

SETAC Europe 26th Annual Meeting, Nantes, 23 May 2016

# A model and tool to calculate life cycle inventories of chemicals discharged down the drain

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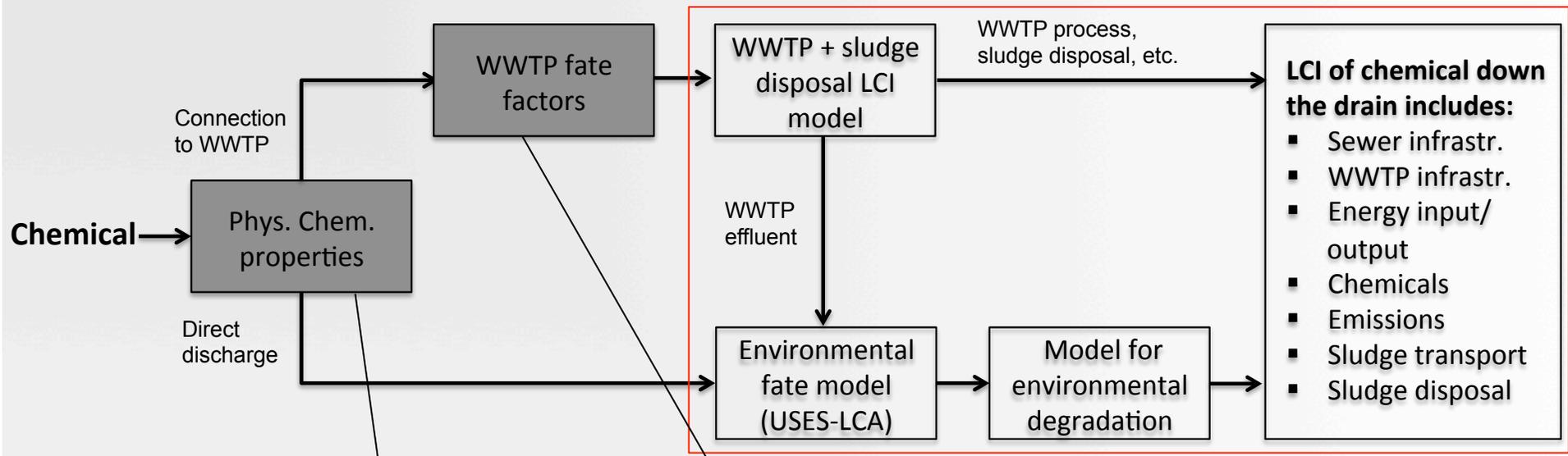
# Background and aim

- The fate of household chemicals following use is generally to municipal wastewater treatment plants (WWTP) although in some countries this may be limited
- Current WWTP models in LCA, e.g. Ecoinvent (Doka 2007):
  - Reflect average conditions in WWTPs, rather than the specific fate of particular chemicals (e.g. Degradability)
  - Omit the impact of direct discharges
- Our goal was to develop a model that calculates chemical-specific LCIs of chemicals discharged down the drain or to the environment

Doka, G. (2007) Life Cycle Inventories of Waste Treatment Services. Final report ecoinvent 2000 No. 13, EMPA St. Gallen, Swiss Centre for Life Cycle Inventories, Duebendorf, Switzerland.

# Concept, scope and data

WW LCI



**LCI of chemical down the drain includes:**

- Sewer infrastr.
- WWTP infrastr.
- Energy input/output
- Chemicals
- Emissions
- Sludge transport
- Sludge disposal

- Organic/inorganic
- Composition (C, H, O, N, S, P, Cl)
- Molecular weight
- Vapour pressure
- Solubility
- Kow
- Half-lives in the environment (soil, water, air)

- Fraction degraded
- Fraction volatilized
- Fraction to sludge
- Anaerobic degradability

- % population connected to WWTPs
- WWTP includes N and P removal
- Country
- Sludge disposal scenario

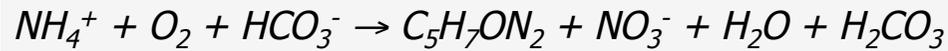


# WWTP model

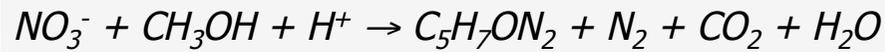
**Aerobic degradation of carbonaceous organic matter:**



