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chemicals

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Bundesämter

Special LCA forum, December 5, 2003
ETH Lausanne / Session „Chemicals"

Chemicals

Part I

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Statistics: Chemicals in ecoinvent

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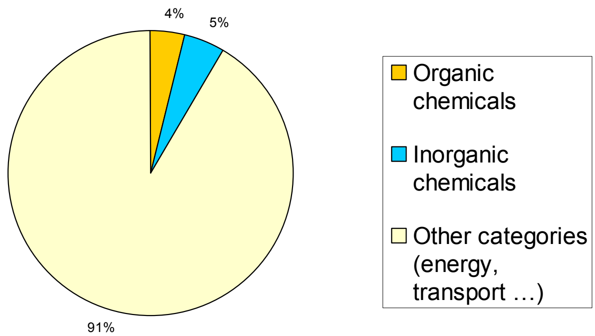

Further chemicals are contained in other categories such as detergants, plastics, etc.

Chemicals in ecoinvent

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- **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

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- Acetone
- Acetic acid
- Formaldehyde
- **Isopropanol**
- **Methanol**
- Methylchloride
- **Toluene**
- Xylene
- Aniline
- Benzene
- Methyldichloride
- Methylethylketone
- Methyl tert-butyl ether
- Nitrobenzene
- Tetrachloroetylene

➡ 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

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- Chemical formula: CH_3OH
- 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

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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)

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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)

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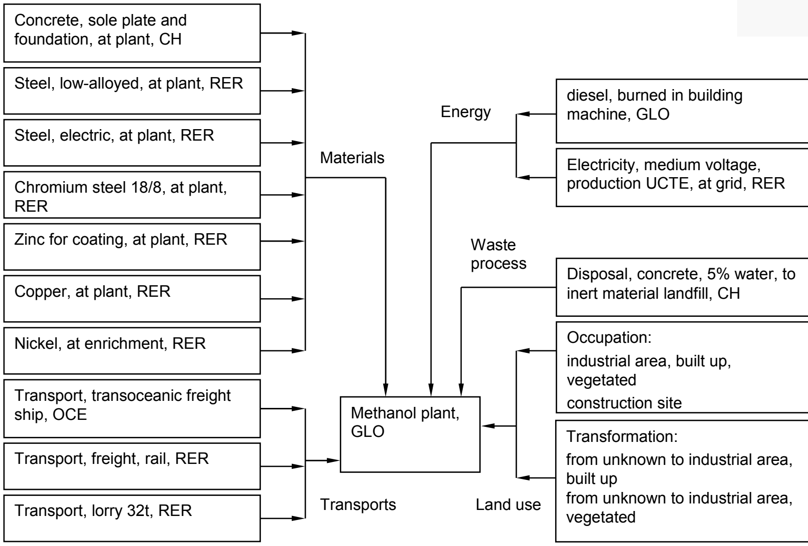

Methanol plant (GLO): raw data

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Technos-phere	electricity, medium voltage, production UCTE, at grid, UCTE	5.66E+6	kWh
	diesel, burned in building machine, GLO	4.75E+7	MJ
	zinc for coating, at regional storage, RER	1.02E+6	kg
	nickel, 99.5%, at plant, GLO	3.77E+4	kg
	steel, electric, un- and low-alloyed, at plant, RER	4.68E+6	kg
	steel, low-alloyed, at plant, RER	1.99E+6	kg
	chromium steel 18/8, at plant, RER	1.72E+6	kg
	copper, at regional storage, RER	4.30E+5	kg
	concrete, sole plate and foundation, at plant, CH	4.89E+2	m3
	disposal, concrete, 5% water, to inert material landfill, CH	1.13E+6	kg
	transport, lorry 32t, RER	7.38E+6	tkm
	transport, transoceanic freight ship, OCE	5.41E+6	tkm
	transport, freight, rail, RER	1.44E+6	tkm
Ressources	Occupation, construction site	4.30E+6	m2a
	Occupation, industrial area, built up	9.69E+6	m2a
	Occupation, industrial area, vegetation	3.21E+6	m2a
	Transformation, from unknown	4.30E+5	m2
	Transformation, to industrial area, built up	3.23E+5	m2
	Transformation, to industrial area, vegetation	1.07E+5	m2
Emissionen	Heat, waste, air, low population density	1.54E+7	MJ

