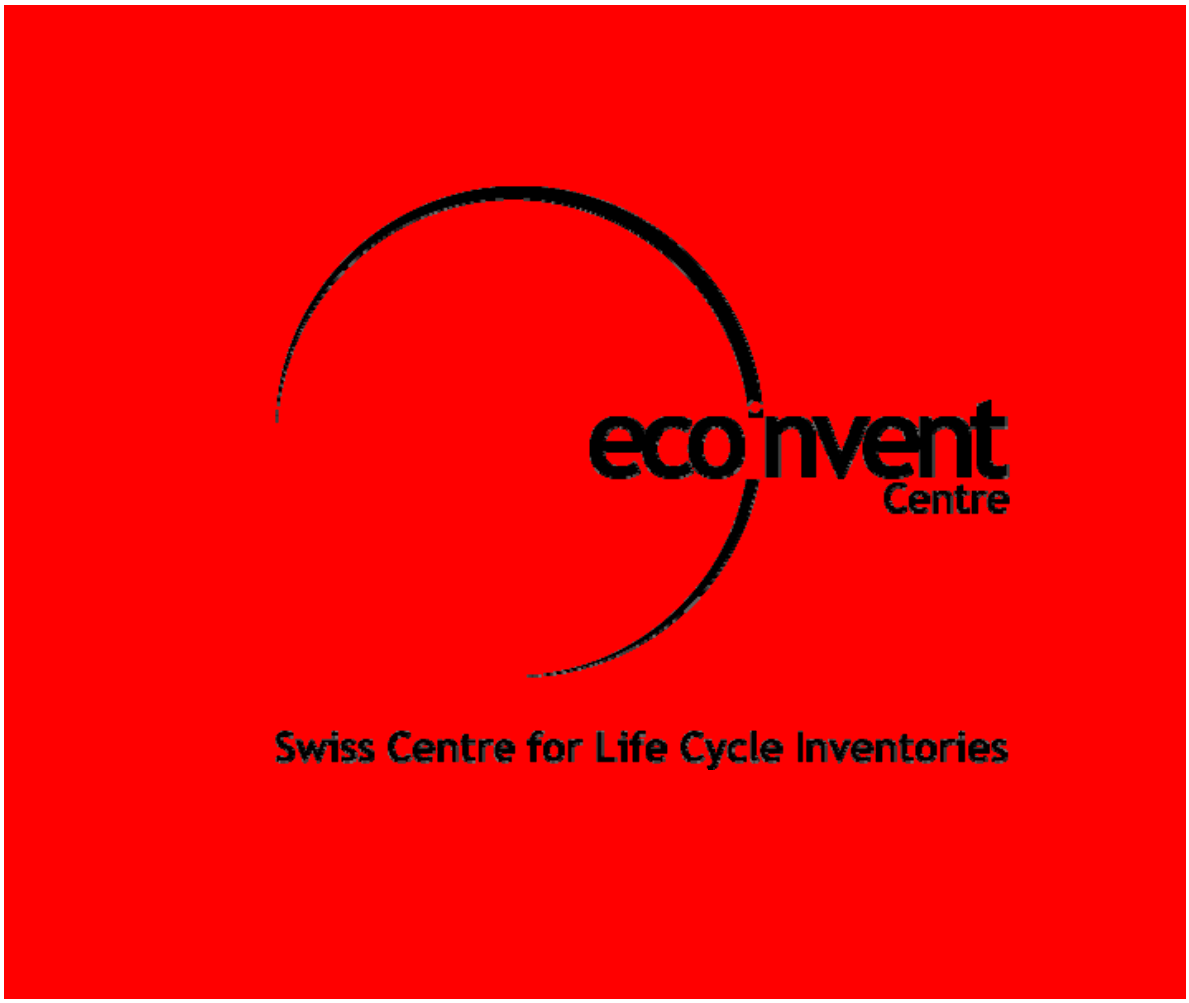

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ETH
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2nd International ecoinvent Meeting
Lausanne, March 14, 2008

eco'nvent Centre

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

Gregor Wernet, Jürgen Sutter, ecoinvent Centre

New ecoinvent data v2.0

- Two projects:
  - petrochemical solvents
  - highly pure chemicals
- Detailed information on project goals, contents, dataset quality
- Examples of data generation