**N removal:**

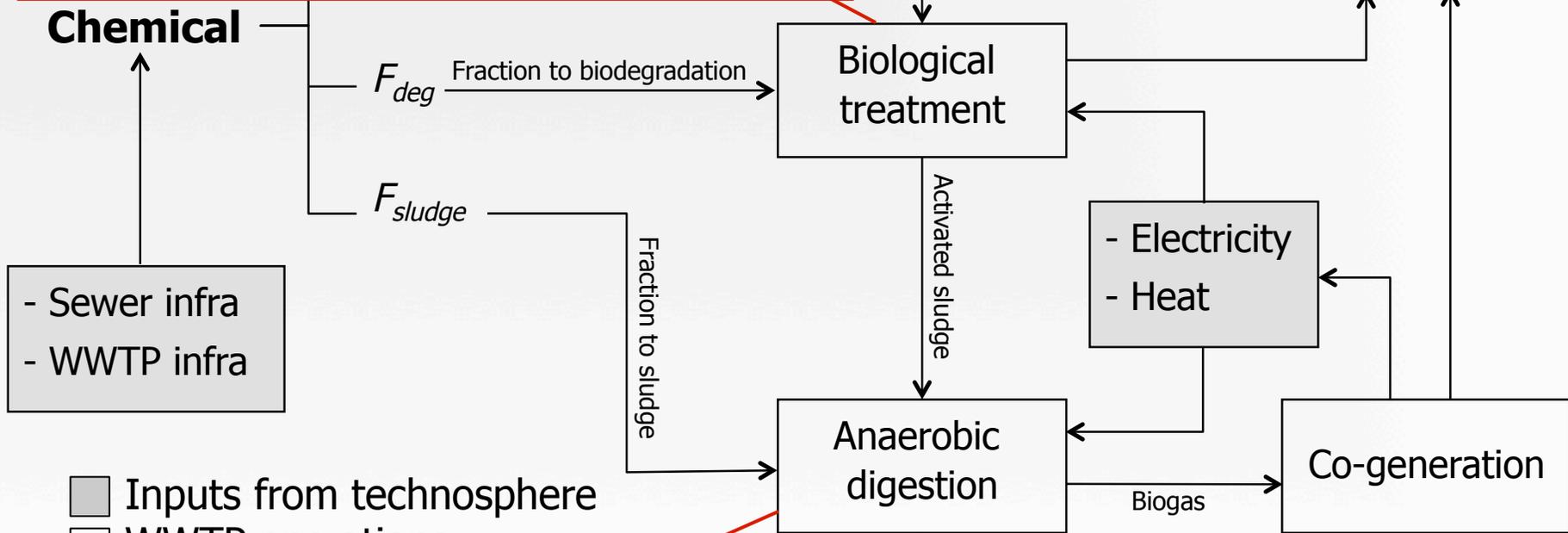


Denitrification

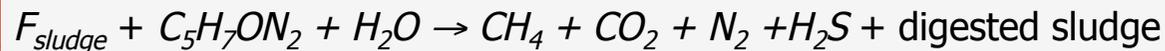


alcohol (N removal)  
chloride (P removal)

**P removal:**



**Anaerobic digestion:**



# WW LCI: key features

- All calculations in a single Excel file: WW LCI.xlsx
- 30 chemicals can be assessed at a time, separately or as a mixture
- Entirely parameterized, all values can be changed by the user
- Resulting LCIs use ecoinvent 3 nomenclature
- WW LCI does not include impact assessment calculations
- LCIs can be exported as CSV files to LCA software: SimaPro

# WW LCI in Excel

## Sheet 'WWTP input'

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	<b>Scenario data</b>																					
2	WWTP	Connection to WWTP (%)						100%														
3		Nitrogen Removal in WWTP						yes														
4		Phosphorus removal in WWTP						yes														
5	Sludge	Sludge to landfarming (%)						100%														
6		Sludge to landfilling (%)						0%														
7		Sludge to incineration (%)						0%														
8	Country						DE															
9	Chemical mixture						yes															
10																						
11	<b>Chemical-specific data</b>																					
12	Name	CAS number	Type	Composition (no of atoms in a molecule)						Molecular weight (g/mol)	Biogenic carbon?	Mass in mixture (%)	Fate in WWTP (%)				If emitted to water					
13				C	H	O	N	S	P				Cl	Fair	Fdeg	Fsludge	Anaerobic deg?	Deg <sub>s</sub>	Deg <sub>w</sub>	Deg <sub>sed</sub>	Deg <sub>g</sub>	Deg <sub>a</sub>
14																						
15	DTPMP	15827-60-8	Organic	9	28	15	3		5	573	no	100.00%	0.00%	0.00%	85.00%	no	0.00%	53.10%	42.14%	0.00%	0.09%	
16	Sodium carbonate	497-19-8	Inorganic	1		3				106	n.a.		0.00%	0.00%	0.00%	n.a.	0.00%	0.00%	0.00%	0.00%		
17	Ethanol	64-17-5	Organic	2	6	1				46	yes		0.43%	87.05%	0.01%	yes	13.14%	86.45%	0.05%	0.35%	23.16%	
18	TAED	10543-57-4	Organic	10	16	4	2			228	no		0.00%	97.00%	0.10%	yes	0.00%	99.09%	0.91%	0.00%	0.03%	
19	Zeolite A	1344-00-9	Inorganic	54	75					2190	n.a.		0.00%	0.00%	90.00%	no	0.00%	0.00%	0.00%	0.00%		
20	STPP	7758-29-4	Inorganic		10					368	n.a.		0.00%	0.00%	0.00%	no						
21	Water		Inorganic	2	1					18	n.a.		0.00%	0.00%	0.40%	n.a.						
22																						
23																						
24																						
25																						
26																						
27																						
28																						

