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LCI model and tool for chemicals discharged down the drain

Case study on detergent formulations

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Background and aim

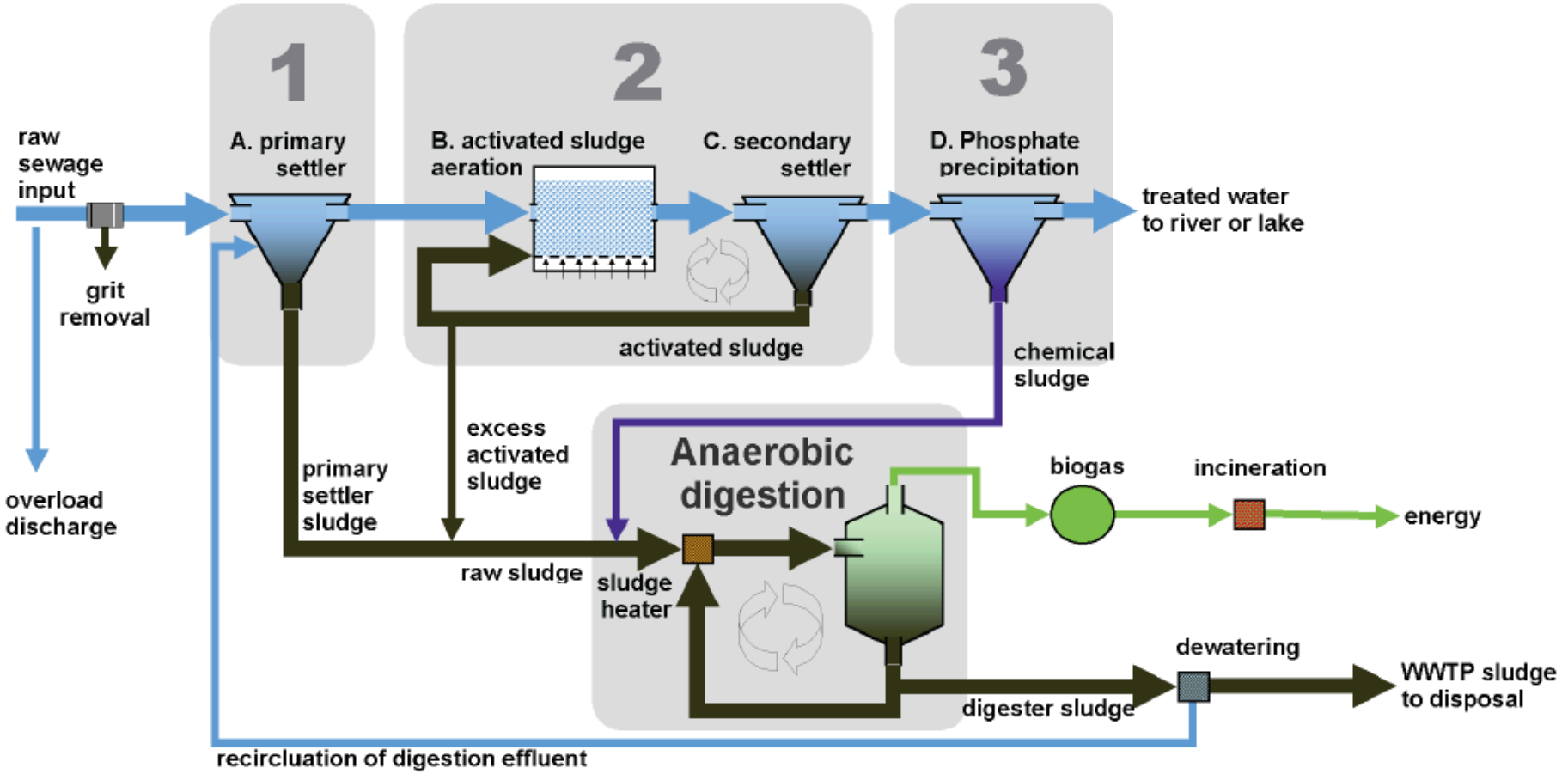
- There is a need to better assess in LCA the disposal of chemicals down the drain including fate in wastewater treament and direct discharge scenarios
- Current wastewater treatment plant (WWTP) models in LCA, e.g. Ecoinvent (Doka 2007):
  - Reflect average conditions in WWTPs, rather than model the specific fate of chemicals (e.g. Degradability)
- We recently developed WW LCI, a model that calculates chemical-specific LCIs of chemicals discharged down the drain
- We compared two models for strengths and weaknesses: Ecoinvent model and WW LCI using three detergent formulations.