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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

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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

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List of the 50 solvents

Aliphatic Hydrocarbons
- Pentane
- Hexane
- Isohexane
- Heptane

Alicyclic Hydrocarbons
- Cyclohexane
- Methyl cyclohexane

Aromatic Hydrocarbons
- Ethyl benzene
- Toluene
- Xylene

Chlorinated Hydrocarbons
- Chlorobenzene
- Methylene chloride

Aldehydes
- Benzaldehyde
- Formaldehyde
- Propionaldehyde

Alcohols
- Benzyl alcohol
- 1-Butanol
- 2-Butanol
- Isobutanol
- Butylene glycol
- Ethanol
- Methanol
- Pentanol
- 2-Methyl-2-butanol
- Isoamyl alcohol
- 1-Propanol
- Isopropanol

Acids
- Formic acid
- Acetic acid

Ketones
- Acetone
- Cyclohexanone
- Methyl ethyl ketone
- Methyl isobutyl ketone

Esters
- Methyl formiate
- Butyl acetate
- Ethyl acetate
- Isobutyl acetate
- Isopropyl acetate
- Isoamyl acetate
- Methyl acetate

Ethers and glycolethers
- Diethyl ether
- Dioxane
- Ethylene glycol dimethyl ether
- Ethylene glycol monoethyl ether
- Ethylene glycol diethyl ether
- Methyl-tert-butyl ether
- Tetrahydrofuran

Amides and other N-compounds
- Acetonitrile
- N,N-Dimethylformamide

Other solvents
- Dimethylsulfoxide
- Acetic anhydride
- N-Methyl-2-pyrrolidone

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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 pyrolisis gasoline are separated.

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Solvent Production Routes

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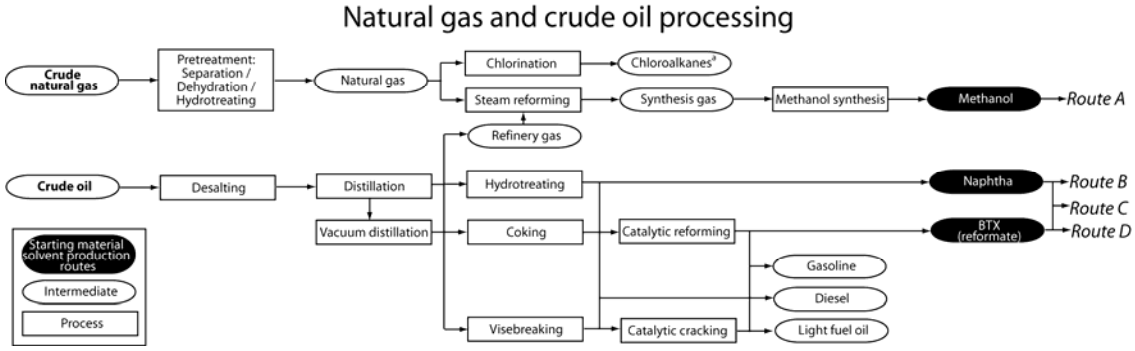