## Sheet 'USES-LCA input'

	A	B	C	D	E	F	G	H	I	J	K	L	
1													
2	<b>Chemical-specific data</b>												
3													
4	Row number	Name	CAS number	ChemType	Neutral/Acid/Base	MW (g/mol)	Vapour pressure 25 deg. C (Pa)	Solubility 25 deg (mg/L)	Melting point (deg. C)	Kow	Koc	Henry's Law Constant (Pa·m <sup>3</sup> /mol)	
5	1	Ethanol	64-17-5	organic	-	46	7910	1000000	-114	0.48977882	1.04	0.506625	
6	2	TAED	10543-57-4	organic	-	228	4.80E-06	1500	152	0.83176377	15	1.682E-11	
7	3	DTPMP	15827-60-8	organic	A	573	1.67E-10	500000	90	0.00039811		7.3967E-13	
8	4												
9	5												
10	6												

# WW LCI in Excel

## Sheet 'LCI output'

	A	B	C	D	H	I	J	K	L	M	N	O	P			
1	LCI for WWTP+sludge disposal+environmental degradation				TAED	Zeolite A	STPP	Water	LAS	Diuron	0	0	0			
2	Inputs	From technosphere		Product in wastewater (kg)	1	1	1	1	1	1	0	0	0			
3				Methanol (kg)	0.094473229	0	0	0	0	0	0	0	0	0	0	
4				FeCl3 (kg)	0	0	1.589673913	0	0	0	0	0	0	0	0	
5				Electricity (kWh)	0.2978645	0.012124	0.01795287	0.00008176	0	0.000597856	0	0	0	0	0	
6				Heat (MJ)	0	0.192555	0.285296478	0.00095436	0	0.009165816	0	0	0	0	0	
7				WWTP infrastructure (unit)	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	6.0643E-13	0	0	0
8				Sewer infrastructure (km)	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	1.2376E-10	0	0	0
9				Sludge transport	transport to sludge disposal facilities, lorry (kgkm)		27.31475067	0	0	26.87351304	0.005773196	0.609239766	0.848	0	0	0
10				Compost plant infrastructure (units)			0	0	0	0	0	0	0	0	0	0
11				Sludge composting	Electricity (kWh)		0	0	0	0	0	0	0	0	0	0
12				Diesel (MJ)			0	0	0	0	0	0	0	0	0	0
13				Transport to landfarming (kgkm)			0	0	0	0	0	0	0	0	0	0
14				process-specific burdens, municipal waste incineration (kg)			0	0	0	0	0	0	0	0	0	0
15				process-specific burdens, slag compartment (kg)			0	0	0	0	0	0	0	0	0	0
16				process-specific burdens, residual material landfill (kg)			0	0	0	0	0	0	0	0	0	0
17				electricity from waste, at municipal waste incineration plant (kWh)			0	0	0	0	0	0	0	0	0	0
18				heat from waste, at municipal waste incineration plant (MJ)			0	0	0	0	0	0	0	0	0	0
19				iron (III) chloride, 40% in H2O, at plant (kg)			0	0	0	0	0	0	0	0	0	0
20				cement, unspecified, at plant (kg)			0	0	0	0	0	0	0	0	0	0
21				disposal, cement, hydrated, 0% water, to residual material landfill			0	0	0	0	0	0	0	0	0	0
22				transport, freight, rail (tkm)			0	0	0	0	0	0	0	0	0	0
23				transport, lorry 28t (tkm)			0	0	0	0	0	0	0	0	0	0
24				natural gas, burned in industrial furnace low-NOx >100kW (MJ)			0	0	0	0	0	0	0	0	0	0
25				electricity, low voltage, at grid (kWh)			0	0	0	0	0	0	0	0	0	0
26				light fuel oil, burned in boiler 100kW, non-modulating (MJ)			0	0	0	0	0	0	0	0	0	0
27				natural gas, burned in boiler modulating >100kW (MJ)			0	0	0	0	0	0	0	0	0	0
28				iron sulphate, at plant (kg)			0	0	0	0	0	0	0	0	0	0
29				aluminium sulphate, powder, at plant (kg)			0	0	0	0	0	0	0	0	0	0
30				process-specific burdens, sanitary landfill (kg)			0	0	0	0	0	0	0	0	0	0
31				municipal waste incineration plant (unit)			0	0	0	0	0	0	0	0	0	0
32				process-specific burdens, municipal waste incineration (kg)			0	0	0	0	0	0	0	0	0	0
33				slag compartment (unit)			0	0	0	0	0	0	0	0	0	0
34				process-specific burdens, slag compartment (kg)			0	0	0	0	0	0	0	0	0	0
35				residual material landfill facility (unit)			0	0	0	0	0	0	0	0	0	0
36				process-specific burdens, residual material landfill (kg)			0	0	0	0	0	0	0	0	0	0
37				electricity from waste, at municipal waste incineration plant (kWh)			0	0	0	0	0	0	0	0	0	0
38				heat from waste, at municipal waste incineration plant (MJ)			0	0	0	0	0	0	0	0	0	0
39				sodium hydroxide, 50% in H2O, production mix, at plant (kg)			0	0	0	0	0	0	0	0	0	0
40				quicklime, milled, packed, at plant (kg)			0	0	0	0	0	0	0	0	0	0
41				hydrochloric acid, 30% in H2O, at plant (kg)			0	0	0	0	0	0	0	0	0	0
42				chemicals inorganic, at plant (kg)			0	0	0	0	0	0	0	0	0	0
43				cement, unspecified, at plant (kg)			0	0	0	0	0	0	0	0	0	0
44				disposal, cement, hydrated, 0% water, to residual material landfill			0	0	0	0	0	0	0	0	0	0
45				transport, freight, rail (tkm)			0	0	0	0	0	0	0	0	0	0
46				transport, lorry 28t (tkm)			0	0	0	0	0	0	0	0	0	0
47				ammonia, liquid, at regional storehouse (kg)			0	0	0	0	0	0	0	0	0	0
48				natural gas, burned in industrial furnace low-NOx >100kW (MJ)			0	0	0	0	0	0	0	0	0	0
49				titanium dioxide, production mix, at plant (kg)			0	0	0	0	0	0	0	0	0	0
50				chromium oxide, flakes, at plant (kg)			0	0	0	0	0	0	0	0	0	0
51				Product to air (kg)			0	0	0	0	0	0	0	0	0	0
52				CO2 to air, biogenic (kg)			0.008383035	0	0	0	0	0	0	0	0	0
53				CH4 to air, biogenic (kg)			8.48738E-06	0	0	0	0	0	0	0	0	0
54				CO2 to air, fossil (kg)			1.574951965	0	0	0	1.385615811	0	0	0	0	0
55				CH4 to air, fossil (kg)			0.000646717	0	0	0	0.001402863	0	0	0	0	0