Ecoinvent model (Doka 2007)

- Developed for ecoinvent v2
- Programmed in Excel
- Weighted average technology for Switzerland in the early 2000's
- Sludge disposal includes incineration and landfarming only
- The functional unit is 1 m^3 of wastewater, as characterized by the user
- Wastewater characterization based on general descriptors (BOD, TOC, N, P, etc.)
- Based on a complete mass balance using average transfer factors for each descriptor

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.

Ecoinvent model (Doka 2007)



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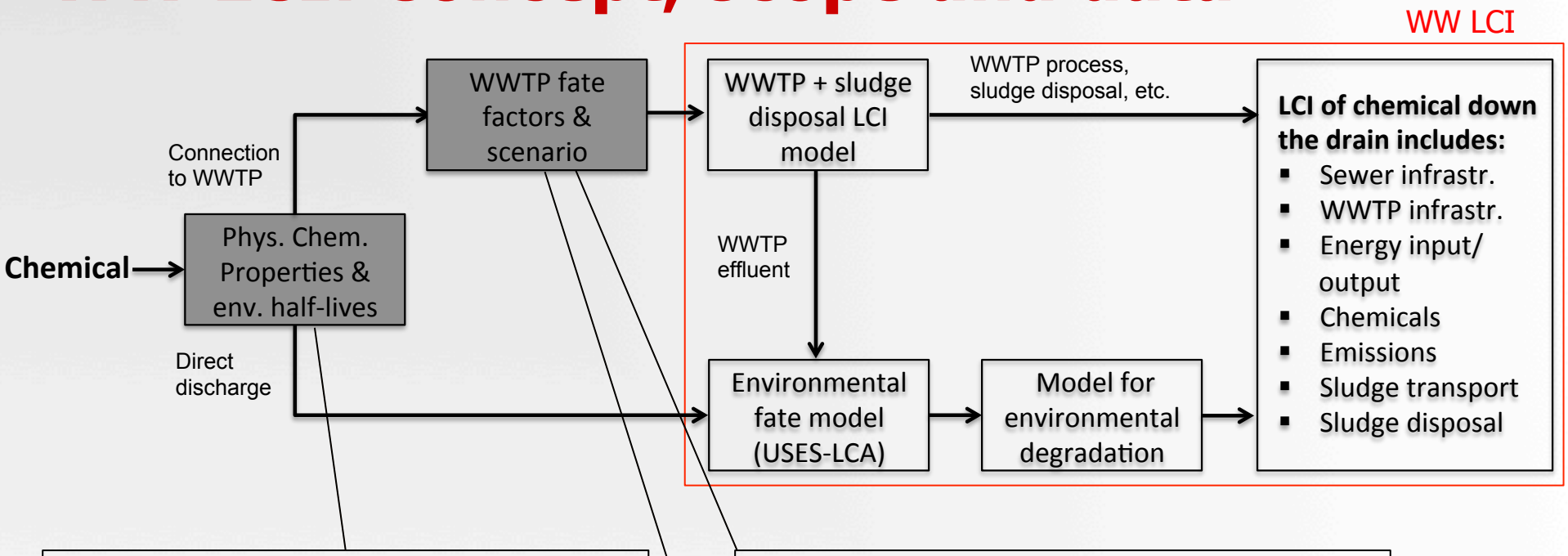
WW LCI: Concept, scope and data



