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ETH Lausanne / Session „Chemicals“

Chemicals
Part I

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Further chemicals are contained in other categories such as detergents, plastics, etc.

Chemicals in ecoinvent

- Solvents (acetone, methanol)
- Inorganic bases (ammonia)
- Inorganic acids (sulfuric acid, nitric acid, hydrochloric acid)
- Organic acids (acetic acid)
- Organic bases (triethanolamine)
- Inorganic gases (Kr, Xe)
- Inorganic reactive chemicals (sodium chlorate, hydrogen peroxide)
- Organic reactive chemicals (phosphorous chloride, epichlorhydrin, ethylene oxide, phosgene)
- Salts (NaCl, sodium sulphate)
- Organic natural substances (soya oil, palm oil)
- Etc.
Example: solvents in ecoinvent

- Acetone
- Acetic acid
- Formaldehyde
- Isopropanol
- Methanol
- Methyl chloride
- Toluene
- Xylene
- Aniline
- Benzene
- Methyl dichloride
- Methyl ethyl ketone
- Methyl tert-butyl ether
- Nitrobenzene
- Tetrachloroethylene

Different solvent groups represented (such as alcohols, aldehydes, aromatic hydrocarbons, aliphatic carboxylic acid, chlorinated hydrocarbons, ether, and ketones). Methanol, toluene, and isopropanol belong to the most used solvents, mass-wise, in the pharmaceutical and specialty chemical industry.

Methanol: description

- Chemical formula: CH$_3$OH
- Worldwide annual demand: 28.2 million tons
- Use in chemical synthesis (formaldehyde, MTBE, acetic acid) and as solvent and detergent
- More than 90% of methanol is produced of natural gas
- Methanol is produced worldwide, increasingly at remote locations with resources of natural gas
Methanol in ecoinvent

Three data sets:

1. Methanol plant, GLO
   Infrastructure (per plant)

2. Methanol, at plant, GLO
   Average production of 1 kg pure methanol

3. Methanol, at regional storage, CH
   Production and transport of 1 kg methanol to Switzerland

Methanol plant (GLO)

Reference: 1 plant in Sibiria
Capacity: 2700 t/day
Availability: 91%
Operation time: 30 years

37.2*10^{-12} units per kg methanol
Methanol plant (GLO)

Concrete, sole plate and foundation, at plant, CH
Steel, low-alloyed, at plant, RER
Steel, electric, at plant, RER
Chromium steel 18/8, at plant, RER
Zinc for coating, at plant, RER
Copper, at plant, RER
Nickel, at enrichment, RER
Transport, transoceanic freight ship, OCE
Transport, freight, rail, RER
Transport, lorry 32t, RER

Energy
- Electricity, medium voltage, production UCTE, at grid, UCTE
- Diesel, burned in building machine, GLO

Materials
- Concrete, sole plate and foundation, at plant, CH
- Zinc for coating, at plant, RER
- Copper, at plant, RER
- Nickel, at enrichment, RER
- Steel, low-alloyed, at plant, RER
- Chromium steel 18/8, at plant, RER
- Steel, electric, at plant, RER

Waste process
- Disposal, concrete, 5% water, to inert material landfill, CH
- Disposal, concrete, 5% water, to inert material landfill, CH

Occupation
- Industrial area, built up, vegetated construction site
- Industrial area, built up, vegetated construction site

Transformation
- from unknown to industrial area, built up from unknown to industrial area, vegetated

Methanol plant, GLO

Transports
- Transport, transoceanic freight ship, OCE
- Transport, freight, rail, RER
- Transport, lorry 32t, RER