The Methanol route

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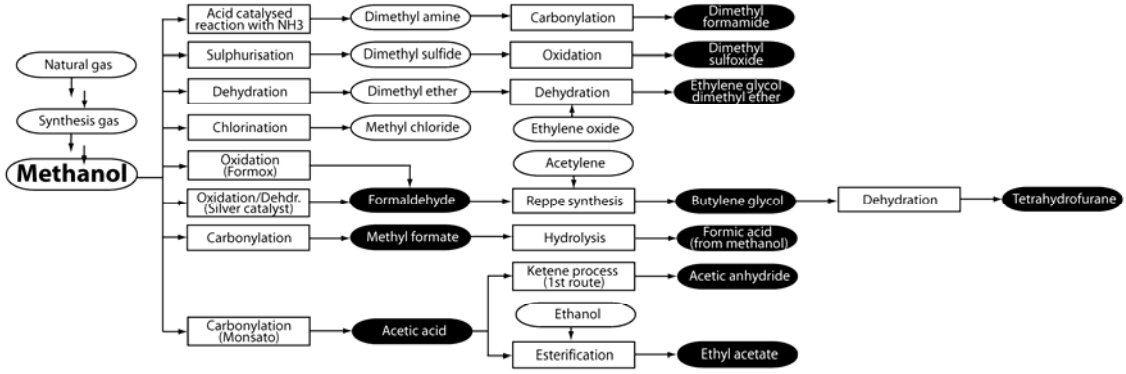

The Methanol route: CED

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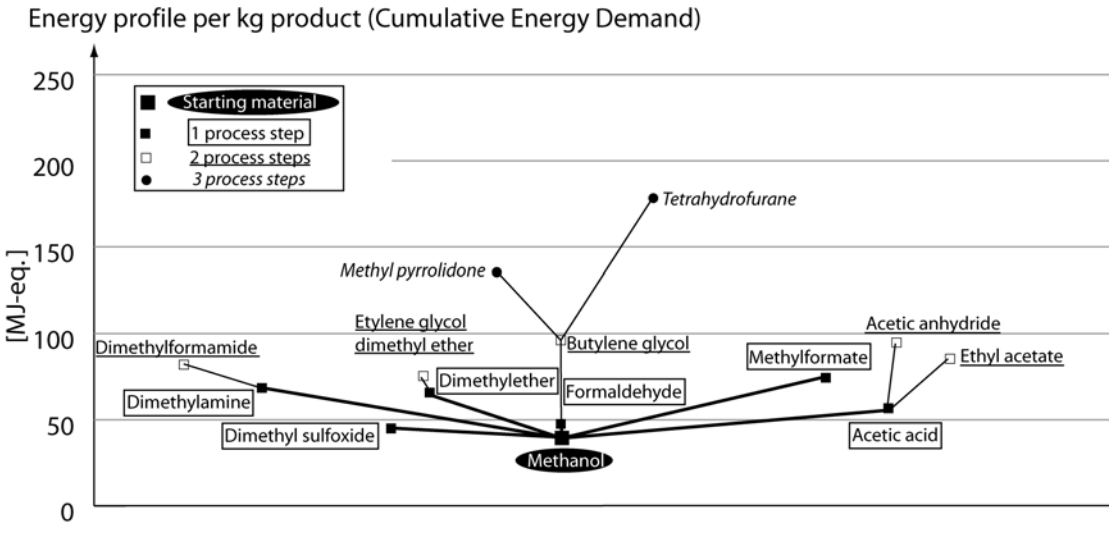
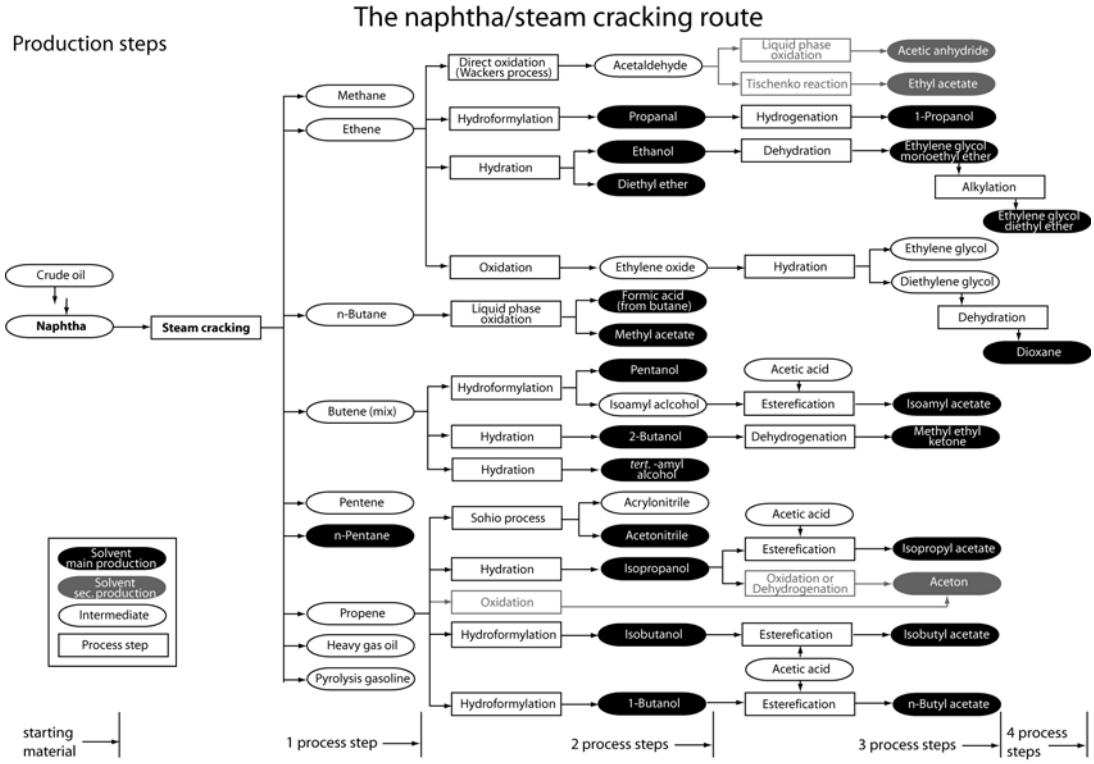