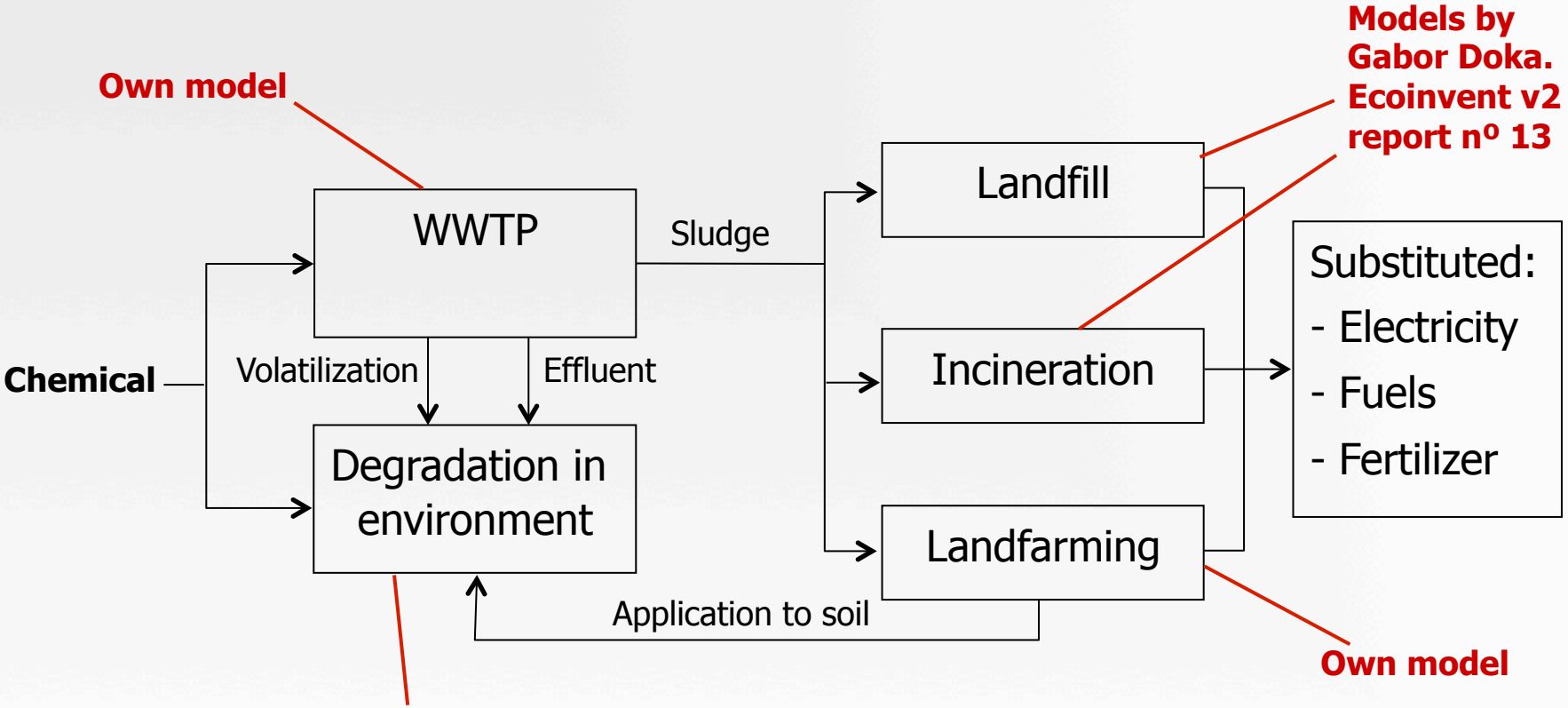
- Organic/inorganic
- Composition (C, H, O, N, S, P, Cl)
- Molecular weight
- Vapour pressure
- Solubility
- Kow
- Half-lives in the environment (soil, water, air)

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

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

WW LCI: Concept, scope and data

- Mass and energy balances
- Functional unit is 1 kg of chemical
- Multifunctionality solved by substitution (credits)