Land use

Methanol plant (GLO): raw data

<table>
<thead>
<tr>
<th>Technosphäre</th>
<th>Wert</th>
<th>Ressourcen</th>
<th>Wert</th>
<th>Emissionen</th>
<th>Wert</th>
</tr>
</thead>
<tbody>
<tr>
<td>electricity, medium voltage, production UCTE, at grid, UCTE</td>
<td>5.66E+6 kWh</td>
<td>Occupation, construction site</td>
<td>4.30E6 m2a</td>
<td>Heat, waste, air, low population density</td>
<td>1.54E+7 MJ</td>
</tr>
<tr>
<td>diesel, burned in building machine, GLO</td>
<td>4.75E+7 MJ</td>
<td>Occupation, industrial area, built up</td>
<td>9.69E+6 m2a</td>
<td>Occupation, industrial area, vegetation</td>
<td>3.21E+6 m2a</td>
</tr>
<tr>
<td>zinc for coating, at regional storage, RER</td>
<td>1.02E+6 kg</td>
<td>Transformation, from unknown</td>
<td>4.30E+5 m2</td>
<td>Transformation, to industrial area, built up</td>
<td>3.22E+5 m2</td>
</tr>
<tr>
<td>nickel, 99.5%, at plant, GLO</td>
<td>3.77E+4 kg</td>
<td>Transformation, to industrial area, vegetation</td>
<td>1.07E+5 m2</td>
<td>Occupation, construction site</td>
<td>4.30E6 m2a</td>
</tr>
<tr>
<td>steel, electric, un- and low-alloyed, at plant, RER</td>
<td>4.69E+6 kg</td>
<td>Heat, waste, air, low population density</td>
<td>1.54E+7 MJ</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Production of methanol

Methanol, at plant, GLO
### Methanol: direct emissions to air (example)

<table>
<thead>
<tr>
<th>Substance</th>
<th>Methanol production process</th>
<th>Values for this inventory</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Steam reforming</td>
<td>Combined reforming</td>
</tr>
<tr>
<td></td>
<td>kg</td>
<td>kg</td>
</tr>
<tr>
<td>CO₂</td>
<td>0.47 *10⁻³</td>
<td>0.31</td>
</tr>
<tr>
<td>NOₓ</td>
<td>0.69 *10⁻³</td>
<td>0.18 *10⁻³, 0.2 *10⁻³</td>
</tr>
<tr>
<td>SOₓ</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.98 *10⁻³</td>
<td>-</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>0.53 *10⁻³</td>
<td>-</td>
</tr>
</tbody>
</table>

### Methanol: cumulated inventory data (selected results)

<table>
<thead>
<tr>
<th>Value</th>
<th>Unit</th>
<th>Methanol, at plant per kg methanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Land occupation</td>
<td>m²</td>
<td>3.0 E-03</td>
</tr>
<tr>
<td>Carbon dioxide, fossil</td>
<td>kg</td>
<td>0.61</td>
</tr>
<tr>
<td>NMVOC</td>
<td>kg</td>
<td>3.3 E-04</td>
</tr>
<tr>
<td>Nitrogen oxides</td>
<td>kg</td>
<td>0.00091</td>
</tr>
<tr>
<td>Sulphur dioxide</td>
<td>kg</td>
<td>6.5 E-04</td>
</tr>
<tr>
<td>Particulates &lt;2.5um</td>
<td>kg</td>
<td>4.4 E-05</td>
</tr>
<tr>
<td>BOD to water</td>
<td>kg</td>
<td>0.00034</td>
</tr>
<tr>
<td>Cadmium to soil</td>
<td>kg</td>
<td>2.6 E-11</td>
</tr>
</tbody>
</table>
Methanol, at regional storage (CH)

- Methanol, at plant, GLO
- Transport, transoceanic tanker, OCE
- Transport, barge tanker, RER
- Transport, freight, rail, RER
- Transport, lorry 28t, CH

Material

Emissions

Emissions, to air CH$_2$OH

methanol, at regional storage, CH

Liquid storage tank, chemicals, organics, RER

Transports

Infrastructure

Methanol, at plant, GLO

0.05

0.24

0.34

3.7

43

0.05

0.05

0.05

0.05

Average distance

0.05

0.05

0.05

0.05

Share for

CH

Overseas

ship

Inland

ship

Rail

Lorry

%   tkm   tkm   tkm   tkm

Continental European production

40   0.05

Norwegian production

13   1.5  0.56  0.05

Overseas production

47   7.5  0.56  0.05

Average distance

100  3.7  0.34  0.24  0.05
Chemicals - 2nd part
Examples for multioutput & weak documented processes

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Reaction Scheme

- **Anode**: chlorine ions are oxidised - chlorine (Cl₂) is formed. The chemical reaction therefore is:
  \[ 2 \text{Cl}^{-(aq)} \rightarrow \text{Cl}_2(g) + 2 \text{e}^- \]

