ecoinvent data v2.0
Life-Cycle Inventories of Petrochemical Solvents and Highly Pure Chemicals

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New ecoinvent data v2.0

- Two projects:
  - petrochemical solvents
  - highly pure chemicals

- Detailed information on project goals, contents, dataset quality

- Examples of data generation

Petrochemical Solvents

- Annual solvent consumption in Europe alone was 4 million tonnes in 2004
- Roughly 250 to 300 solvents are generally available to chemists, but not all are used on a large scale
- Uses in
  - paint and coatings industry
  - chemical industry (production of pharmaceuticals, agrochemicals, specialty chemicals)
  - metal cleaning and degreasing
  - rubber and plastics manufacture
  - detergents and personal care products
Petrochemical Solvents

- Project size was limited to 50 chemicals

- Solvents were classified into various chemical groups (alcohols, aliphatic and aromatic hydrocarbons, ethers, ...)

- Important representative chemicals of all groups were selected based on production data, technical literature and a survey of the Swiss chemical industry

### List of the 50 solvents

<table>
<thead>
<tr>
<th>Aliphatic Hydrocarbons</th>
<th>Alcohols</th>
<th>Esters</th>
<th>Ethers and glycolethers</th>
<th>Acids</th>
<th>Ketones</th>
<th>Amides and other N-compounds</th>
<th>Other solvents</th>
</tr>
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<tbody>
<tr>
<td>• Pentane</td>
<td>• Benzy alcohol</td>
<td>• Methyl formiate</td>
<td>• Diethyl ether</td>
<td>• Formic acid</td>
<td>• Acetone</td>
<td>• Acetonitrile</td>
<td>• Dimethylsulfoxide</td>
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<td>• Hexane</td>
<td>• 1-Butanol</td>
<td>• Butyl acetate</td>
<td>• Dioxane</td>
<td>• Cyclohexanone</td>
<td>• Cyclohexanone</td>
<td>• N,N-Dimethylformamide</td>
<td>• Acetic anhydride</td>
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<tr>
<td>• Isohexane</td>
<td>• 2-Butanol</td>
<td>• Ethyl acetate</td>
<td>• Ethylene glycol dimethyl ether</td>
<td>• Methyl ethyl ketone</td>
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<td>• N-Methyl-2-pyrrolidone</td>
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<td>• Methyl isobutyl ketone</td>
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<td>• Butylene glycol</td>
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Swiss Centre For Life Cycle Inventories
A joint initiative of the ETH domain and Swiss Federal Offices
Solvent Production Routes

- Most solvents are created in one of four chemical routes:
  - **Methanol route**: methanol production from natural gas
  - **Naphta/steam cracking route**: Naphta from crude oil is treated in a steam cracking process
  - **BTX/Naphta separation route**: Naphta from crude oil or BTX reformate is separated in a molecular sieve
  - **BTX splitting route**: BTX reformate or pyrolysis gasoline are separated.

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**Natural gas and crude oil processing**

- Crude oil:
  - Desalting
  - Distillation
  - Vacuum distillation
- Crude oil:
  - Sweetening (sweetening process)
  - Gas processing

**Natural gas**:
- Chirnacterisation
- Steam reforming
- Synthesis gas
- Methanol synthesis
- Methanol

**Route A**

**Naphta**
- Crude oil:
  - Distillation
- Hydrocracking
- Catalytic cracking
- Catalytic reforming
- Gasoline
- Diesel
- Light fuel oil

**Route B**

**Route C**

**Route D**
The Naphta/steam cracking route

Production steps

1. Crude oil
   - Naphtha
   - Steam cracking

2. Methane
   - Hydration
   - Ethylene glycol
   - Dehydration
   - 1-Butanol

3. Butane
   - Hydroformylation
   - Butene
   - Ethylene glycol
   - Dehydration
   - 1-Butanol

4. 2-Butanol
   - Acrylonitrile
   - Propylene glycol
   - Dehydration
   - 1-Butanol

5. Propene
   - Propylene glycol
   - Dehydration
   - 1-Butanol

6. Heavy gas oil
   - Propene
   - Propylene glycol
   - Dehydration
   - 1-Butanol

Energy profile per kg product (Cumulative Energy Demand)

- Formic acid
- Methyl acetate
- Methylene chloride
- Dichloromethane
- Butanol
- Butenes
- MTBE
- Pentane
- Propene
- Isopropyl alcohol
- Isobutyl alcohol
- Isobutyl acetate
- 1-Butanol
- 1-Propanol
- Butyric acid
- Ethylene oxide
- Ethylene glycol
- Diethyl ether
- Monoethyl ether

