Input analysis

Summary

The input analysis is a method for detecting first weak points of products and processes. It is based on the norm ISO 14040 for the carrying out of ecobalances. In contrast to an ecobalance an impact assessment is not included. The estimation is based on the analysis of material and energy flows.

The following example of an input analysis should demonstrate the methodical procedure of the analysis. The achieved results of the example will be discussed elsewhere (see text “Environmental Aspects of the Energy Supply of Chemical Reactions”).

Input Analysis as an Example

The reaction “acid catalysed acetalisation of 3-nitrobenzaldehyde with ethanediol to 2-(3-nitrophenyl)-1,3-dioxolane” was examined by means of input analysis. Thereby the classical carrying out of the reaction was compared with the alternative usage of microwaves. Within the classical method the heating facilities oil bath and heating-mantle were used for comparison. There were different levels considered in the analysis. In the first level, the reaction level, only material and energy flows are examined that are directly connected with the reaction. The second level, the synthesis level, contains the input of the reaction and the work up. The third and last level has a holistic point of view. In this level all input flows are balanced from the exploration of the raw materials to the final product (the disposal of the waste and residual materials were not taken into account because we assume constant amounts and waste treatment). In Fig. 1 the underlying analytical area is illustrated schematically.

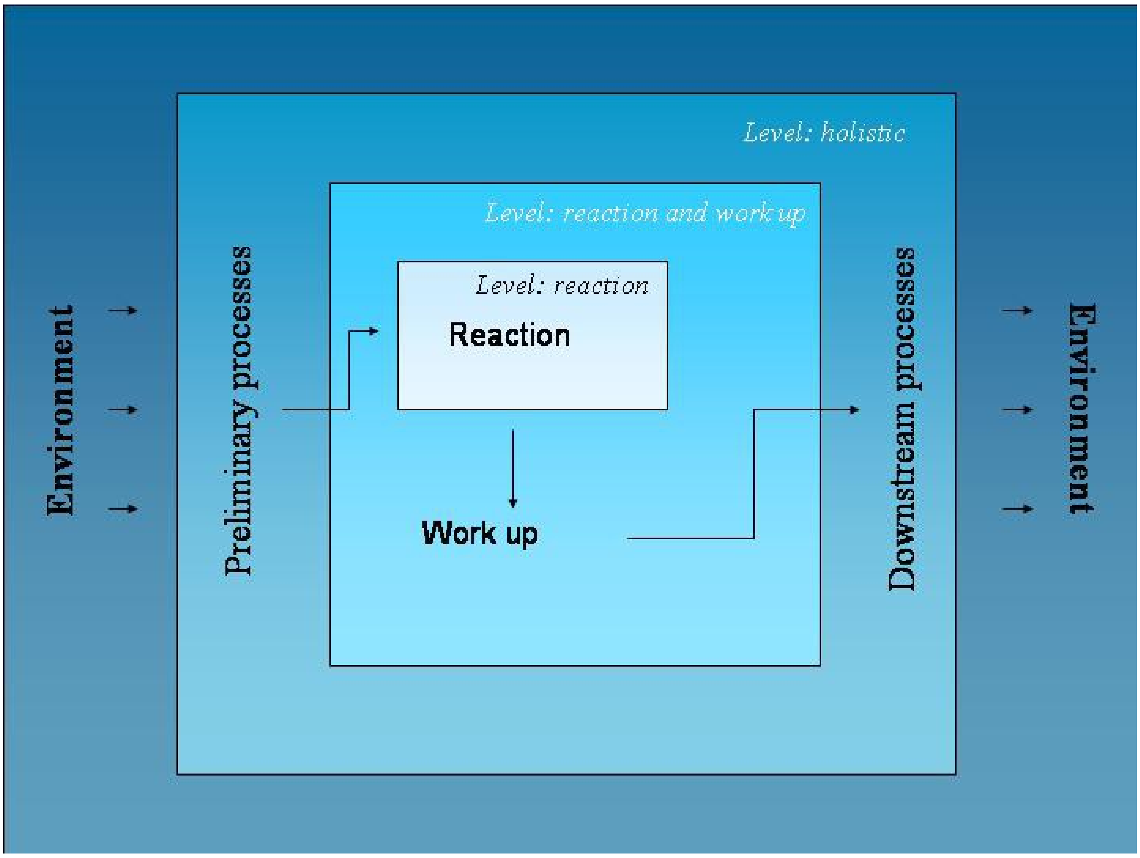

Fig. 1: Different consideration levels in the examination of the synthesis

The input analysis records the consumption of materials regarding to the amount. The potentials of toxicity of each substance are not taken into account in this method. On this way it is not possible to derive absolute statements referring to the environmental pollution. However, the procedure is able to reveal the weak points relating to the process with small expenses and contribute to an improvement of procedures.