- **Cathode**: While in the diaphragm and membrane cell, water decomposes to form hydrogen (H₂) and hydroxide ions (OH⁻), in the mercury process, a sodium/mercury amalgam (formed at the anode) reacts with water in a decomposer cell (cathode) to form H₂ and OH⁻. All in all, the chemical reaction at the cathode is:
  \[ 2 \text{Na}^{+(aq)} + 2 \text{H}_2\text{O} + 2 \text{e}^- \rightarrow \text{H}_2(g) + 2 \text{Na}^{+(aq)} + 2 \text{OH}^{-(aq)} \]

- **Overall reaction** of the electrolysis of the salt solution:
  \[ 2 \text{Na}^{+(aq)} + 2 \text{Cl}^{-(aq)} + 2 \text{H}_2\text{O} \rightarrow 2 \text{Na}^{+(aq)} + 2 \text{OH}^{-(aq)} + \text{Cl}_2(g) + \text{H}_2(g) \]

Products

- **Chlorine** (Cl₂, CAS-No. 7782-50-5):
  - a greenish-yellow gas with a strong, irritating odor
  - slightly soluble in water

- **Sodium hydroxide** (NaOH, CAS-No. 1310-73-2):
  - white odorless pellet or solid
  - very soluble and often used in water solutions

- **Hydrogen** (H₂, CAS-No. 1333-74-0):
  - colorless, very flammable gas
### System Boundaries

- **Mercury cell electrolysis**
- **Diaphragm cell electrolysis**
- **Membrane cell electrolysis**

Flows:
- Salt brine (NaCl solution)
- Chlorine (Cl₂) - gaseous
- Chlorine (Cl₂) - liquid
- Sodium hydroxide (NaOH)
- Hydrogen (H₂)

Chlorine, liquid, (average)
- Chlorine, gaseous, mercury cell
- Chlorine, gaseous, diaphragm cell

Sodium hydroxide (NaOH)
- Sodium hydroxide, membrane cell
- Sodium hydroxide, mercury cell
- Sodium hydroxide, diaphragm cell

1 kg Chlorine, liquid, at plant (RER)

### Data Sources


Allocation

- **Economic properties**
  - Chlorine and sodium hydroxide are used in very different applications, having therefore very different markets with each one its own dynamic!

- **Energy content**
  - Chlorine and sodium hydroxide are not used as fuels!

- **Mass** (production amount)
  - Different chemicals are produced in fixed amounts due to stoichiometry

⇒ Allocation according to mass (i.e. 46.4% Cl₂, 52.3% NaOH, 1.3% H₂)

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**Input Data**

<table>
<thead>
<tr>
<th>Name</th>
<th>Location</th>
<th>Unit</th>
<th>Economic properties</th>
<th>Energy content</th>
<th>Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water, unspecified natural origin</td>
<td>CH</td>
<td>m³</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Water, unspecified natural origin</td>
<td>CH</td>
<td>m³</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Mercury, liquid, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Iron, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sodium chloride, CaCl₂, at storage, sodium</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sodium hydroxide, 50% in H₂O, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sulphuric acid, liquid, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Barite, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Calcium chloride, CaCl₂, at storage, barite</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hydrochloric acid, 30% in H₂O, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sulphite, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Chemical plant, organics</td>
<td>CH</td>
<td>unit</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Waste disposal, sludge, NaCl electrolysis Hg, 0% water, to residual material landfill CH</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Waste disposal, spent activated carbon with mercury, 0% water, to underground deposit DE</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**Outputs**

<table>
<thead>
<tr>
<th>Name</th>
<th>Location</th>
<th>Unit</th>
<th>Economic properties</th>
<th>Energy content</th>
<th>Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorine, gaseous, mercury cell, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sodium hydroxide, 50% in H₂O, mercury cell, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hydrogen, liquid, mercury cell, at plant</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Air Heat, waste</td>
<td>CH</td>
<td>MJ</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Chlorine</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon dioxide, fossil</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Mercury</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Methane, tetrachloro-, CFC-10</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Chlorate</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Bromate</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Chloride</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Chlorinated solvents, unspecified</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sulfate</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Mercury</td>
<td>CH</td>
<td>kg</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Cumulated Data (LCI)
mercury cell electrolysis