Production of methanol

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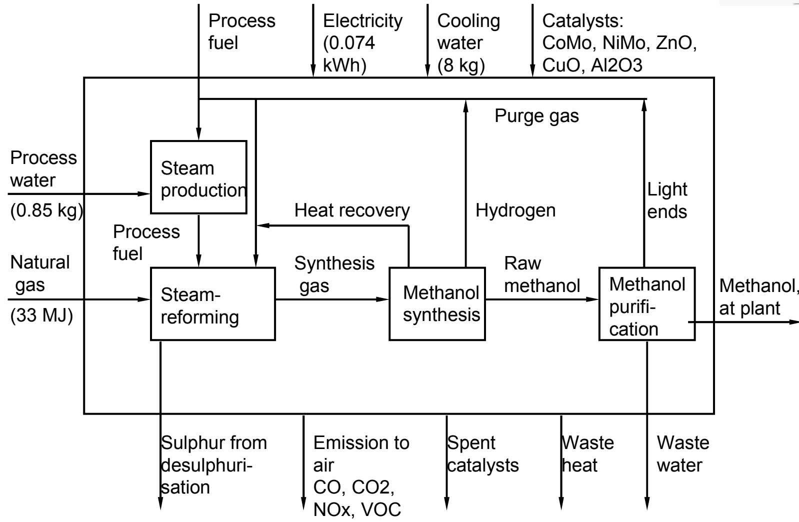

Methanol, at plant, GLO

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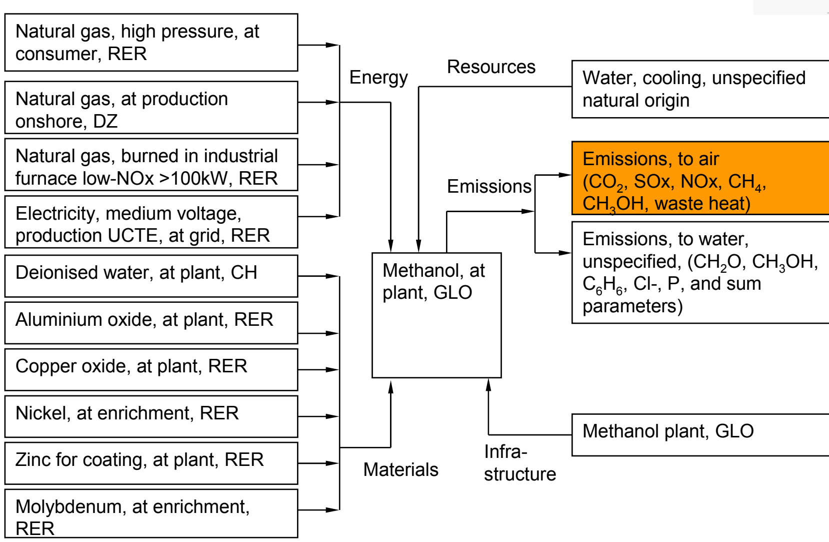

Methanol: direct emissions to air (example)

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Sub-stance	Methanol production process			Values for this inventory	
	Steam reforming	Combined reforming	Autothermal reforming	Included in furnace process	Additional emissions
	kg	kg	kg	kg	kg
CO_2	0.47 -	0.31	0.33	0.431	-
NOx	0.69 *10^{-3} -	0.18 *10^{-3}, 0.2 *10^{-3}	0.05 *10^{-3}, 0.1 *10^{-3}	0.18 *10^{-3}	0.15 *10^{-3}
SOx	-	-	-	4.2 *10^{-6}	13.8 *10^{-6}
CH_4	0.98 *10^{-3}			-	0.98 *10^{-3}
CH_3OH	0.53 *10^{-3}	-	-	-	0.53 *10^{-3}