The Naphta/steam cracking route



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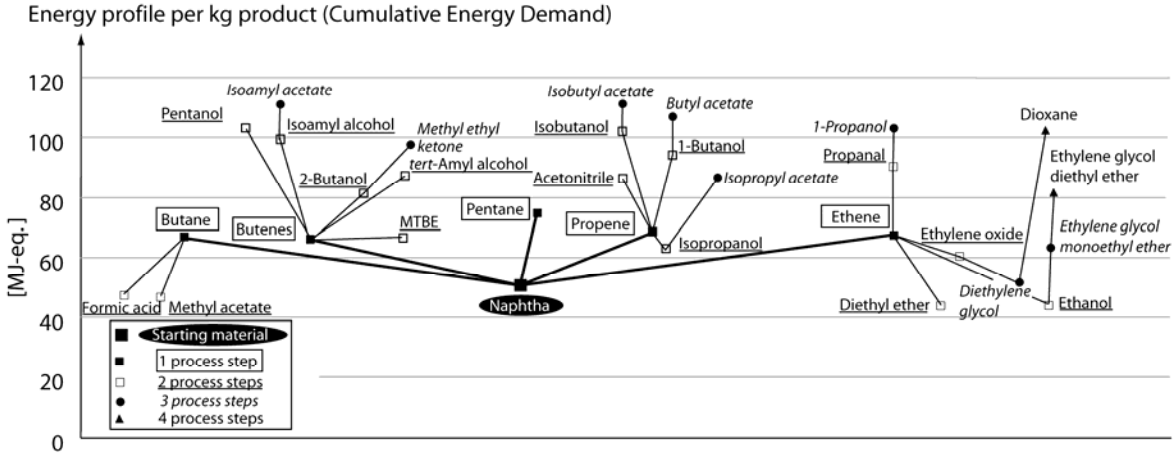
The Naphta/steam cracking route



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The BTX/ Naphta separation route