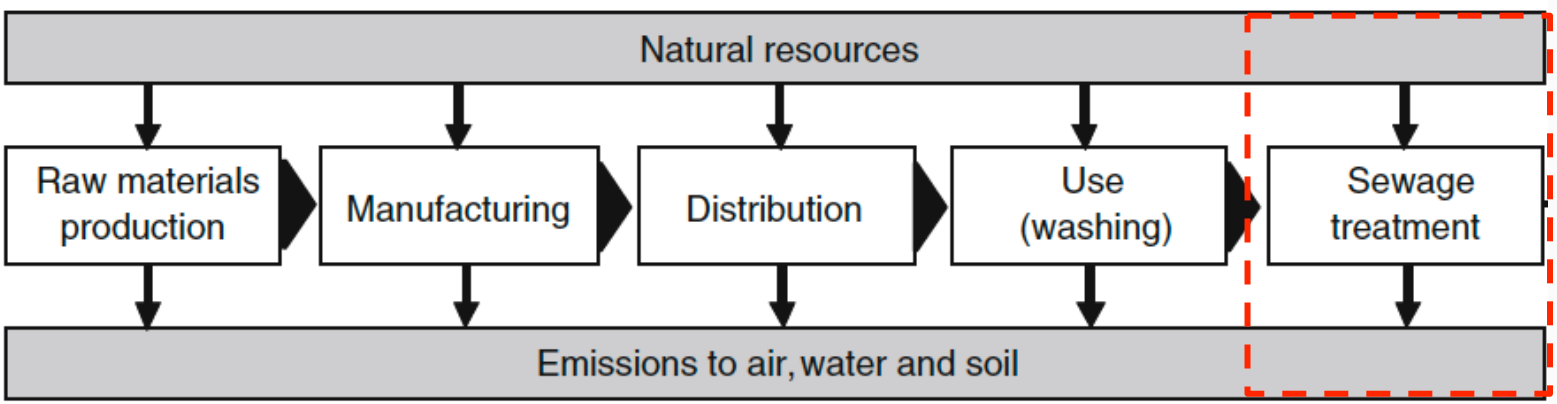


Muñoz, I. et al. (2013) Accounting for greenhouse gas emissions from the degradation of chemicals in the environment . IJLCA, 18:252–262.

WW LCI: key features

- All calculations performed in an Excel file: WW LCI.xlsx
- 30 chemicals can be assessed at a time
- All input values transparently displayed and can be specified by the user
- Output: LCIs use ecoinvent 3 nomenclature
- LCIs can be exported as CSV files to LCA software SimaPro for further analysis.

Case study: scope



- Functional unit is one wash in a washing machine in Germany
- The washing machine uses 50 L water/wash
- Three average detergent formulations (Van Hoof et al. 2011):
  - Powder: 85 g/wash + 50 L water
  - Liquid dilute: 122 g/wash + 50 L water
  - Liquid concentrate: 39 g/wash + 50 L water

Case study: scope

Ingredient	CAS number	Composition (% in weight) Powder	Liquid	Concentrated
Water		7.80	74.43	45.59
Sodium carbonate	497-19-8	22.18		
Sodium sulfate	7757-82-6	19.89		
Sodium percarbonate	15630-89-4	13.28		
Na, linear alkylbenzene sulfonate	68411-30-3	8.69	5.02	14.43
Zeolite	1318-02-1	7.04		
Sodium silicate	1344-00-9	4.71		
Bentonite	1302-78-9	4.48		
C15 alkylethoxysulphate (3EO)		3.09	4.58	
TAED	10543-57-4	2.83		
Acrylic acid	79-10-7	1.48		
Carboxymethylcellulose	9000-11-7	1.23		
Citric acid	77-92-9	1.00		
Polyacrylate	9007-04-7	0.58		
HEDP Na	3794-83-0	0.54	0.47	0.45
Enzymes		0.35	0.34	1.28
Sodium chloride		0.073		
Dye CI 15630	1103-38-4	0.0085	0.0011	0.0013
C12 alkylethoxysulphate (3EO)			3.21	6.12
Sodium dodecanate	629-25-4		2.88	6.04
Propyleneglycol	57-55-6		2.36	6.71
Citrate	68-04-2		2.22	3.42
Ethanol	64-17-5		1.55	
Sodium metaborate	231-891-6		0.67	0.42
C25AE7 petro	66455-15-0		1.75	12.13
Glycerin	56-81-5			1.24
PEI ethoxylate	68130-99-4			0.75
biphenyl disulfonate (FWA5)	27344-41-8			0.09
Perfume (excluded)		0.76	0.54	1.33

Van Hoof, G. et al. Ecotoxicity impact assessment of laundry products: comparison of USEtox and Critical Dilution Volume methods. IJLCA, 2011, 16(8), 803-818