Methanol: cumulated inventory data (selected results)

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		Methanol, at plant
Value	Unit	per kg methanol
Land occupation	m^2a	3.0 E-03
Carbon dioxide, fossil	kg	0.61
NMVOC	kg	3.3 E-04
Nitrogen oxides	kg	0.00091
Sulphur dioxide	kg	6.5 E-04
Particulates <2.5um	kg	4.4 E-05
BOD to water	kg	0.00034
Cadmium to soil	kg	2.6 E-11

Methanol, at regional storage (CH)

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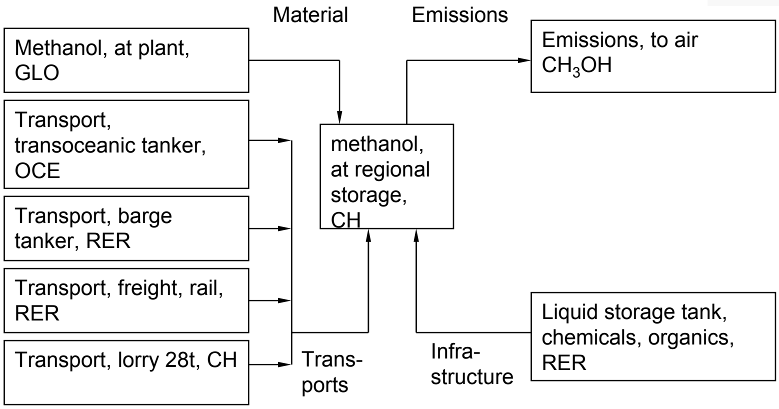

Präsentation Roland Hischier

Methanol, at regional storage (CH)

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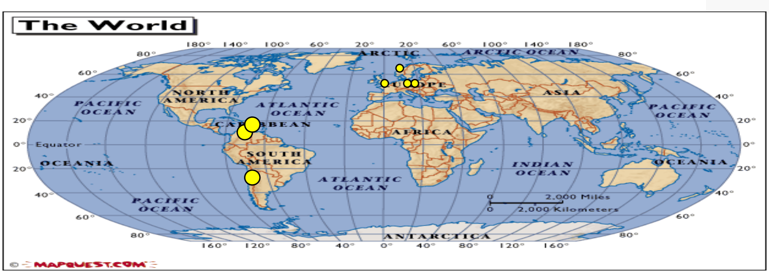

Location of Plant / Vehicle	Share for CH	Overseas ship	Inland ship	Rail	Lorry
	%	tkm	tkm	tkm	tkm
Continental European production	40	0	0	0.6	0.05
Norwegian production	13	1.5	0.56	0	0.05
Overseas production	47	7.5	0.56	0	0.05
Average distance	**100**	**3.7**	**0.34**	**0.24**	**0.05**

Präsentation Roland Hischier

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EPF Lausanne / Session „Chemicals“

Chemicals - 2nd part

Examples for multioutput & weak documented processes

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Example of a Multioutput Process:

Chlorine electrolysis (RER)

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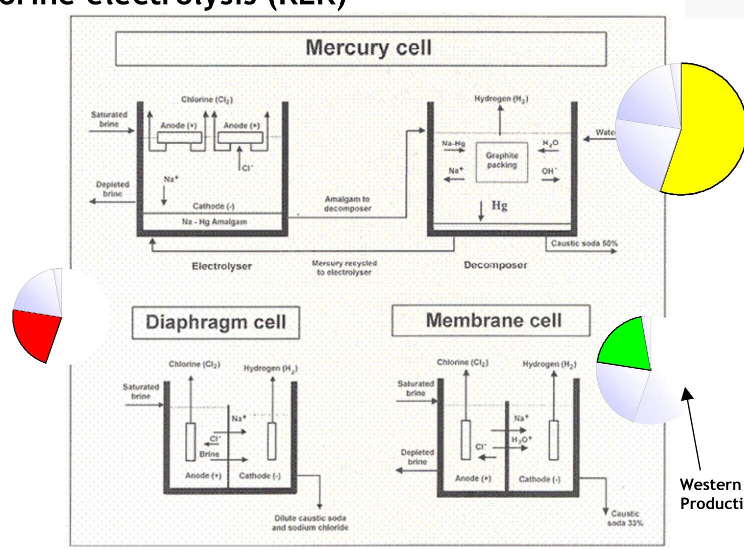