# WW LCI: import to SimaPro

The screenshot displays the SimaPro LCA Explorer interface. On the left, a sidebar contains navigation options: Wizards, Goal and scope, Inventory, Impact assessment, Interpretation, and General data. The main area is divided into a tree view of processes and a list view. The tree view shows a hierarchy starting with 'Material', followed by 'Agricultural', 'Animal feed', and 'Plant production'. The list view displays a table of processes with their names and associated environmental impact data. A large text overlay 'Data sets in SimaPro' is centered on the list. At the bottom, there is a filter section and a status bar showing '24060 items' and '0 items selected'.

Name
Alcohol ethoxylate (C10-14), 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Diuron, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Enzyme, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Ethanol, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Fake chemical, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
FWA-1, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
LAS, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Melamine, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Pendimethalin, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Phosphonate (ATMP), 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Polyacrylate, Na salt, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Propane, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Sodium carbonate, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Sodium sulphate, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
TAED, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}
Zeolite A, 100% connect., 30% landfarm, 50% landfill, 25% incineration {DE}

Wastewater LCI model by 2.-0 LCA consultants, version 1.0, June 2015

Filter on  and  or   Clear 16

24060 items 0 items selected

2.0 LCA Consultants 2 Manager 8.0.4.26 Analyst Multi user

# WW LCI: import to SimaPro

File Edit Calculate Tools Window Help

Documentation Input/output Parameters System description

Known outputs to technosphere. Products and co-products

Name	Amount	Unit	Quantity	Allocation %	Waste type	Category
TAED, 100% connect., N&P rem., 30% dm, 42% landfarm, 0% landfill, 58% incin. (DE)	1	kg	Mass	100 %	not defined	_WW LCI initiative\Article
(Insert line here)						

Known outputs to technosphere. Avoided products

Name	Amount	Unit	Distribution	SD^2 or 2*SDMin	Max	Comment
(Insert line here)						

Inputs

Known inputs from nature (resources)

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*SDMin	Max	Comment
(Insert line here)							

Known inputs from technosphere (materials/fuels)

