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

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Background and aim

- There is a need to better assess the disposal of chemicals via wastewater in LCA taking into account differences in:
  - Specific behaviour of individual chemicals
  - Wastewater collection and treatment levels in different countries
  - Wastewater treatment technologies
  - Sludge disposal practices in different countries

- We recently developed WW LCI, a model that calculates chemical-specific LCIs of chemicals in wastewater\(^1\)

- We present WW LCI v2, where we expand the scope of its predecessor, including features from another model, SewageLCI\(^2\)

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\(^2\) Birkved M, Dijkman TJ (2012) SewageLCI 1.0, an inventory model to estimate chemical specific emissions via sewage treatment systems. 6th SETAC World Congress, Berlin 20-24 May 2012.
**WW LCI: the concept**

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

**WW LCI**

**Chemical**

- Connection to WWTP
  - Phys. Chem. Properties & env. half-lives
  - Direct discharge

- WWTP fate factors & scenario
  - WWTP + sludge disposal LCI model
    - WWTP process, sludge disposal, etc.
    - Environmental fate model (USES-LCA)
    - Model for environmental degradation
      - Fraction degraded
      - Fraction volatilized
      - Fraction to sludge
      - Anaerobic degradability

- LCI of chemical down the drain includes:
  - Sewer infrastr.
  - WWTP infrastr.
  - Energy input/output
  - Chemicals
  - Emissions
  - Sludge transport
  - Sludge disposal

- % population connected to WWTPs
- WWTP includes N and P removal
- Country
- Sludge disposal scenario
WW LCI (v1): technological scope

- **Direct discharges**
  - Discharge to aquatic environment
- **Includes emissions of GHG**
- **Sludge landfarming, incineration and landfilling available**
- **WWTP with biological treatment, including N removal & chemical P removal**
- **Anaerobic digestion of sludge, biogas used in cogeneration**

Diagram:
- **Wastewater**
  - **Sewer**
    - **Primary settling**
      - **Biological treatment**
        - **Phosphorus removal**
        - **Anaerobic digestion**
          - **Thickening, dewatering**
            - **Transport**
              - **Sludge Landfarming**
              - **Incineration**
                - **Transport**
                - **Landfiling**

- **Untreated wastewater flow**
- **Treated wastewater flow**
- **Sludge flow**
**WW LCI v2: expanded technological scope**

- **Connection to sewer but no treatment**
- **WWTPs with only primary treatment**

**Database with wastewater/sludge treatment practices for 57 countries**

- **Septic tanks**
- **WWTPs with tertiary treatment (sand filter)**

**Sludge composting**

**Transport**

- **Septic tank sludge disposal**
- **Thermal drying of sludge**
WW LCI v2: new processes

- Septic tanks
  - Production and installation of septic tank
  - Degradation/removal of chemicals in wastewater:
    \[
    F_{\text{deg,septic}} = 0.3 \cdot F_{\text{deg,WWTP}} \\
    F_{\text{sludge,septic}} = 0.3 \cdot F_{\text{sludge,WWTP}}
    \]
  - Transport of sludge (3% dry mass) to WWTP

- WWTPs with primary treatment only
  - Lower energy use and land occupation
  - No anaerobic digestion of sludge
  - Degradation/removal of chemicals in wastewater: 
    ➔ As in septic tanks
WW LCI v2: new processes

- WWTPs with tertiary treatment
  - We only include sand filtration
  - Additional energy use, cleaning chemicals and land occupation
  - Removal of chemicals based on chemical-specific sorption to sludge:

\[
F_{\text{sludge,tert}} = \frac{\rho_{\text{sludge}} \cdot K_d}{1 + \rho_{\text{sludge}} \cdot K_d}
\]

\[
K_d = f_{oc} \cdot 0.41 \cdot K_{ow}
\]
**WW LCI v2: new processes**

- **Thermal drying of sludge**
  - Pre-treatment for incineration
  - Electricity and heat demand to evaporate excess water
  - Chemical content assumed unaltered

- **Sludge composting**
  - Optional before application to agricultural soil
  - Open composting only
  - Inputs include composting plant and energy use
  - Complete mass balance:

### Mass balance for sludge composting, all amounts in kg

<table>
<thead>
<tr>
<th>Chemical in sludge</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Chemical</td>
<td>O₂</td>
</tr>
<tr>
<td>DTPMP (persistent)</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>TAED (degradable)</td>
<td>1</td>
<td>0.13</td>
</tr>
</tbody>
</table>
WW LCI v2: country database

- **Statistics on wastewater treatment (in %):**
  - Connection to sewer
    - Without treatment
    - With treatment - primary
    - With treatment - secondary
    - With treatment - tertiary
  - Connection to independent collection
    - With treatment
    - Without treatment

- **Statistics on sludge disposal (in %):**
  - Composting
  - Landfarming
  - Landfilling
  - Incineration

<table>
<thead>
<tr>
<th>Region</th>
<th>Countries</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Europe</strong></td>
<td>Austria, Bosnia Herzegovina, Belgium, Bulgaria, Switzerland, Cyprus, Czech Republic, Germany, Denmark, Estonia, Spain, Finland, France, United Kingdom, Greece, Croatia, Hungary, Ireland, Iceland Italy, Lithuania, Luxembourg, Latvia, FYR of Macedonia, Malta, The Netherlands, Norway, Poland, Portugal, Romania, Serbia, Sweden, Slovenia, Slovakia, Turkey, Ukraine, Montenegro</td>
</tr>
<tr>
<td><strong>America</strong></td>
<td>Brazil, Canada, Chile, Mexico, Peru, United states</td>
</tr>
<tr>
<td><strong>Asia Pacific</strong></td>
<td>Australia, China, Indonesia, India, Iran, Japan, Republic of Korea, Malaysia, Russia, Saudi Arabia, Thailand, Taiwan</td>
</tr>
<tr>
<td><strong>Africa</strong></td>
<td>Tanzania, South Africa</td>
</tr>
</tbody>
</table>
WW LCI v2: key features of the Excel tool

- 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 v2 in Excel

| Scenario data | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z | AA |
| Quality       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| Choice of country data set | Database | Automated error flags | No errors |  |
| Wastewater treatment processes | Connection to urban wastewater collecting systems - total (%) | 100% | 100% |  |
| | Connection to urban wastewater collecting systems - without treatment (%) | 5% | 5% |  |
| | Connection to urban wastewater collecting systems - with treatment (%) | 5% | 5% |  |
| | Connection to urban wastewater treatment - primary treatment (%) | 1% | 1% |  |
| | Connection to urban wastewater treatment - secondary treatment (%) | 1% | 1% |  |

### Sludge scenarios

| Nutrient removal rate | 100% | 100% |  |
| Chemical maturity | 100% | 100% |  |

### Chemical-specific data

#### Sludge transport

<table>
<thead>
<tr>
<th>Product in wastewater (kg)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol (kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PVC (kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electricity (kWh)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Sludge composting

<table>
<thead>
<tr>
<th>Product in wastewater (kg)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
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<td></td>
<td></td>
</tr>
<tr>
<td>PVC (kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electricity (kWh)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Sludge landfilling

<table>
<thead>
<tr>
<th>Product in wastewater (kg)</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol (kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PVC (kg)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electricity (kWh)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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### CSVmaker

![CSVmaker Diagram](image)

**Inputs**

1. WWTP input
2. USELCA input
3. LCI output
4. LCI output, raw data
5. Ready to CSV output
6. Ready to CSV output, raw data
7. Database
8. Parameters
9. Env deg calc
10. Calc deg
11. Summary

---

**Outputs**

- Normal View
- Ready
- LCI output
- LCI output, raw data
- Ready to CSV output
- Ready to CSV output, raw data
- Database
- Parameters
- Env deg calc
- Calc deg
- Summary

---

**Data**

- Normal View
- Ready
- LCI output
- LCI output, raw data
- Ready to CSV output
- Ready to CSV output, raw data
- Database
- Parameters
- Env deg calc
- Calc deg
- Summary