Western European Chlorine Production Capacity (2000)

Reaction Scheme

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- **Anode**: chlorine ions are oxidised - chlorine (Cl_2) is formed. The chemical reaction therefore is:

$$2\ Cl^-(aq) \rightarrow Cl_2(g) + 2\ e^-$$

- **Cathode**: While in the diaphragm and membrane cell, water decomposes to form hydrogen (H_2) 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 H_2 and OH^-. All in all, the chemical reaction at the cathode is:

$$2\ Na^+(aq) + 2\ H_2O + 2\ e^- \rightarrow H_2(g) + 2\ Na^+(aq) + 2\ OH^-(aq)$$

- **Overall reaction** of the electrolysis of the salt solution:

$$2\ Na^+(aq) + 2\ Cl^-(aq) + 2\ H_2O \rightarrow 2\ Na^+(aq) + 2\ OH^-(aq) + Cl_2(g) + H_2(g)$$

Products

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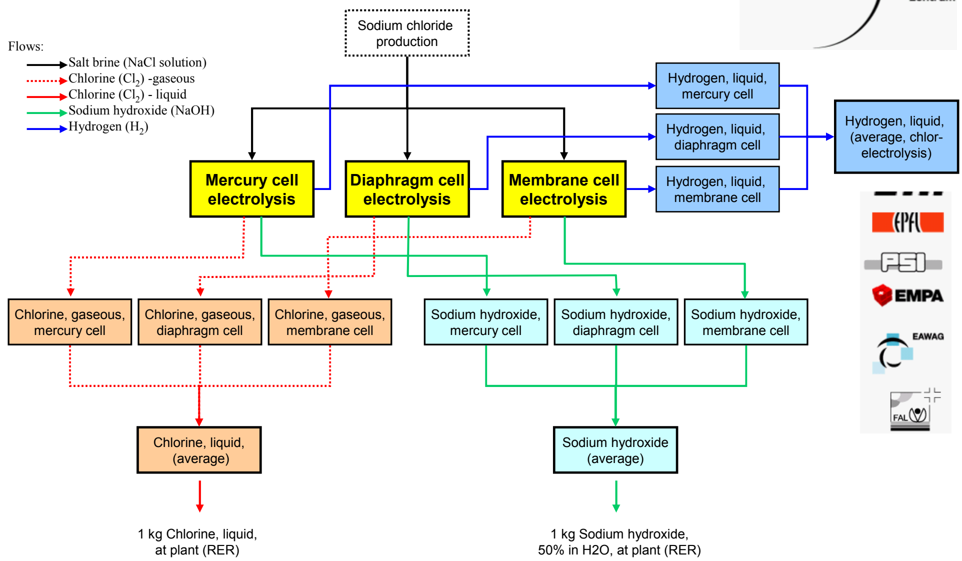
- Chlorine (Cl_2, CAS-No. 7782-50-5):
  - a greenish-yellow gas with a strong, irritating odor
  - slightly soluble in water
- Sodium hydroxide (NaOH, CAS-No. 1310-73-2):
  - white odorless pellet or solid
  - very soluble and often used in water solutions
- Hydrogen (H2, CAS-No. 1333-74-0):
  - colorless, very flammable gas

System Boundaries



Data Sources

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- European Commission (2000) Integrated Pollution Prevention and Control (IPPC) - Reference Document on Best Available Techniques in the Chlor-Alkali Manufacturing Industry. Institute for Prospective Technological Studies, Sevilla
- Ayres R. (1997) The Life-Cycle of Chorine, Part I: Chlorine Production and the Chlorine-Mercury Connection. In: Journal of Industrial Ecology, 1(1), pp. 81 - 94.
- Landbank (1994) The Phosphate Report - A life cycle study to evaluate the envi-ronmental impact of phosphates and zeolite A-PCA as alternative builders in UK laundry detergent formulations. Landbank Environmental Research and Consult-ing, London.