<table>
<thead>
<tr>
<th>Name</th>
<th>Location</th>
<th>Unit Infrastructure</th>
<th>Unit</th>
<th>RER/kg</th>
<th>RER/kg</th>
<th>RER/kg</th>
<th>RER/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>cumulative energy demand</td>
<td>non-renewable (fossil)</td>
<td>MJ-Eq</td>
<td>1.2E+1</td>
<td>1.2E+1</td>
<td>1.2E+1</td>
<td>1.2E+1</td>
<td>1.2E+1</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>non-renewable (nuclear)</td>
<td>MJ-Eq</td>
<td>9.0E+0</td>
<td>9.0E+0</td>
<td>9.0E+0</td>
<td>9.0E+0</td>
<td>9.0E+0</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>renewable (water)</td>
<td>MJ-Eq</td>
<td>1.4E+0</td>
<td>1.4E+0</td>
<td>1.4E+0</td>
<td>1.4E+0</td>
<td>1.4E+0</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>renewable (wind, solar, geothermic)</td>
<td>MJ-Eq</td>
<td>2.3E-1</td>
<td>2.3E-1</td>
<td>2.3E-1</td>
<td>2.3E-1</td>
<td>2.3E-1</td>
</tr>
</tbody>
</table>

-> all substances show equal values (mass allocation !)

Cumulated Data (LCI)
chlorine production of all cell types

<table>
<thead>
<tr>
<th>Name</th>
<th>Location</th>
<th>Unit Infrastructure</th>
<th>Unit</th>
<th>RER/kg</th>
<th>RER/kg</th>
<th>RER/kg</th>
<th>RER/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>cumulative energy demand</td>
<td>non-renewable (fossil)</td>
<td>MJ-Eq</td>
<td>1.2E+1</td>
<td>1.0E+1</td>
<td>9.6E+0</td>
<td>1.1E+1</td>
<td>1.1E+1</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>non-renewable (nuclear)</td>
<td>MJ-Eq</td>
<td>9.0E+0</td>
<td>7.7E+0</td>
<td>7.4E+0</td>
<td>8.7E+0</td>
<td>8.7E+0</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>renewable (water)</td>
<td>MJ-Eq</td>
<td>1.4E+0</td>
<td>1.2E+0</td>
<td>1.1E+0</td>
<td>1.3E+0</td>
<td>1.3E+0</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>renewable (wind, solar, geothermic)</td>
<td>MJ-Eq</td>
<td>2.3E-1</td>
<td>2.0E-1</td>
<td>1.9E-1</td>
<td>2.2E-1</td>
<td>2.2E-1</td>
</tr>
</tbody>
</table>

-> small differences between different types
-> mercury cell seems to have higher impact than other cell types
Cumulated Data (LCIA) / II
chlorine (mercury cell electrolysis)

*Cumulative Data (LCIA) / II*

- Direct emissions
- Waste
- Transports
- Infrastructure
- Energy
- Mercury (for cells)
- Auxillaries
- Raw material

**Conclusion Multioutput Example**

- Database contains *allocated unit processes*, based on the chosen allocation factors (standard data)

- Database contains *unallocated process* on a unit process basis
  - Total input / output numbers can be identified
  - Allocation factors for each number are clearly defined
  - Allocation factors can be changed for own purposes

- Database offers (i) **maximum flexibility** for user of data AND (ii) **clearly defined** standard data
Example of an Estimated Process: Propylene glycol (RER)

- HOCH₂CH(CH₃)OH, CAS-No. 57-55-6
- Clear, odorless liquid at room temperature
- Raw material for production of unsaturated polyester resins - used in automotive plastics, fiberglass boats, construction area
- Production by direct hydrolysis of propylene oxide and water with subsequent distillation
- Data sources: Ullmann’s Encyclopedia, Well’s handbook, EMAS declaration of a German “Chemiepark”

Establishing Unit Process Data

1. Reaction equation according to Ullmann’s:

   \[ \text{CH}_2\text{OC(CH}_3\text{)H} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{CH(CH}_3\text{)OH} \]