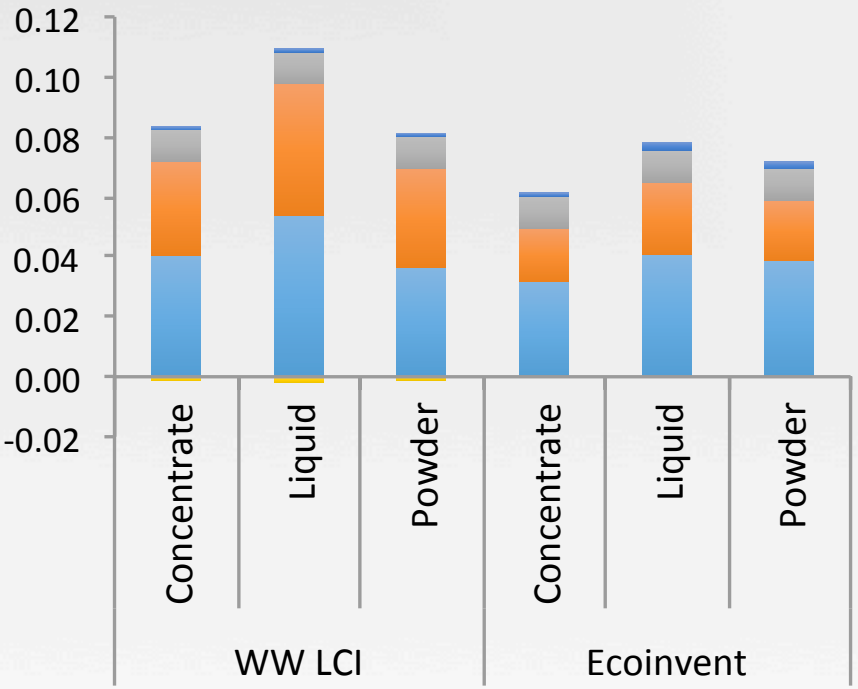
Case study: data used

- WW LCI: data sources for ingredients
  - Published risk assessments, e.g. ECHA, HERA* (composition, phys-chem properties, fate in WWTP, etc.)
  - Some WWTP factors based on expert judgement due to lack of data, e.g. Bentonite, PEI ethoxylates, dye…
- Ecoinvent model: data sources for ingredients
  - Only composition needed (TOC, N, P, etc.)
- Sludge disposal in Germany: 42% agriculture, 58% incineration

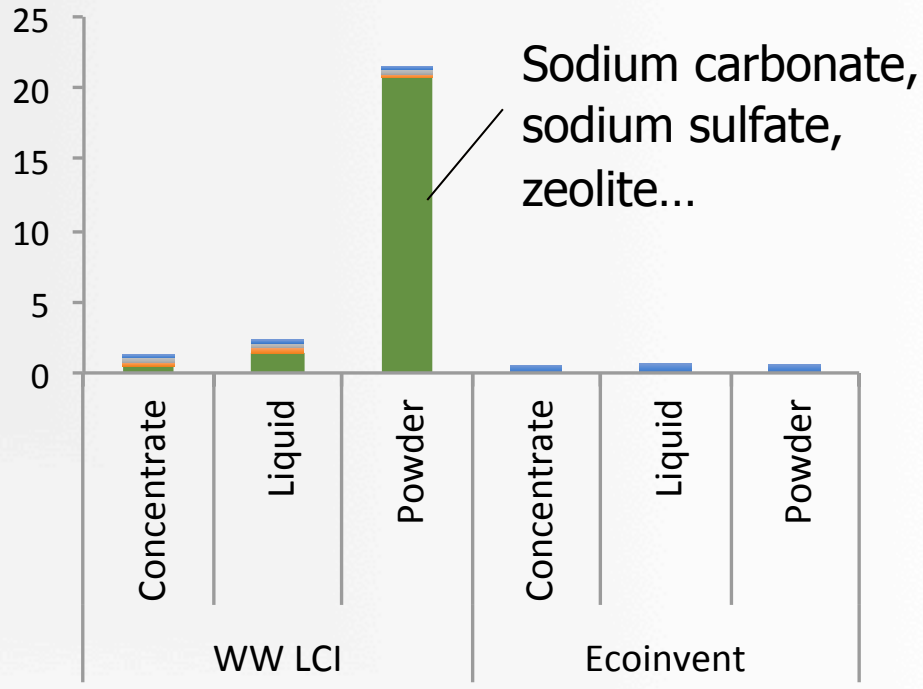
* Human and environmental risk assessment of ingredients in household cleaning products. http://www.heraproject.com/