Allocation

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- **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 stoechiometry

⇒ Allocation according to **mass** (i.e. 46.4% Cl_2, 52.3% NaOH, 1.3% H_2)

Input Data

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		Name	Location	Unit	Mercury cell	ALLOKATION FACORS		
						Cl2	NaOH	H2
		Unit			kg	kg	kg	kg
Inputs	Ressource	Water, unspecified natural origin		m3	1.90E-03	46.4	52.3	1.3
		Water, cooling, unspecified natural origin		m3	1.00E-01	46.4	52.3	1.3
	from Techno-sphere	sodium chloride, powder, at plant	RER	kg	1.75E+00	46.4	52.3	1.3
		mercury, liquid, at plant	GLO	kg	6.75E-06	46.4	52.3	1.3
		soda, powder, at plant	RER	kg	1.15E-02	46.4	52.3	1.3
		barite, at plant	RER	kg	3.50E-03	46.4	52.3	1.3
		calcium chloride, CaCl2, at regional storage	CH	kg	1.78E-02	46.4	52.3	1.3
		hydrochloric acid, 30% in H2O, at plant	RER	kg	2.50E-02	46.4	52.3	1.3
		sulphite, at plant	RER	kg	1.00E-04	46.4	52.3	1.3
		sodium hydroxide, 50% in H2O, production mix, at plant	RER	kg	6.00E-03	46.4	52.3	1.3
		sulphuric acid, liquid, at plant	RER	kg	8.62E-03	100	0	0
		carbon tetrachloride, at plant	RER	kg	1.00E-05	100	0	0
		electricity, medium voltage, production UCTE, at grid	UCTE	kWh	3.56E+00	46.4	52.3	1.3
		transport, lorry 32t	RER	tkm	1.89E-01	46.4	52.3	1.3
		transport, freight, rail	RER	tkm	1.40E-02	46.4	52.3	1.3
		chemical plant, organics	RER	unit	4.00E-10	46.4	52.3	1.3
	Waste	disposal, sludge, NaCl electrolysis Hg, 0% water, to residual material landfill	CH	kg	1.53E-02	46.4	52.3	1.3
		disposal, spent activated carbon with mercury, 0% water, to underground deposit	DE	kg	2.90E-04	46.4	52.3	1.3
Outputs	Products	chlorine, gaseous, mercury cell, at plant	RER	kg	1	100	0	0
		sodium hydroxide, 50% in H2O, mercury cell, at plant	RER	kg	1.128	0	100	0
		hydrogen, liquid, mercury cell, at plant	RER	kg	0.028	0	0	100
	Air emissions	Heat, waste		MJ	1.28E+01	46.4	52.3	1.3
		Hydrogen		kg	5.50E-04	46.4	52.3	1.3
		Chlorine		kg	8.00E-06	46.4	52.3	1.3
		Carbon dioxide, fossil		kg	3.10E-03	46.4	52.3	1.3
		Mercury		kg	1.15E-06	46.4	52.3	1.3
		Methane, tetrachloro-, CFC-10		kg	2.25E-06	100	0	0
	Water emissions	Chlorate		kg	2.10E-03	46.4	52.3	1.3
		Bromate		kg	2.75E-04	46.4	52.3	1.3
		Chloride		kg	1.50E-02	46.4	52.3	1.3
		Chlorinated solvents, unspecified		kg	6.00E-07	46.4	52.3	1.3
		Sulfate		kg	7.90E-03	46.4	52.3	1.3
		Mercury		kg	3.30E-07	46.4	52.3	1.3