Name	Amount	Unit	Distribution	SD^2 or 2*SDMin	Max	Comment
Methanol (GLO)   market for   Conseq, U	0.0944732291233778	kg	Undefined			
Electricity, medium voltage (DE)   market for   Conseq, U	0.578145350582864	kWh	Undefined			
Heat, district or industrial, natural gas (CH)   market for heat, district or industrial, natural gas	0.513847686067642	MJ	Undefined			
Wastewater treatment facility, capacity 4.7E10/year (GLO)   market for   Conseq, U	8.42263888888889E-10	p	Undefined			
Sewer grid, 4.7E10/year, 583 km (GLO)   market for   Conseq, U	1.71888888888889E-7	km	Undefined			
Transport, freight, lorry, unspecified (GLO)   market for   Conseq, U	18.9447165755555	kgkm	Undefined			
Municipal waste incineration facility (GLO)   market for   Conseq, U	1.37349195172778E-10	p	Undefined			
Process-specific burdens, municipal waste incineration (GLO)   market for   Conseq, U	0.549396780691111	kg	Undefined			
Slag landfill (GLO)   market for   Conseq, U	6.87755137133613E-10	p	Undefined			
Process-specific burdens, slag landfill (GLO)   market for   Conseq, U	0.386862264637657	kg	Undefined			
Residual material landfill (GLO)   market for   Conseq, U	4.91847593725435E-13	p	Undefined			
Process-specific burdens, residual material landfill (GLO)   market for   Conseq, U	0.000236086844988209	kg	Undefined			
Electricity, medium voltage (DE)   market for   Conseq, U	0.289650670353426	kWh	Undefined			
Heat, district or industrial, natural gas (Europe without Switzerland)   market for heat, district	1.88137608615912	MJ	Undefined			
Sodium hydroxide, without water, in 50% solution state (GLO)   market for   Conseq, U	0.000107415053668396	kg	Undefined			
Quicklime, milled, packed (GLO)   market for   Conseq, U	1.90331937201894E-5	kg	Undefined			
Hydrochloric acid, without water, in 30% solution state (RER)   market for   Conseq, U	1.33647546953005E-7	kg	Undefined			
Chemical, inorganic (GLO)   market for chemicals, inorganic   Conseq, U	2.22745911588341E-7	kg	Undefined			
Cement, unspecified (GLO)   market for   Conseq, U	9.44347379952835E-5	kg	Undefined			
Transport, freight train (Europe without Switzerland)   market for   Conseq, U	0.00507181904027039	tkm	Undefined			
Transport, freight, lorry, unspecified (GLO)   market for   Conseq, U	0.0159156712225795	tkm	Undefined			
Ammonia, liquid (RER)   market for   Conseq, U	0.00201398080284601	kg	Undefined			
Heat, district or industrial, natural gas (CH)   market for heat, district or industrial, natural gas	0.196408038652177	MJ	Undefined			
Titanium dioxide (RER)   market for   Conseq, U	5.76499323496558E-5	kg	Undefined			
Chromium oxide, flakes (GLO)   market for   Conseq, U	1.17652923162563E-6	kg	Undefined			
Nitrogen fertiliser, as N (GLO)   market for   Conseq, U	-0.0115631309551324	kg	Undefined			
(Insert line here)						

Known inputs from technosphere (electricity/heat)

Name	Amount	Unit	Distribution	SD^2 or 2*SDMin	Max	Comment
(Insert line here)						

Outputs

Emissions to air

Name	Sub-compartment	Amount	Unit	Distribution	SD^2 or 2*SDMin	Max	Comment
Carbon dioxide, biogenic		0.0083830349	kg	Undefined			
Methane, biogenic		8.4873821127	kg	Undefined			
Carbon dioxide, fossil		1.5749519651	kg	Undefined			
Methane, fossil		0.0006467173	kg	Undefined			
Ammonia		0.0008489087	kg	Undefined			
Dinitrogen monoxide		0.0009871233	kg	Undefined			
Nitrogen oxide		0.0034075016	kg	Undefined			