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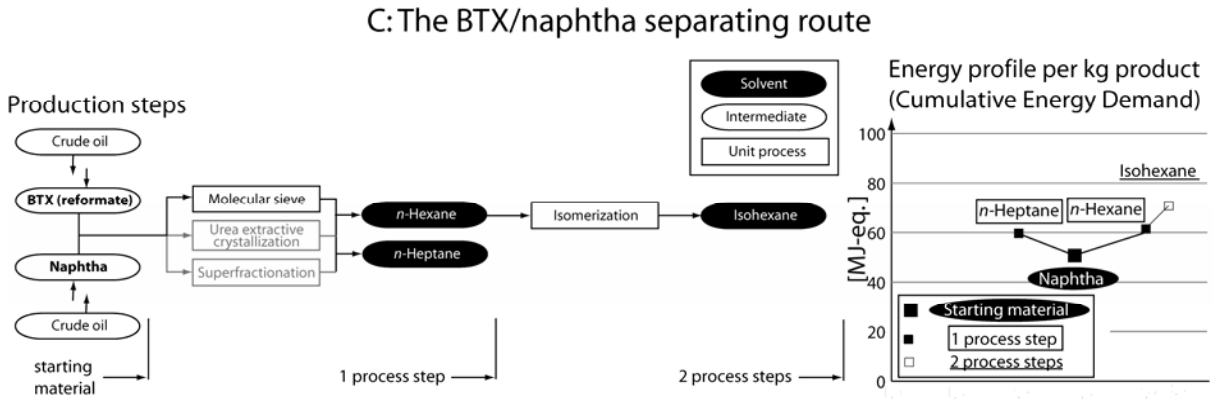

The BTX splitting route

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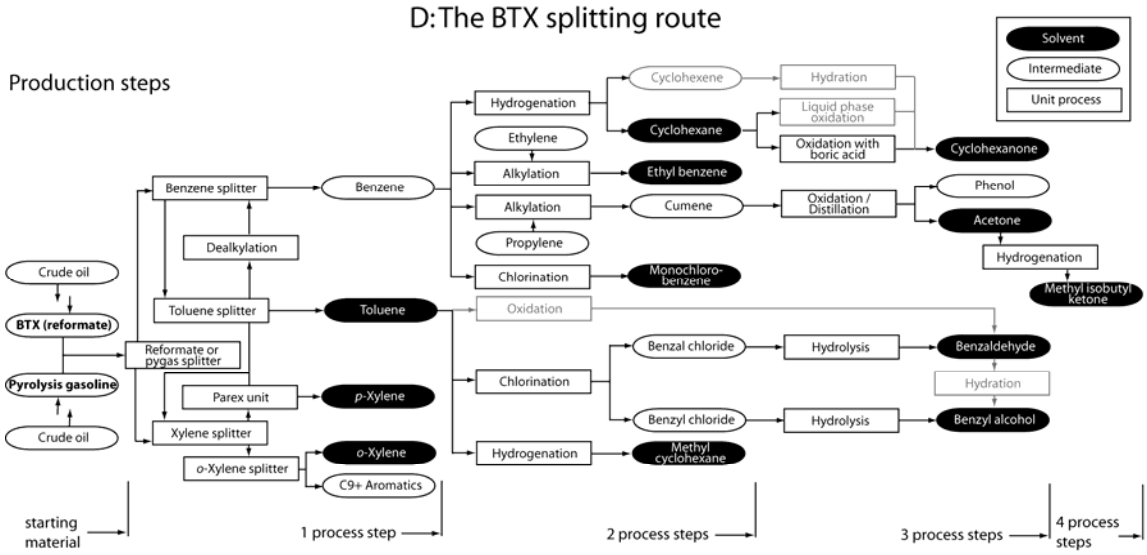