Cumulated Data (LCI)
mercury cell electrolysis

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		Name	Unit	chlorine, gaseous, mercury cell, at plant	sodium hydroxide, 50% in H2O, mercury cell, at plant	hydrogen, liquid, mercury cell, at plant
		Location		RER	RER	RER
		Unit	Unit	kg	kg	kg
		Infrastructure		0	0	0
LCIA results						
	cumulative energy demand	non-renewable (fossil)	MJ-Eq	1.2E+1	1.2E+1	1.2E+1
	cumulative energy demand	non-renewable (nuclear)	MJ-Eq	9.0E+0	9.0E+0	9.0E+0
	cumulative energy demand	renewable (water)	MJ-Eq	1.4E+0	1.4E+0	1.4E+0
	cumulative energy demand	renewable (wind, solar, geothermic)	MJ-Eq	2.3E-1	2.3E-1	2.3E-1
	cumulative energy demand	renewable (biomass)	MJ-Eq	1.7E-1	1.7E-1	1.7E-1
LCI results						
resource	Land occupation	total	m2a	2.8E-2	2.8E-2	2.8E-2
air	Carbon dioxide, fossil	total	kg	9.3E-1	9.2E-1	9.3E-1
air	NMVOC	total	kg	2.6E-4	2.6E-4	2.6E-4
air	Nitrogen oxides	total	kg	1.9E-3	1.9E-3	1.9E-3
air	Sulphur dioxide	total	kg	3.7E-3	3.6E-3	3.6E-3
air	Particulates, < 2.5 um	total	kg	3.0E-4	3.0E-4	3.0E-4
water	BOD	total	kg	7.4E-4	7.4E-4	7.4E-4
soil	Cadmium	total	kg	1.3E-9	1.3E-9	1.3E-9

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

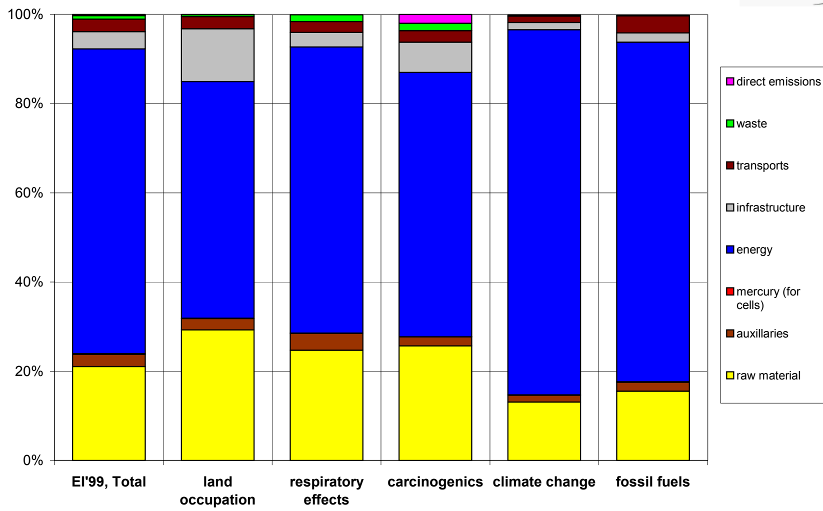
Cumulated Data (LCI)
chlorine production of all cell types

		Name	Unit	gaseous (mercury cell)	gaseous (diaphragma cell)	gaseous (membrane cell)	liquid (production mix)
		Location		RER	RER	RER	RER
		Unit	Unit	kg	kg	kg	kg
		Infrastructure		0	0	0	0
LCIA results							
	cumulative energy demand	non-renewable (fossil)	MJ-Eq	1.2E+1	1.0E+1	9.9E+0	1.1E+1
	cumulative energy demand	non-renewable (nuclear)	MJ-Eq	9.0E+0	7.7E+0	7.4E+0	8.7E+0
	cumulative energy demand	renewable (water)	MJ-Eq	1.4E+0	1.2E+0	1.1E+0	1.3E+0
	cumulative energy demand	renewable (wind, solar, geothermic)	MJ-Eq	2.3E-1	2.0E-1	1.9E-1	2.2E-1
	cumulative energy demand	renewable (biomass)	MJ-Eq	1.7E-1	1.5E-1	1.4E-1	1.6E-1
LCI results							
resource	Land occupation	total	m2a	2.8E-2	2.6E-2	2.5E-2	2.8E-2
air	Carbon dioxide, fossil	total	kg	9.3E-1	8.0E-1	7.8E-1	9.0E-1
air	NMVOC	total	kg	2.6E-4	2.3E-4	2.4E-4	2.6E-4
air	Nitrogen oxides	total	kg	1.9E-3	1.7E-3	1.7E-3	1.9E-3
air	Sulphur dioxide	total	kg	3.7E-3	3.2E-3	3.1E-3	3.6E-3
air	Particulates, < 2.5 um	total	kg	3.0E-4	2.7E-4	2.6E-4	2.9E-4
water	BOD	total	kg	7.4E-4	6.7E-4	6.8E-4	7.3E-4
soil	Cadmium	total	kg	1.3E-9	1.2E-9	1.3E-9	1.3E-9