Data set in SimaPro

# WW LCI compared to Ecoinvent model

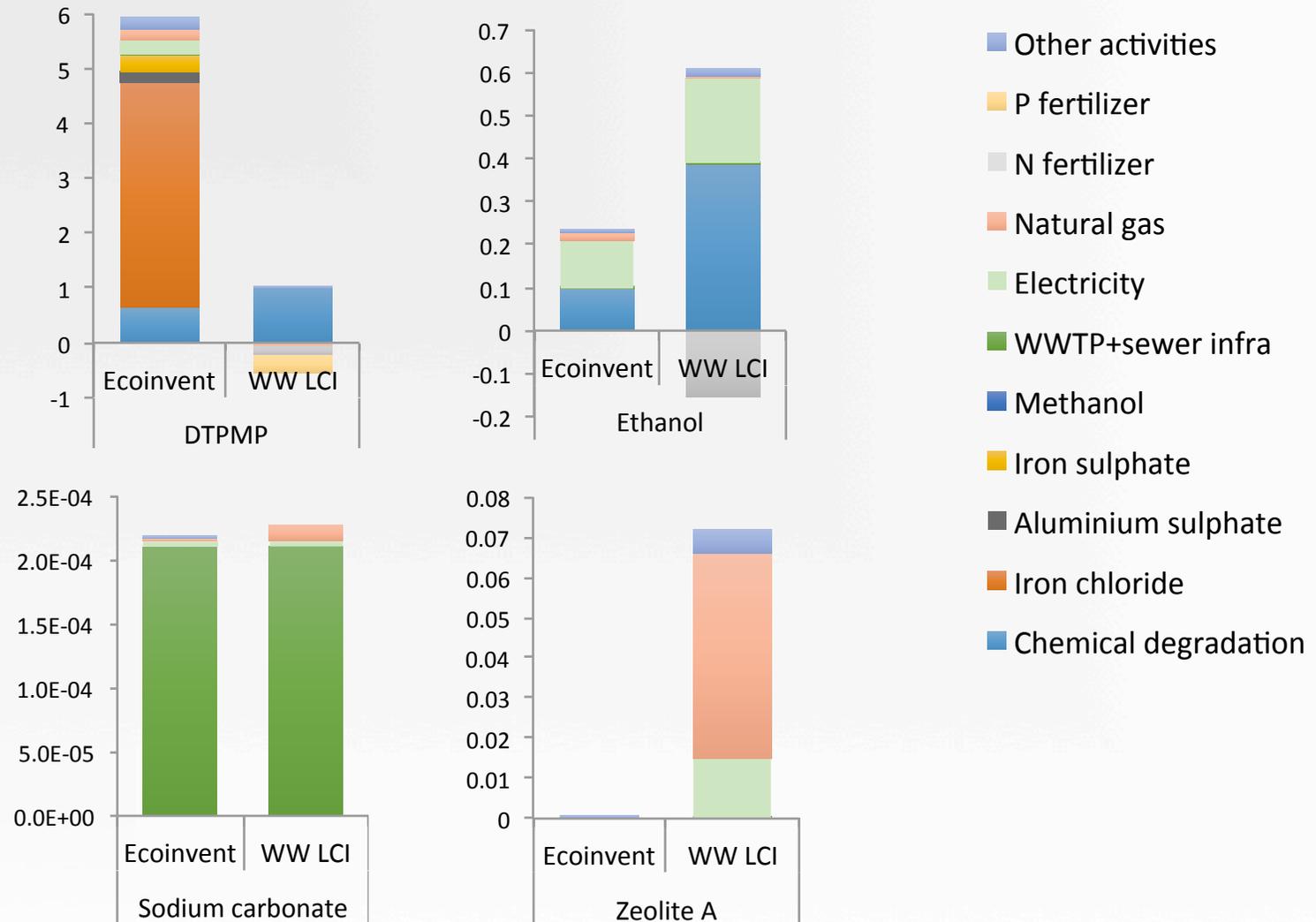
Name	CAS number	Key features
Tetraacetythylenediamine (TAED)	10543-57-4	Organic, degradable, contains N and fossil C
Ethanol	64-17-5	Organic, degradable, contains biogenic C
Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)	15827-60-8	Organic, poorly degradable, contains N and P, contains fossil C
Sodium carbonate	497-19-8	Inorganic, soluble
Zeolite A	1344-00-9	Inorganic, insoluble
Sodium tripolyphosphate (STPP)	7758-29-4	Inorganic, soluble, contains P

- Same connection level to WWTP: 100%
- Same sludge disposal: 58% incineration, 42% agriculture (DE)
- Same sewer-WWTP size: 4.7E10 L/year
- Same functional unit: 1 kg chemical in wastewater influent