2. Assumptions for Input / Output - Data:
   - Energy & water consumption: data from chemical plant (D)
   - Raw materials: stoechiometry & yield = 95%
   - Emissions: Assumption (air) r.s.p. mass balance (water)
   - Waste water treatment: efficiency/distribution from ESU’96
   - Infrastructure / transport: standard approach of ecoinvent
   - waste: not taken into account
Input Data

[per kg propylene glycol]

<table>
<thead>
<tr>
<th>INPUTS</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene oxide</td>
<td>kg 0.803 stoechiometric calc., 95% yield</td>
</tr>
<tr>
<td>Water, unspecified</td>
<td>m³ 2.49E-04 stoechiometric calc., 95% yield</td>
</tr>
<tr>
<td>Electricity, medium voltage</td>
<td>kWh 0.333 estimation</td>
</tr>
<tr>
<td>Natural gas, burned in industrial furnace &gt;100kW</td>
<td>MJ 2 estimation</td>
</tr>
<tr>
<td>Water, cooling, unspecified</td>
<td>m³ 2.40E-02 estimation</td>
</tr>
<tr>
<td>Transport, by train</td>
<td>ftm 4.82E-01 standard distances &amp; means</td>
</tr>
<tr>
<td>Transport, by lorry</td>
<td>ftm 8.03E-02 standard distances &amp; means</td>
</tr>
<tr>
<td>chemical plant, organics</td>
<td>unit 4.00E-10 approximation for infrastructure</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>OUTPUTS</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>waste heat, to air</td>
<td>MJ 1.20E+00 calculated from electricity input</td>
</tr>
<tr>
<td>propylene oxide, to air</td>
<td>kg 1.60E-03 estimated as 0.2% of input</td>
</tr>
<tr>
<td>carbon dioxide, fossil, to air</td>
<td>kg 7.88E-02 from waste water treatment</td>
</tr>
<tr>
<td>propylene oxide, to water</td>
<td>kg 3.85E-03 calculated from mass balance</td>
</tr>
<tr>
<td>COD, BOD</td>
<td>kg 5.91E-02 calculated from water emissions</td>
</tr>
<tr>
<td>TOC, DOC</td>
<td>kg 1.85E-02 calculated from water emissions</td>
</tr>
</tbody>
</table>

Cumulated Data (LCI)

<table>
<thead>
<tr>
<th>Name</th>
<th>propylene glycol, liquid, at plant</th>
<th>propylene oxide, liquid, at plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene glycol, liquid, at plant</td>
<td>RER</td>
<td>RER</td>
</tr>
<tr>
<td>propylene oxide, liquid, at plant</td>
<td>kg</td>
<td>kg</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Name</th>
<th>Land occupation</th>
<th>air Carbon dioxide, fossil</th>
<th>air Nitrogen oxides</th>
<th>air Sulphur dioxide</th>
<th>air Particulates, &lt; 2.5 μm</th>
<th>water BOD</th>
<th>soil Cadmium</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resource</td>
<td>m²a</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
<td>kg</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>MJ-Eq</td>
<td>7.6E+1</td>
<td>8.6E+1</td>
<td>2.6E+1</td>
<td>3.6E+0</td>
<td>8.6E+1</td>
<td>8.6E-2</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>MJ-Eq</td>
<td>3.6E+1</td>
<td>3.6E+1</td>
<td>3.6E+1</td>
<td>3.6E+1</td>
<td>5.6E+1</td>
<td>6.6E-1</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>MJ-Eq</td>
<td>5.6E+1</td>
<td>6.6E-1</td>
<td>5.6E+1</td>
<td>6.6E-1</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
</tr>
<tr>
<td>cumulative energy demand</td>
<td>MJ-Eq</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
<td>9.6E-1</td>
</tr>
</tbody>
</table>
Conclusion Estimated Process

- Substance is reported on a **unit process** base
- **Best data** for **raw material inputs**, as based on the reaction scheme according to stoechiometry
- **Major concerns** with the input rsp. output values in the area of **energy, emissions** (air / water), **waste**
- Data can only be used, when **dataset** doesn't represent a **central element** of the respective study