-> small differences between different types
-> mercury cell seems to have higher impact than other cell types

Cumulated Data (LCIA) / II

chlorine (mercury cell electrolysis)



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Conclusion Multioutput Example

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- Database contains **allocated unit processes**, based on the choosen 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)

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- $HOCH_2CH(CH_3)OH$, CAS-No. 57-55-6
- Clear, odorless liquid at room temperature
- Raw material for production of unsaturated polyester resins – used in automotive plastics, fibreglass 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

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1. Reaction equation according to Ullmann's :

$$CH_2OC(CH_3)H + H_2O \rightarrow HOCH_2CH(CH_3)OH$$

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

Input Data

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[per kg propylene glycol]			Remark
INPUTS			
propylene oxide	kg	0.803	stoechiometric calc., 95% yield
Water, unspecified	m3	2.49E-04	stoechiometric calc., 95% yield
Electricity, medium voltage	kWh	0.333	estimation
Natural gas, burned in industrial furnace >100kW	MJ	2	estimation
Water, cooling, unspecified	m3	2.40E-02	estimation
Transport, by train	tkm	4.82E-01	standard distances & means
Transport, by lorry	tkm	8.03E-02	standard distances & means
chemical plant, organics	unit	4.00E-10	approximation for infrastructure
OUTPUTS			
waste heat, to air	MJ	1.20E+00	calculated from electricity input
propylene oxide, to air	kg	1.60E-03	estimated as 0.2% of input
carbon dioxide, fossil, to air	kg	7.88E-02	from waste water treatment
propylene oxide, to water	kg	3.85E-03	calculated from mass balance
COD, BOD	kg	5.91E-02	calculated from water emissions
TOC, DOC	kg	1.85E-02	calculated from water emissions

Cumulated Data (LCI)

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		Name Location Unit Infrastructure	Unit	**propylene glycol, liquid, at plant** **RER** **kg** **0**	propylene oxide, liquid, at plant RER kg 0
LCIA results					
	cumulative energy demand	non-renewable energy resources, fossil	MJ-Eq	**7.6E+1**	8.8E+1
	cumulative energy demand	non-renewable energy resources, nuclear	MJ-Eq	**2.3E+1**	2.6E+1
	cumulative energy demand	renewable energy resources, water	MJ-Eq	**3.5E+0**	3.9E+0
	cumulative energy demand	renewable energy resources, wind, solar, geothermal	MJ-Eq	**5.8E-1**	6.6E-1
	cumulative energy demand	renewable energy resources, biomass	MJ-Eq	**4.5E-1**	5.0E-1
LCI results					
resource	Land occupation	total	m2a	**8.0E-2**	8.6E-2
air	Carbon dioxide, fossil	total	kg	**3.5E+0**	3.8E+0
air	NMVOC	total	kg	**4.6E-3**	3.5E-3
air	Nitrogen oxides	total	kg	**8.8E-3**	1.0E-2
air	Sulphur dioxide	total	kg	**1.2E-2**	1.4E-2
air	Particulates, < 2.5 um	total	kg	**8.9E-4**	1.0E-3
water	BOD	total	kg	**1.6E-1**	1.2E-1
soil	Cadmium	total	kg	**3.9E-9**	4.1E-9

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