Starting materials
- 1 process step
- 2 process steps
- 3 process steps
- 4 process steps
The BTX/ Naphtha separation route

C: The BTX/naphtha separating route

Production steps

Crude oil → BTX (naphtha) → Naphtha → Crude oil

Starting material

Molecular sieve Ultra molecular sieve crystallization Superfractionation

α-Hexane Isomerization Isohene

1 process step

Energy profile per kg product (Cumulative Energy Demand)

α-Heptane

BTX splitting route

D: The BTX splitting route

Production steps

Crude oil → BTX (naphtha) → Paraxene splitter

Starting material

1 process step

Solvent Intermediate Unit process
The BTX splitting route

Energy profile per kg product (Cumulative Energy Demand)

New Inventories in ecoinvent 2.0

- 50 solvents were selected for relevance
- LCI data for 11 of these solvents had already been published in ecoinvent 1.1
- LCI data for 3 solvents existed in ecoinvent 1.1 but were replaced by new inventories during the project
- New LCI data were created for 36 solvents
Data Sources

- Whenever possible, actual production data was used to determine inventory flows
- Basic information was gathered from technical reference books
- Necessary estimations were made based on Hischier et al 2004 (Establishing Life Cycle Inventories of Chemicals Based on Differing Data Availability)

Data quality

- Actual production data available: 6 solvents
- Data for raw materials and energy available: 13 solvents
- Data for energy available: 5 solvents
- Energy approximated with similar process: 8 solvents
- All data estimated: 7 solvents
Example: Chlorobenzene

- Multi-output process: benzene chlorination
- Benzene + Chlorine $\rightarrow$ Monochlorobenzene + o-Dichlorobenzene + p-Dichlorobenzene
- Data available from US database (Overcash 1998-2001)
- Production data from US chemical industry
- Data available for use of raw materials, auxiliaries, and energy
- Data available for emissions to air and emissions to water
- Data available for yield of co-products $\rightarrow$ allocation

Example: Acetates

- Ethyl acetate (esterification of ethanol and acetic acid)
  - Ethanol + acetic acid $\rightarrow$ ethyl acetate
  - Energy consumption: steam 8.84 MJ/kg, electricity 0.00725 kWh/kg

- These data are used as approximation for energy consumptions of other esterifications:
  - Butyl acetate (1-Butanol + Acetic acid)
  - Isoamyl acetate (Isoamyl alcohol + Acetic acid)
  - Isobutyl acetate (Isobutanol + Acetic acid)
  - Isopropyl acetate (Isopropanol + Acetic acid)
Highly Pure Chemicals

- Part of the ecoinvent 2.0 project *Life cycle Inventories of electric and electronic equipment*
- **IT-services**: report 18_IV
- **Devices**: report 18_III
- **Modules**: report 18_II
- **Components**: report 18_I
- **Disposal**: report 18_V
- **Raw materials**: report 10 (metals)
- **Auxilliaries**: *report 19 (chemicals for IT)*

Chemicals for IT

- *EMPA St. Gallen*: list of **77 chemicals** for IT
  - Batteries: 7 chemicals
  - Hard disc drive: 1 chemical
  - Semiconductors: 16 chemicals
  - Printed wiring board: 26 chemicals
  - Other components: 13 chemicals
  - Others: 4 chemicals
  - Preliminary products: 10 chemicals
- Mostly chemicals not included in previous versions of ecoinvent
List of Chemicals

- Lithium
- Alcohol ethoxylate
- Alkyl oxidized salts
- Ammonia-2-ethanol
- Butyl acetate
- Cellulose acetate
- Diacetone alcohol
- Dibutyl phthalate
- Dimethyl acetylamide
- Dimethylamine borane
- Ethanol
- Ethyl acetate
- Ethyl cellulose
- 4-Fluoro-1,3-dioxolan-2-one
- Fluorouracil
- Hexafluoroethane
- Hexamethyldisilazane
- Hydroxyl monoethanolamine
- Lactic acid
- Methanesulfonic acid
- Methoxy propanol
- Methyl-3-methoxypropionate
- M-Pyrrol
- N-Methyl Pyrrolidone
- Polyacetal
- Polylactone
- Polyglycol mixture
- Polyphenyl oxide
- Polystyrene
- Polyvinyl pyrrolidone
- Polyvinyl sulfide
- Rosin
- Rosin, modified
- Tetramethyl ammonium hydroxide