The BTX splitting route

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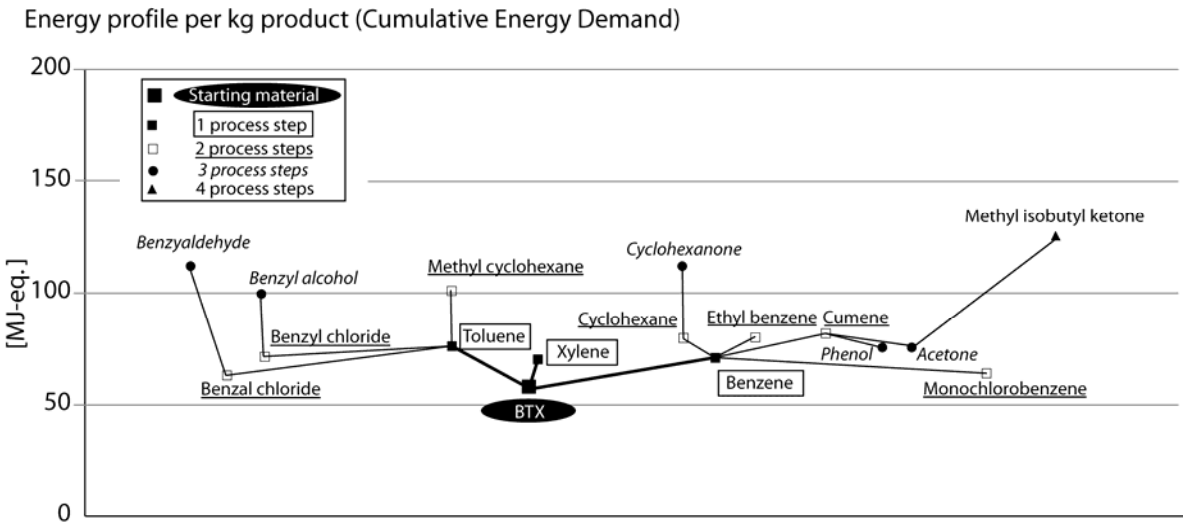

New Inventories in ecoinvent 2.0

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- 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

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A joint initiative of the ETH domain and Swiss Federal Offices

- 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

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- 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

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

Example: Acetates

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- Ethyl acetate (esterification of ethanol and acetic acid)
  - Ethanol + acetic acid → 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

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- 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

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A joint initiative of the ETH domain and Swiss Federal Offices

- *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

metals
- Lithium

organics
- Alcohol ethoxylate
- Alkyl oxylated salts
- Amino-2-ethanol
- Butyl acetate
- Cellulose acetate
- Diacetone alcohol
- Dibutyl phtalate
- Dimethyl acetamide
- Dimethylamine borane
- Ethanol
- Ethyl acetate
- Ethyl cellulose
- 4-Fluoro-1,3-dioxolan-2-one
- Fluoroform
- Hexafluoroethane
- Hexamethyldisilazane
- Hydroxyl monoethanolamine
- Lactic acid
- Methanesulfonic acid
- Methoxy propanol
- Methyl-3-methoxypropionate
- M-Pyrrol
- N-Methyl Pyrrolidone
- Polyacetal
- Polyglycol mixture
- Polyphenyl oxide
- Polyvinyl pyrrolidone
- Polyvinyl sulfide
- Rosin
- Rosin, modified
- Tetramethyl ammonium hydroxide

inorganics
- Ammonium chloride
- Arsine
- Carbonic acid
- Chloride as ion
- Diborane
- Dinitrogen 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
- Glas cleaner
- Solder leveller (HAZL)

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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"*

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Data Sources (cf. Solvent Project)

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- 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)

