios provided in the WW LCI v2 database.

Figure 2: Screenshot of WW LCI v2 showing part of the LCI output tab.

Wastewater treatment and sludge disposal scenario			DK	IN
Wastewater treatment scenario	Connection to WWTP - primary treatment		2%	0%
	Connection to WWTP - secondary treatment		3%	21%
	Connection to WWTP - tertiary treatment		84%	0%
	Connection to septic tank		11%	39%
	Direct discharge		0%	39%
Sludge disposal scenario	Composting		6%	0%
	Landfarming		50%	100%
	Landfilling		0%	0%
	Incineration		44%	0%

Table 1: Wastewater treatment and sludge disposal scenario in Denmark and India based on WW LCI v2 database.

Figure 3: GHG emissions (left) and freshwater ecotoxicity (right) results per kg ibuprofen discharged in wastewater in Denmark and India. Impact assessment calculations carried out in the software SimaPro. GHG emissions assessed with global warming potential (GWP) for a time horizon of 100 years. Freshwater ecotoxicity assessed with USEtox v1.



### 4. Conclusions

WW LCI 2.0 makes it possible to obtain a chemical-specific and comprehensive LCI of chemicals discharged down the drain, including not only treatment in the WWTP but also sludge disposal and degradation of chemicals in the environment when there is no connection to a WWTP. This is particularly important since emissions from direct discharges can be important. The model provides substantially different outcomes depending on the expected behaviour and composition of chemicals as well as on the existing level of treatment where they happen to be discharged. This model takes a step forward from its predecessors, WW LCI v1 and SewageLCI, enabling a more realistic assessment of the impact of chemicals at their end of life, thus contributing to better decision making and data availability in the context of the life cycle of chemicals.

### 5. References

[1] Muñoz I, Otte N, Van Hoof G, Rigarlfsord G (2016) A model and tool to calculate life cycle inventories of chemicals discharged down the drain. Int J Life Cycle Assess. doi: 10.1007/s11367-016-1189-3

[2] Birkved M, Dijkman TJ (2012) SewageLCI 1.0, an inventory model to estimate chemical specific emissions via sewage treatment systems. 6<sup>th</sup> SETAC World Congress 2012.