# WW LCI compared to Ecoinvent model

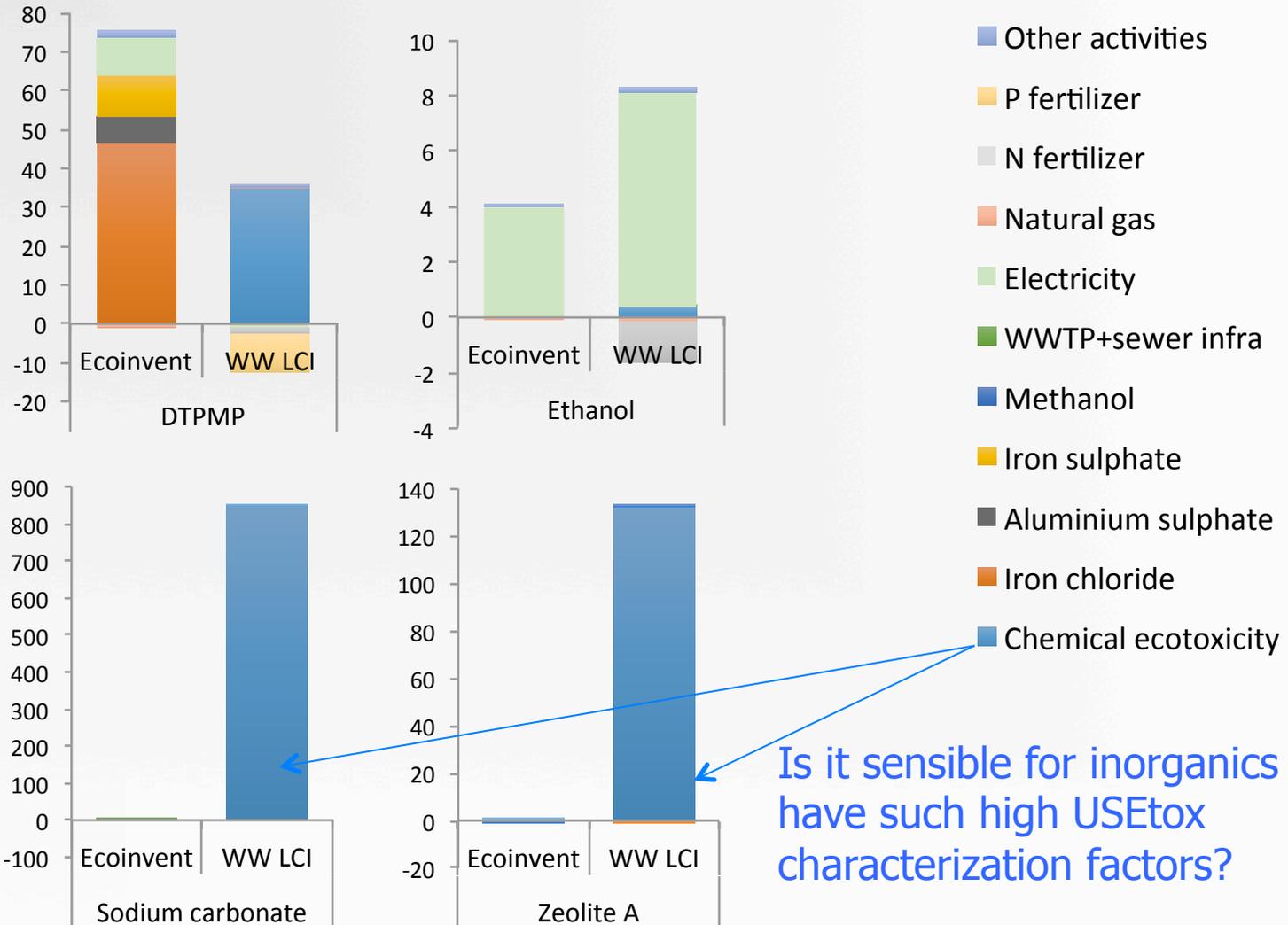
GHG emissions, in kg CO<sub>2</sub>-eq/kg chemical (IPCC 2013)  
 (biogenic CO<sub>2</sub> considered neutral)

Note different  
Y axis scale



# WW LCI compared to Ecoinvent model

Freshwater ecotoxicity, in CTU-eq/kg chemical (USEtox)