Case study: results

GHG emissions, kg CO_2-eq/wash



Freshwater Ecotox, CTU/wash



Ingredients degradation
Energy use
WWTP+sewer infra
Displaced fertilizers
Other activities
Ingredients ecotox

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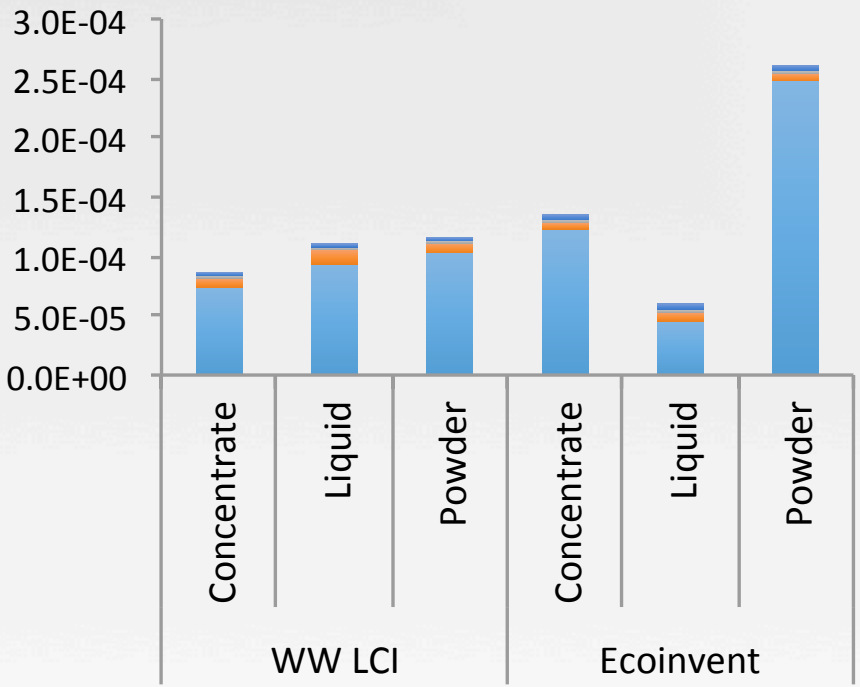
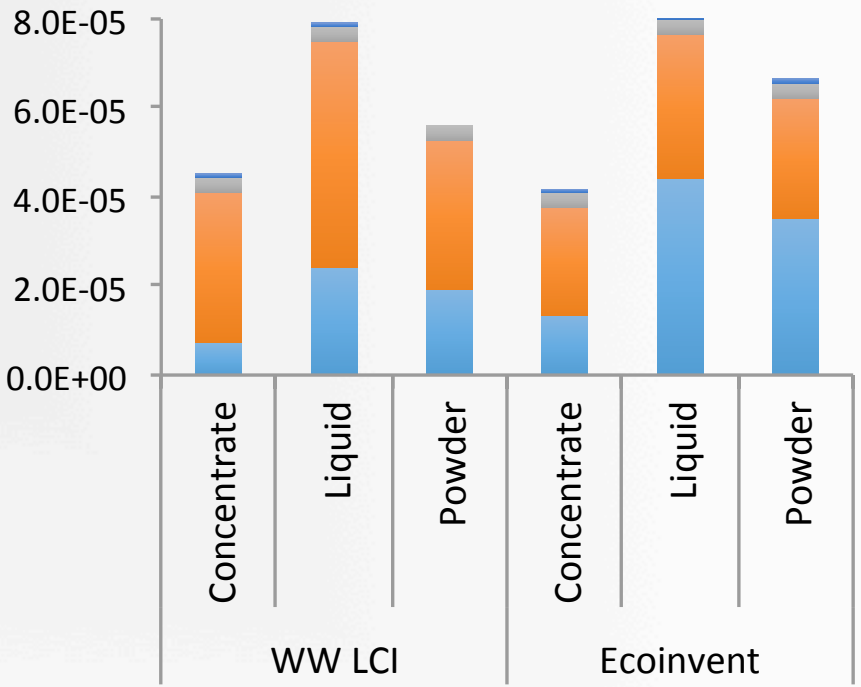
Case study: results