At the Reaction Registered Data

IInput and output flows of the different consideration levels registered through measurements are described in the following paragraph. The masses of the used materials was taken as described in the instruction. The data of the energy consumption were recorded by means of a usual in trade measuring instrument. The consumption of the cooling water was measured.

Material and Energy Flows of the Reaction – Input

		Oil bath	Heating-mantle	Microwave	
Substances and auxiliaries	3-Nitrobenzaldehyde	7.55	7.55	7.55	g
	Ethylene glycol	3.42	3.42	3.42	g
	4-Toluenesulfonic acid monohydrate	0.40	0.40	0.40	g
	Cyclohexane	90.0	90.0	---	cm^3
	Cooling water	12.1	12.1	---	dm^3
Energy demand	Provision of thermical energy	1444	1008	180	kJ
	Stirring	18	18	54	kJ
	Oil pump/cryostatic temperature regulator	43	43	43	kJ

Table 1: Material and energy flows of the reaction – input

Material and Energy Flows of the Synthesis (Reaction and Work up) – Input

		Oil bath	Heating-mantle	Microwave	
Substances and auxiliaries	3-Nitrobenzaldehyde	7.55	7.55	7.55	g
	Ethylene glycol	3.42	3.42	3.42	g
	4-Toluenesulfonic acid monohydrate	0.40	0.40	0.40	g
	Cyclohexane	90.0	90.0	---	cm^3
	Cooling water	12.8	12.5	0.4	dm^3
	Petrolether (40-60)	25.0	25.0	25.0	cm^3
	Diethyl ether	25.0	25.0	25.0	cm^3
Energy demand	Provision of thermical energy	1627	1044	216	kJ
	Stirring	18	18	54	kJ
	Oil pump/Cryostat	86	86	86	kJ

Table 2: Material and energy flows of the synthesis – Input

Material and Energy Flows of the Synthesis – Output

		Oil bath	Heating-mantle	Microwave	
	Wastes	108.16	108.16	47.31	g
	1,3-Dioxolane	7.8	7.8	7.8	g
	Cooling water	12.8	12.5	0.4	dm^3

Table 3: Material and energy flows of the synthesis – Output

The in- and output of the reaction and synthesis level were comparatively easy to determine because of the limited number of different flows. It is clearly more difficult to register the material flows in a holistic view. For this data must be gathered from different databanks and linked respectively.

Material and Energy Flows – Holistic View

The material and energy flows of the holistic view are very extensive. Because of this they were set into the appendix of this description. After the determination of the material and energy flows the data of the different experiments will be compared with each other and will be evaluated. The analysed levels are considered.

Evaluation

The evaluation of the experiments follows two aspects. On the one hand the material flows and on the other hand the energy flows are evaluated.

Energy Consumption

It is easy to see that in this case the usage of microwaves represents the most favourable method from the energetical point of view. The short reaction time plays an out jutting role here. Under the classical variations the supply of energy using a heating-mantle should be preferred. The reason for this is the better isolation of the heating basket compared to an oil bath. Table 4 shows the electrical energy needed for each process version.

	Microwave	Oil bath	Heating-mantle	
Energy demand reaction	277	1505	1069	kJ
Energy demand work up	79	227	79	kJ
Total energy demand	356	1732	1148	kJ

Table 4: Energy consumption of each process version

Among the differences in energy consumption of the reaction variants its distribution within the synthesis is interesting. Regarding the examined synthesis it can be shown that the participation of the work up in the energy consumption is negligible compared to the energy of the reaction. Thats why possible improvements should apply to the reaction and not to the method of the work up. The rate of the working up is shown in Fig. 2 in relation to the whole energy consumption.

