ecosolvent: A tool for waste-solvent management in chemical industry

Christian Capello, Stefanie Hellweg, Christina Seyler, Konrad Hungerbühler
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- Project goals
- Inventory models
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Waste solvent in Swiss chemical industry

- Swiss chemical industry operates mainly in the field of pharmaceutical and specialty chemicals (>90% of the total turnover)
- High consumption of organic solvents (~250’000 tonnes of fresh solvents / year)
- 45 organic solvents were identified to be important (industry survey)
- Waste-solvent management is controlled by economic and logistic factors
- So far, no instruments are available for quantifying the environmental impact of waste-solvent treatment
Project goals

- Development of an easy usable tool for the comparative environmental assessment of waste-solvent treatment technologies for specific, user-defined waste-solvent mixtures
- Environmental assessment using the LCA methodology
- Close collaboration with industry (data and requirements)
Model overview

- **Incineration** → Avoidance of fossil fuels
- **Distillation** → Avoidance of petrochemical solvent production
- Both treatment options enable a reduction of the demand of non-renewable resources

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LCI-models incineration: Multi-input allocation models

- **Allocation:**
  - Elemental composition (e.g. NaOH consumption)
  - Net calorific value (e.g. process steam as co-product)
  - Waste-solvent mass (e.g. electricity consumption)

- **Models:**
  - Waste-solvent incineration plant (capacity 35’000 t/a) 
    *(Seyler et al. 2005, J. of Cleaner Production 13, 1211-1224)*
  - Incineration in cement kilns (Swiss average, 8 plants) 
    *(Seyler et al. 2004, Int. J. of LCA 10 (2), 120-130)*

- **Input information needed:**
  - Elemental waste-solvent composition and water content
LCI-model wastewater treatment plant: Multi-input allocation model

- Currently:
  - Allocation based on TOC-content
  - All consumption and emission factors are based on industry data
  - Differentiation between well degradable alcohols (e.g. methanol and ethanol) and other solvents.

- Planned improvement:
  - More comprehensive model, including various technologies and allocations

(A. Köhler, Dissertation ETH)
LCI-model distillation: A statistical approach

- Problem: Every distillation process is unique (waste composition, distillate purity, technology)
- Solution: Statistical analysis of 150 industrial waste-solvent distillations
- Results: Generic data ranges for each LCI parameter
  (Capello et al. 2005, ES&T 39 (15), 5885-5892)
LCI-model distillation: Case 1

Generic data ranges I: Data ranges based on full sample

Example: Use of cooling water

Generic data range I:
First approximation in case no information is available
(no primary data, no measurements)

95% Interval

Empiric minimum value

Empiric maximum value
LCI-model distillation: Case 2

Generic data ranges II: Data ranges based on sub-samples

Example: Use of nitrogen

Sub-sample 1: Continuous distillation
Sub-sample 2: Batch distillation

m³ / kg waste solvent

95% Interval

Minimum (C) Maximum (C) Minimum (B) Maximum (B)

More

95% Interval

Generic data range II: More accurate approximation in case little information is available (distillation technology, use of ancillaries)
# LCI-model distillation: Model overview

<table>
<thead>
<tr>
<th>Required Information</th>
<th>Additional Information</th>
<th>Additional Information</th>
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<tbody>
<tr>
<td>Waste solvent composition</td>
<td>Distillation technology (batch/continuous)</td>
<td>User defined values for</td>
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<tr>
<td>Recovered solvent</td>
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<td>Solvent recovery</td>
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<td>Solvent recovery</td>
<td>Steam consumption</td>
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<td>Steam consumption</td>
<td>Electricity consumption</td>
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<td>Nitrogen consumption</td>
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<td>Amount of outlet air</td>
<td>Ancillary consumption</td>
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<td>Amount of outlet air</td>
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<td>Ancillaries (purpose)</td>
<td>Amount of wastewater</td>
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<td>pH regulation</td>
<td>Amount of cooling water</td>
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<td>Entrainer (azeotrop)</td>
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<td>Cleaning agents</td>
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</table>