Marine Eutroph, kg N-eq/wash



Freshwater Eutroph, kg P-eq/wash



Ingredients degradation
Energy use
WWTP+sewer infra
Displaced fertilizers
Other activities

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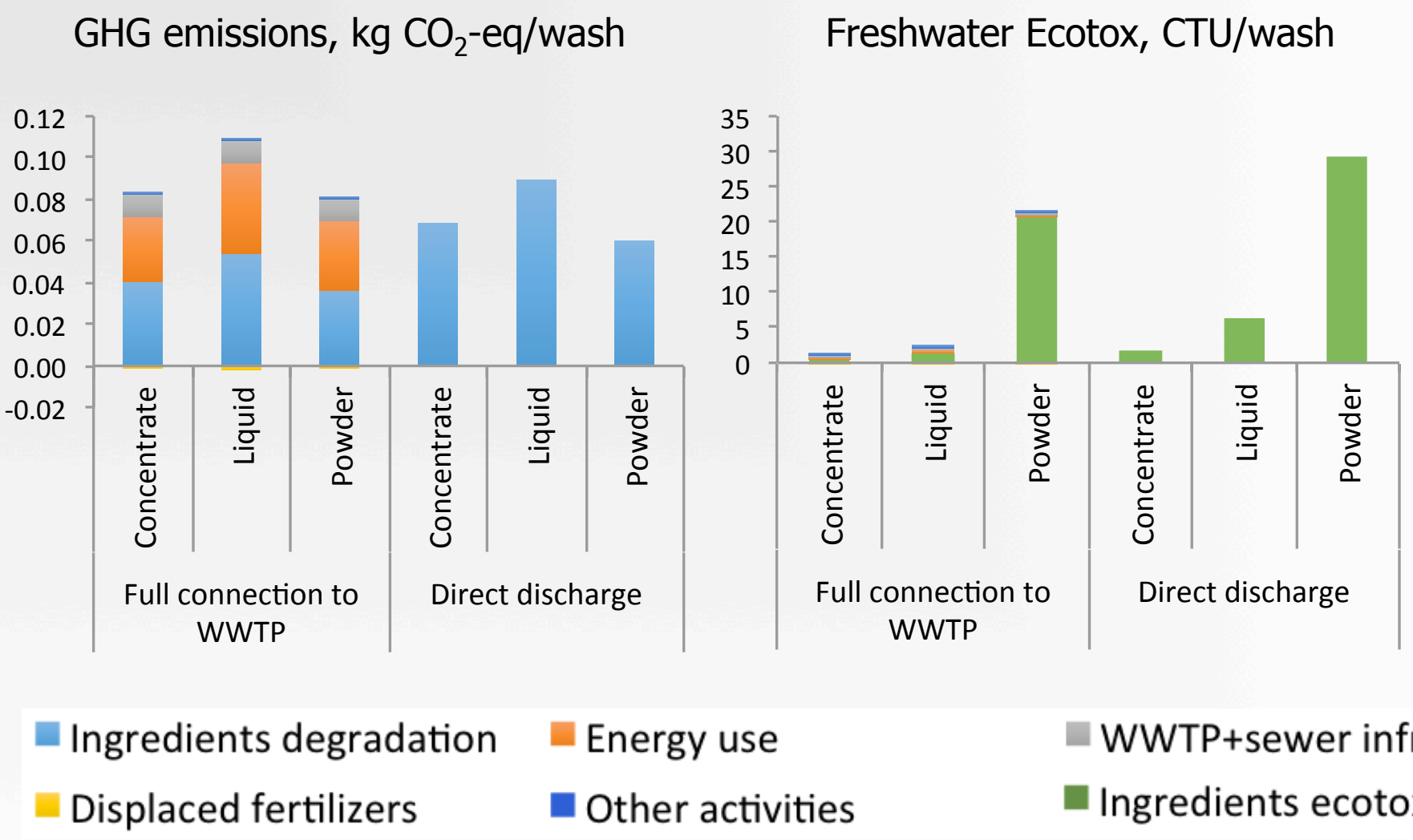
WW LCI: direct discharges