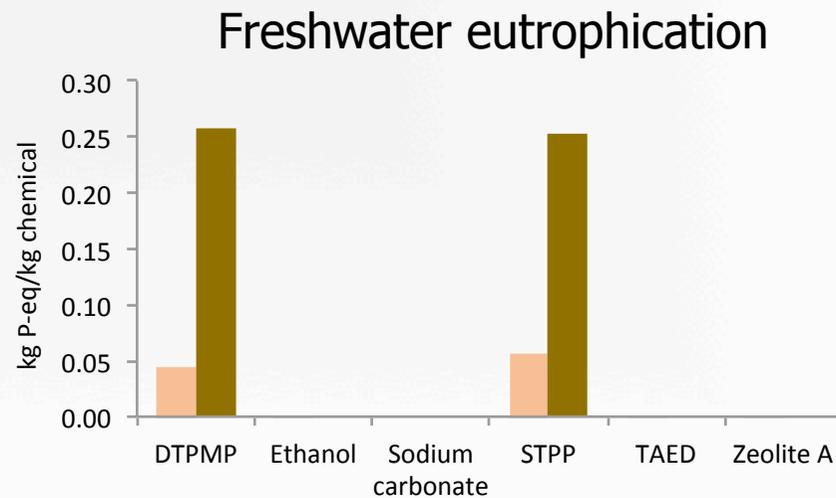
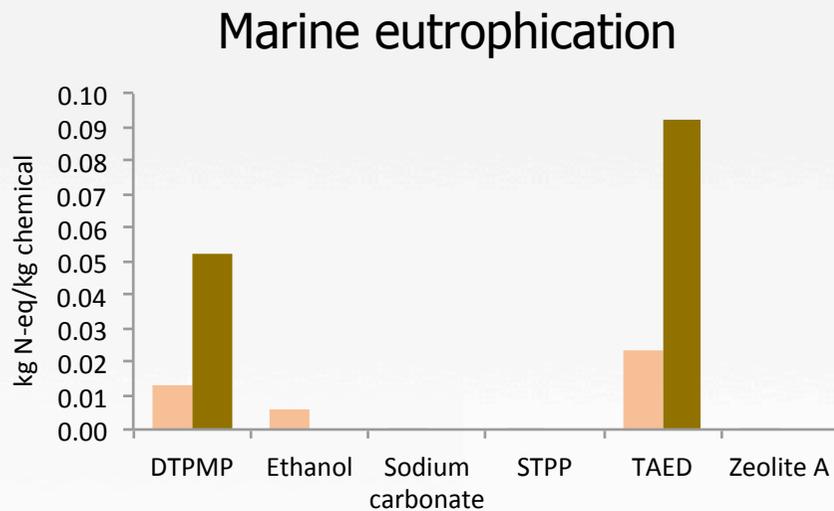
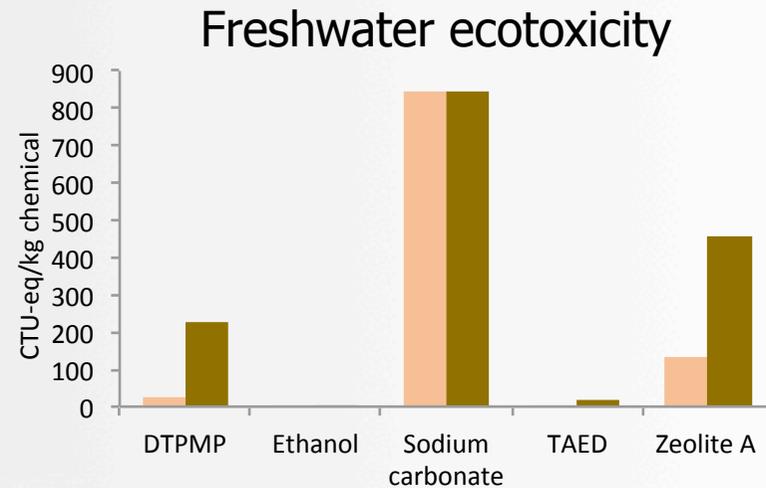
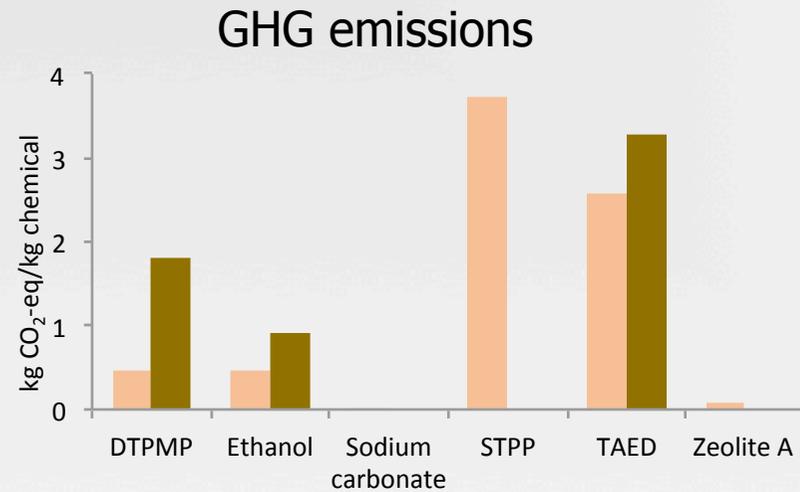


Note different Y axis scale

Is it sensible for inorganics to have such high USEtox characterization factors?

# WW LCI: assessing direct discharges

Population connected to WWTP: 100% vs. 0%



■ WW LCI - 100% connection    
 ■ WW LCI - Direct discharge (0% connection)

## Compared to Ecoinvent model...

- WW LCI can handle a complete substance flow analysis for chemicals in wastewater
- WW LCI addresses specific degradability, sorption to sludge, etc. This has substantial influence in the calculation of energy use, sludge production, N and P removal...
- WW LCI accounts for direct discharges, relevant for developing countries
- WW LCI closes the carbon balance when sludge is applied in agriculture
- WW LCI accounts for displaced energy and fertilizers
- WW LCI can represent scenarios other than Switzerland

# Conclusions & Outlook

- Improvement in modelling the end of life for chemical substances
- Still some limitations:
  - Data-demanding
  - Complete flow analysis only for C, N, P, S and Cl
  - Metals not yet supported
  - Import of data sets only available for SimaPro so far
- Work in progress with Technical University of Denmark (DTU) on integration of **WW LCI** with **Sewage LCI**:
  - Adding treatment by septic tanks
  - Adding WWTPs with primary treatment only
  - Adding WWTPs with tertiary treatment (sand filter)
  - Sludge composting
  - Built-in country scenarios (% connection, sludge disposal)

# Thank you!

More info:

<http://lca-net.com/projects/show/wastewater-lci-initiative/>

Reference:

Muñoz I, Otte N, Van Hoof G, Rigarlsford G. ***A model and tool to calculate life cycle inventories of chemicals discharged down the drain.*** Submitted to the International Journal of Life Cycle Assessment.