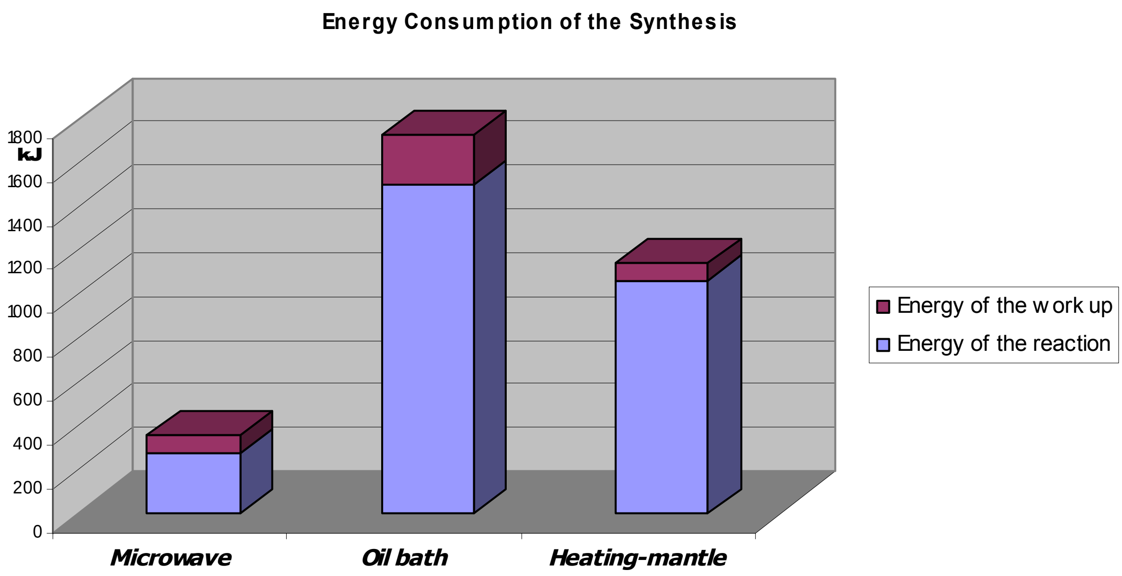

Fig. 2: Energy consumption of the reaction and the working off

Material Consumption

Comparing the analysed variations concerning their material flows the alternative version of heating by microwaves also does better than heating by the classical methods. Using microwaves can be done without entrainer and cooling water by employing same amounts of educts and catalysts. Considering preliminary processes the described advantage of the microwave synthesis becomes more clearly. The renunciation of cyclohexane as entrainer avoids environmental pollution concerning to the production of this substance. From a holistic point of view additionally has to be mentioned that the decrease in energy consumption leads to lower consumptions of the limited existing primary energy sources coal, mineral oil and natural gas.

Appendix

The data given in the following tables represent the input or output respectively of the examined example “Acetalisation”. Materials that cannot be connected directly with the reaction refer to preliminary processes.

Example: Brown coal listed as input of the reaction is used for providing electric power used up in the reaction.

Table: Material and Energy Flows Holistic View – Input

	Heating-mantle		Microwaves		Oil bath	
Chemical basic materials						
Chem. basic materials, inorg.						
Sodium hydrogen carbonate	5.39	g	5.39	g	5.39	g
Oxygen	3.87	g	3.87	g	3.87	g
Chem. basic materials, org.						
Diethyl ether	17.84	g	17.84	g	17.84	g
Petrol ether	16.60	g	16.60	g	16.60	g
tert. Butyl methyl ether	79.81	g	79.81	g	79.81	g
Air	1035.43	g	1035.43	g	1035.43	g
Fine chemicals						
4-Toluenesulfonic acid monohydrate	400.00	mg	400.00	mg	400.00	mg
Cumulated energy demand (CED)	20368.13	kJ	13351.52	kJ	22362.69	kJ
Minerals						
Sodium sulphate	43142.86	mg	43142.86	mg	43142.86	mg
Raw materials in deposits (RiD)						
Energy source (RiD)						
Brown coal	472.88	g	386.99	g	536.03	g
Natural gas	98.38	g	42.36	g	101.62	g
Mineral oil	59.52	g	14.46	g	60.36	g
Wood	3.70	mg	3.70	mg	3.70	mg
Hard coal	137.11	g	105.83	g	158.70	g
Uranium	7.07	mg	7.07	mg	7.07	mg
Not energetically used energy sources (RiD)			0.05	kg	0.05	kg
Bauxite	32.89	mg	9.47	mg	32.89	mg
Bentonite	14.59	mg	2.23	mg	14.59	mg
Calcium sulfate	1.46	mg	0.22	mg	1.46	mg
Dolomite	0.61	mg	0.09	mg	0.61	mg
Iron	55.86	mg	8.24	mg	55.86	mg
Limestone	15323.53	mg	14114.45	mg	16175.79	mg
Gravel	0.15	mg	0.02	mg	0.15	mg
Minerals (RiD)						