Sum = 0
## WW LCI v2 applied to three chemicals

### Chemicals

<table>
<thead>
<tr>
<th>Name</th>
<th>Typical use</th>
<th>Key features</th>
<th>Removal in WWTP (with secondary treatment&lt;sup&gt;1&lt;/sup&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diethylenetriamine penta(methylene phosphonic acid) (DTPMP)</td>
<td>In detergents</td>
<td>Poorly degradable, contains N and P</td>
<td>0% degraded, 85% to sludge</td>
</tr>
<tr>
<td>Atrazine</td>
<td>Pesticide</td>
<td>Poorly degradable, contains N</td>
<td>1% degraded, 2% to sludge</td>
</tr>
<tr>
<td>Ibuprofen</td>
<td>Pharmaceutical</td>
<td>Degradable</td>
<td>72% degraded, 1% to sludge</td>
</tr>
</tbody>
</table>

<sup>1</sup> Estimated with the fate model Simpletreat

### Country data

<table>
<thead>
<tr>
<th></th>
<th>Denmark (DK)</th>
<th>India (IN)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Wastewater treatment scenario</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Connection to sewer</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Without treatment</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>Primary treatment</td>
<td>2%</td>
<td>0%</td>
</tr>
<tr>
<td>Secondary treatment</td>
<td>3%</td>
<td>21%</td>
</tr>
<tr>
<td>Tertiary treatment</td>
<td>84%</td>
<td>0%</td>
</tr>
<tr>
<td><strong>Connection to independent collection</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>With treatment - septic tank</td>
<td>11%</td>
<td>39%</td>
</tr>
<tr>
<td>Without treatment</td>
<td>0%</td>
<td>39%</td>
</tr>
<tr>
<td><strong>Sludge disposal scenario</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Composting</td>
<td>6%</td>
<td>0%</td>
</tr>
<tr>
<td>Landfarming</td>
<td>50%</td>
<td>100%</td>
</tr>
<tr>
<td>Landfilling</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>Incineriation</td>
<td>44%</td>
<td>0%</td>
</tr>
</tbody>
</table>
WW LCI v2 applied to three chemicals

GHG emissions, in kg CO₂-eq/kg chemical (IPCC 2013)

<table>
<thead>
<tr>
<th>Chemical</th>
<th>DTPMP</th>
<th>Direct discharge</th>
<th>Ibuprofen</th>
<th>Direct discharge</th>
<th>Atrazine</th>
</tr>
</thead>
<tbody>
<tr>
<td>DK</td>
<td>0.5</td>
<td>1.7</td>
<td>3.5</td>
<td>4.7</td>
<td>4.1</td>
</tr>
<tr>
<td>IN</td>
<td>1.5</td>
<td>1.7</td>
<td>3.5</td>
<td>4.1</td>
<td>3.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.2</td>
</tr>
</tbody>
</table>

Colors:
- Other Processes
- Heat use in WWTP + sludge disposal
- GHG from chemical's degradation
- P and N fertilizer credit
- Electricity use in WWTP + sludge disposal
WW LCI v2 applied to three chemicals

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

(Log scale)
**WW LCI v2 applied to three chemicals**

Freshwater eutrophication, in kg P-eq/kg chemical (ReCiPe)
Marine Eutrophication, in kg N-eq/kg chemical (ReCiPe)

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Direct discharge DK</th>
<th>Direct discharge IN</th>
<th>Direct discharge DK</th>
<th>Direct discharge IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>DTPMP</td>
<td>0.05</td>
<td>0.00</td>
<td>0.10</td>
<td>0.00</td>
</tr>
<tr>
<td>Ibuprofen</td>
<td>0.20</td>
<td>0.30</td>
<td>0.15</td>
<td>0.30</td>
</tr>
<tr>
<td>Atrazine</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
</tr>
</tbody>
</table>

**Legend:**
- **Blue** Freshwater Eutrophication (kg P-eq.)
- **Red** Marine Eutrophication (kg N-eq.)
Conclusions & options for improvement

- 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
  - No uncertainty quantification
  - Import of data sets only available for SimaPro so far
  - Septic tank sludge scenario is optimistic for developing countries
  - Tertiary treatment includes only sand filter
  - Country database can be expanded
Thank you!

More info:

WW LCI References:
Kalbar P, Muñoz I, Birkved M. **WW LCI v2: a second-generation inventory model for chemicals discharged to wastewater.** Submitted to the International Journal of Life Cycle Assessment

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. DOI: 10.1007/s11367-016-1189-3