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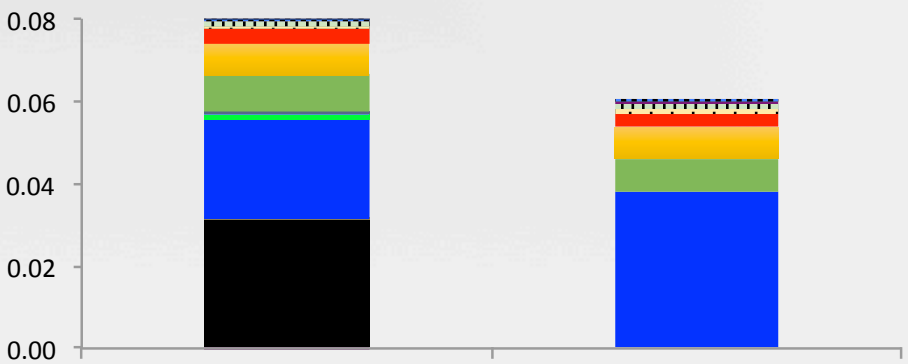
WW LCI: contributions by ingredient

GHG emissions, kg CO_2-eq/wash



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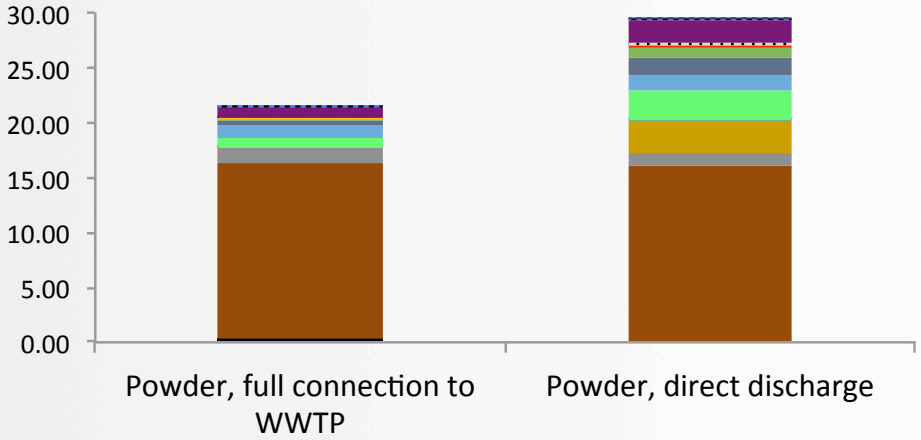
- Enzymes
- Polyacrylate
- Carboxymethylcellulose
- TAED ←
- Bentonite
- Zeolite
- Sodium percarbonate
- Sodium carbonate
- Sodium chloride
- HEDP Na
- Citric acid
- Acrylic acid ←
- C15 alkylethoxysulphate (3EO) ↙
- Sodium silicate
- LAS ←
- Sodium sulfate
- Water ←

Freshwater Ecotox, CTU/wash



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- Water

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Conclusions

- GHG emissions and freshwater eutrophication results are similar with the two models
- Marine eutrophication results differ due to higher N removal rates considered in WW LCI
- Surprisingly high contribution to ecotoxicity from inorganic ingredients like zeolites and carbonates
- Summary of strengths and weaknesses:

	WW LCI	Ecoinvent wastewater model
Strengths	• Complete flow analysis for individual substances • Assesses direct discharges • Results by individual substance	• Low data collection effort
Weaknesses	• High data collection effort	• Does not track fate of individual substances • Does not assess direct discharges • Swiss scenario only

Further developments

- Recently launched WW LCI v.2, in collaboration with the Technical University of Denmark (DTU)
- WW LCI v.2 is the result of integrating **WW LCI** with **Sewage LCI**
- What is new in WW LCI v.2:
  - Treatment by septic tanks
  - Adding WWTPs with primary treatment only
  - Adding WWTPs with tertiary treatment (sand filter)
  - Sludge composting as additional disposal option
  - Built-in scenarios (% connection to WWTP, sludge disposal) for 56 countries
- Article in preparation

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***. International Journal of Life Cycle Assessment, Online First, DOI: 10.1007/s11367-016-1189-3

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