Inorganics
- Ammonium chloride
- Arsenic
- Carbonic acid
- Chloride as ion
- Diborane
- Dinistogen oxide
- Helium
- Hydrogen bromide
- Iron(III)chloride
- Iron oxide
- LaNiH
- Lead borate
- Lithium carbide
- Lithium carbonate
- Lithium hydroxide
- Lithium manganese oxide
- Nitrogen trifluoride
- Phosphine
- Phosphoryl chloride
- Potassium carbonate
- Potassium perchlorate
- Silane
- Sodium persulfate
- Sulphuric peroxide
- Trichloroborane
- Trifluoroborane
- Tungsten fluoride
- Water, ultrapure

Others
- Acid cleaner
- Anti tarnish
- Banking agent
- Diazo film
- Foam Free 940 Defoamer
- Gas cleaner
- Solder leveller (HAZL)

Chemicals for IT

- LCI data created in this project: 30 chemicals (+ precursors)
- Existing LCI in ecoinvent v1.1: 1 chemical
- LCI data from solvents project: 5 chemicals
- LCI data from photovoltaics project: 3 chemicals
- LCI data created by EMPA: 3 chemicals
- Approximated with data from v1.1: 17 chemicals
- Others: Approximated with with DS "chemicals, organic, at plant, RER" or "chemicals, inorganic, at plant, RER"
Data Sources (cf. Solvent Project)

- Whenever possible, actual production data was used to determine inventory flows
- Basic information was gathered from technical reference books
- Necessary estimations were made based on *Hirschier et al 2004* (Establishing Life Cycle Inventories of Chemicals Based on Differing Data Availability)

Example: Water, ultrapure

- Purification steps:
  - tap water $\rightarrow$ water, decarbonised $\rightarrow$ water, ultrapure
- Purification:
  - ion exchangers (resins), membranes, electrodeionization
- Dataset is calculated with literature data for electrodeionization
Example: Lithium route

- Lithium (electrolysis of lithium chloride): data from literature (Wietelmann 2000)
- Lithium chloride (chlorination of lithium carbonate): energy data from literature (Kim 2003)
- Lithium manganese oxide (sintering of lithium carbonate): approximated with data from iron sintering (ecoinvent v1.1)
- Lithium hydroxide (hydration of lithium carbonate): all data estimated
Example: Ammonium thiocyanate

- $\text{CS}_2 + 2\text{NH}_3 \rightarrow \text{NH}_4\text{SCN}$
- All data are estimated
- Raw materials: calculated with an estimated yield of 95%
- Cooling water: estimated with Gendorf 2000
- Energy consumption: estimated with Gendorf 2000
- Transports and infrastructure: ecoinvent standard values
- Emissions to air: estimated as 0.2% of input
- Emissions to water: calculated from mass balance

Thank you for your information

References:

Example: Chlorobenzene

<table>
<thead>
<tr>
<th>input</th>
<th>Chlorination of benzene</th>
<th>kg per kg monochlorobenzene</th>
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<tr>
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<tr>
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<td>Chlorine (kg)</td>
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<td>Sodium hydroxide (kg)</td>
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<td>Electricity (kWh)</td>
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</tr>
</tbody>
</table>

Output

| emissions to air |                          |                             |
| process         |                          |                             |
| Benzene, to air (kg) |                | 0.0266                      |
| Waste heat (MJ)  |                          | 0.0172                      |
| emissions to water |                       |                             |
| Benzene, to water (kg) |           | 0.105                       |
| Monochlorobenzene, to water (kg) | | 0.0969                      |
| Sodium chloride, to water (kg) |         | 0.328                       |
| o-Dichlorobenzene, to water (kg) |       | 0.00469                     |
| COD, BOD (kg)    |                          | 0.638                       |
| TOC, DOC (kg)    |                          | 0.184                       |

Approximations

Highly pure chemical

- Hydroxyl monoethanolamine > monoethanolamine
- Hydrogen bromide > hydrogen chloride
- Diazo film > polyethylene terephthalate
- Anti tarnish > chromium/zinc at a ratio of 4:1
- Glas cleaner > ethanol
- Foam Free 940 Defoamer > polyethylene
- Solder leveller (HAZL) > tin

used ecoinvent DS

Highly pure chemical

- Hydroxyl monoethanolamine > monoethanolamine
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