Example: Water, ultrapure

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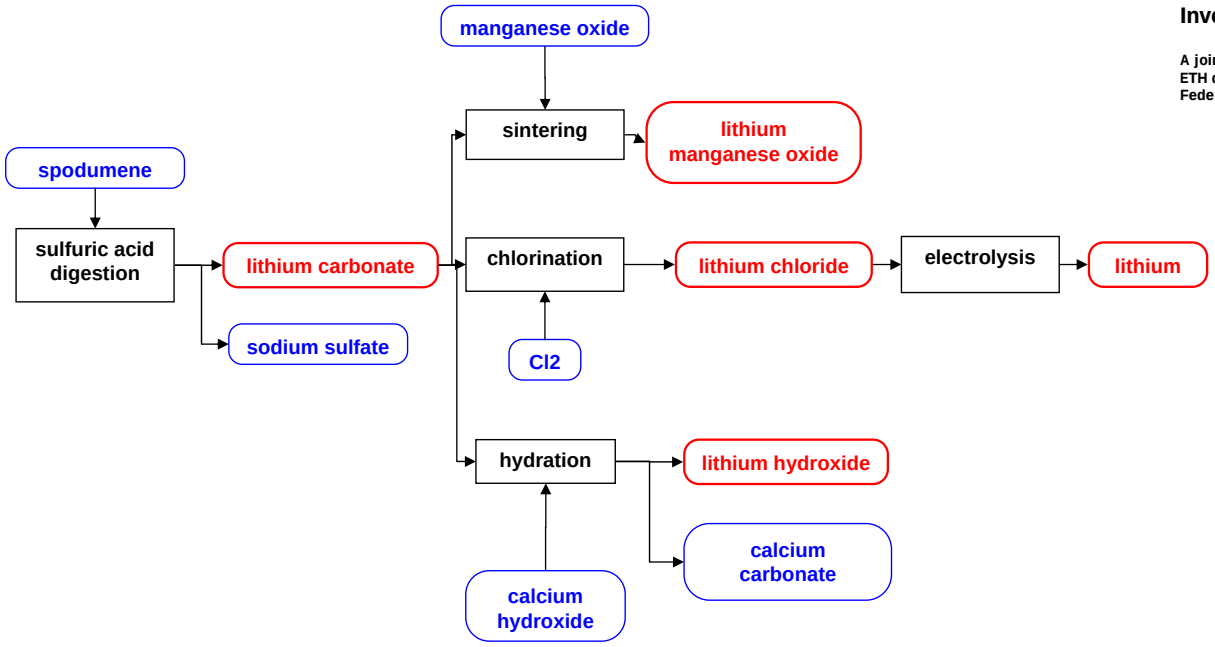
- Purification steps:
  - tap water → water, decarbonised → water, ultrapure
- Purification:
- ion exchangers (resins), membranes, electrodeionization
- Dataset is calculated with literature data for electrodeionization

Example: Lithium route



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Example: Lithium route

- **Lithium** (electrolysis of lithium chloride): data from literature (Wietelmann 2000)
- **Lithium carbonate** (acid digestion of spondumene): data from literature (Wietelmann 2000, Kim 2003)
- **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

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Example:Ammonium thiocyanate

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- $CS_2 + 2NH_3 \rightarrow NH_4SCN$
- 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

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References:

- *Sutter, J. (2007): Life Cycle Inventories of Petrochemical Solvents. Final report, ESU-services, Uster, CH*
- *Sutter, J. (2007): Life Cycle Inventories of Highly Pure Chemicals. Final report, ESU-services, Uster, CH*
- *Hischier, R, Hellweg, S, Capello, C, and Primas, A: 2004. Establishing Life Cycle Inventories of Chemicals Based on Differing Data Availability. International Journal of LCA. 10. (1). 59-67.*

Example: Chlorobenzene

input	Chlorination of benzene	kg per kg monochlorobenzene
raw materials	Benzene (kg)	9.5
	Chlorine (kg)	0.796
	Sodium hydroxide (kg)	0.225
auxilliaries	Process water (kg)	0.9047
	Cooling water (kg)	27.315
energy	Steam (MJ)	1.201
	Electricity (kWh)	0.0478
Output		
emissions to air	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

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Approximations

Highly pure chemical **used ecoinvent DS**

- 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

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