- **Generic data ranges I** (Case 1)
- **Generic data ranges II** (Case 2)
- **Precise user data** (Case 3)

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Methods of uncertainty quantification

- **Method 1: “Bounding analysis”**
  - Total minimum / maximum values based on minimum / maximum values of all consumption and emission factors (incineration) and 95% interval (LCI-parameter distillation)

- **Method 2: Stochastic modelling (Monte Carlo)**
  - Fitted probability functions for all model parameters (incineration and distillation)
  - Uncertainty of the background-inventories (ecoinvent database or generic uncertainty factors)

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The ecosolvent tool: Schematic overview

User Input
- User specified
- Waste solvent composition
- Recovered solvent
- Additional information on the distillation process

Calculation
- Calculation of
  - Elementary composition
  - Net calorific value
- Incineration
- Distillation
  - Analysis of entered information

LCI Output
- Run of waste solvent incinerator model
- Run of cement kiln model
- Generic data range I (Case 1)
- Generic data range II (Case 2)
- Precise user data (Case 3)

LCA Output
- Calculated LCI
- Calculated LCI
- Calculated LCI
- X Assessment factors

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Case study 1: Ethyl acetate mixture

- 1 kg waste solvent: Ethyl acetate (92 wt%), ethanol (1 wt%), water (1 wt%), organic solids (6 wt%)
Case study 1: Ethyl acetate mixture

- Distillation is the environmentally superior treatment option
Case study 2: Acetic acid / water mixture

Solvent recovery:
0.89 kg acetic acid / kg waste solvent

Waste-solvent incinerator
Worst-case scenario
Average scenario
Best-case scenario

Distillation
Worst-case scenario
Average scenario
Best-case scenario

Increasing solvent recovery

Minimum solvent recovery:
- acetic acid 0.31 kg
- Waste solvent composition:
  - acetic acid 0.34 kg
  - water 0.66 kg

Maximum solvent recovery:
- acetic acid 0.97 kg
- Waste solvent composition:
  - 0.98 kg acetic acid
  - 0.02 kg water

Points of equivalent impacts

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Summary & Conclusions

- The *ecosolvent* tool enables to calculate the environmental impact of thermal treatment as well as recovery of specific, user-defined waste solvents.
- All models are based on industry data.
- Only few input information is needed (waste solvent composition and solvent to be recovered).
- Increasing completeness of information leads to more accurate results.
- Due to its flexibility in terms of information needed, the *ecosolvent* tool can be used for the environmental assessment of already operating processes (retrofit) as well as in the stage of process design.
Software release

- Scheduled software release is Juli 2006
- Information available under http://www.sust-chem.ethz.ch
Acknowledgment

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  - Novartis Pharma AG
  - Hoffmann-La Roche AG
  - Sigfried Ltd.
  - Valorec Services AG
Thank you for your attention!

Further information:
- christian.capello@chem.ethz.ch
- http://www.sust-chem.ethz.ch/research/lifecycle/solvents.html

References:
The 45 solvents included in the ecosolvent tool

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<td>Heptane</td>
<td>Diethyl ether</td>
<td>Acetic acid</td>
<td>Cyclohexane</td>
<td>Acetone</td>
<td>Benzaldehyde</td>
<td>Dichloromethane</td>
<td>Butyl acetate</td>
<td>Acetic Anhydride</td>
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<td>Hexane</td>
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<td>Methylcyclohexane</td>
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<td>Monochlorobenzene</td>
<td>Ethyl acetate</td>
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LCIA methods included in the ecosolvent tool

- Aggregated scores:
  - Eco-Indicator 99
  - Method of Ecological Scarcity (UBP’97)
  - Cumulative Energy Demand

- Midpoints:
  - Global Warming Potential
  - Respiratory Inorganics, Climate Change, Fossil Fuels
  - CML Fresh Water Aquatic Toxicity, extended with a characterization factor for TOC from chemical industry

- Elementary flows:
  - CO2