Continuation	Heating-mantle		Microwaves		Oil bath	
Calcium fluoride	0.09	mg	0.09	mg	0.09	mg
Sodium chloride	153.69	mg	95.43	mg	153.69	mg
Olivine	0.46	mg	0.07	mg	0.46	mg
Sand	277.08	mg	269.87	mg	277.08	mg
Slate	4.03	mg	0.65	mg	4.03	mg
Sulphur	35263.64	mg	35255.11	mg	35263.64	mg
Clay	1.25	mg	0.14	mg	1.25	mg
Water	380.30	kg	305.82	kg	389.35	kg
kJ	20368.13	kJ	13351.52	kJ	22362.69	kJ
kg	382.32	kg	307.62	kg	391.46	kg

Table: Material and Energy Flows Holistic View – Output

	Heating-mantle		Oil bath		Microwave	
Wastes						
Wastes for disposal (WfD)						
Wastes for combustion	108.12	g	108.12	g	38.01	g
Wastes, household waste like	62.02	mg	62.02	mg	6.35	mg
Wastes, others (WfD)						
Sewage sludge	2.92	mg	3.57	mg	2.05	mg
Wastes, unspecified	213.75	mg	213.75	mg	153.60	mg
Spoil	3019.41	g	3019.41	g	3018.85	g
Ashes and cinders	8696.78	mg	12917.99	mg	2843.89	mg
Metals	0.48	mg	0.48	mg	0.09	mg
Radioactive wastes (highly radioactive)						
Hazardous waste	2.89	mg	2.89	mg	2.89	mg
Special refuse	42.42	mg	47.90	mg	3.67	mg
Wastes for exploitation (WfE)						
Wastes, others (WfE)						
Ashes and cinders	4907.43	mg	7312.27	mg	1641.61	mg
Filter dust	2301.52	mg	2301.52	mg	2301.52	mg
Gypsum (REA)	7946.59	mg	7946.59	mg	7946.59	mg
Coarse ashes	344.03	mg	344.03	mg	344.03	mg
Sodium sulfate	75.49	mg	75.49	mg	75.49	mg
Pellets of melting chambers	2884.42	mg	2884.42	mg	2884.42	mg
Mixed potential recyclable	10.41	mg	10.41	mg		
Fluidised bed ashes	230.15	mg	230.15	mg	230.15	mg
Wastes unspecified	30.92	mg	41.83	mg	16.10	mg
Diluted nitration acid with traces of nitrate	1075.51	g	1075.51	g	1075.51	g
Chemical basic materials						
Chemical basic materials, inorg.						
Sodium hydrogen carbonate	5.39	g	5.39	g	5.39	g
Chemical basic materials, org.	0.08	kg	0.08	kg	0.08	kg
Benzoic acid	2272.18	mg	2272.18	mg	2272.18	mg
Maleic acid	2272.18	mg	2272.18	mg	2272.18	mg
tert. Butyl methyl ether	79.81	g	79.81	g	79.81	g

Continuation	Heating-mantle		Oil bath		Microwave	
Emissions (soil)						
Metals (W)						
Aluminium	1.63	mg	1.63	mg	0.59	mg
Lead	0.30	mg	0.30	mg	0.30	mg
Manganese	0.58	mg	0.58	mg	0.58	mg
Metals unspecified	21.92	mg	21.92	mg	5.35	mg
Molybdenum	0.07	mg	0.07	mg	0.07	mg
Sodium	14.84	mg	14.84	mg	3.12	mg
Uranium	0.10	mg	0.10	mg	0.10	mg
Vanadium	0.06	mg	0.06	mg	0.06	mg
Emissions (air)						
Particles	0.14	mg	0.14	mg	0.14	mg
Dust	218.43	mg	291.38	mg	61.94	mg
Dust (>PM10)	9.36	mg	9.36	mg	9.36	mg
Dust (PM10)	21.87	mg	21.87	mg	21.87	mg
Compounds inorg. (L)						
Ammonia	22.17	mg	22.83	mg	18.73	mg
Hydrogen chloride	61.60	mg	81.24	mg	33.74	mg
Dinitrogen monoxide	482.77	mg	483.55	mg	481.71	mg
Hydrogen fluoride	8.39	mg	11.10	mg	4.71	mg
Carbon dioxide (L)	1.03	kg	1.15	kg	0.77	kg
Carbon dioxide fossil	1031.75	g	1154.70	g	768.98	g
Carbon monoxide	301.32	mg	315.80	mg	180.62	mg
Metals (L)						
Metals unspecified	0.16	mg	0.16	mg	0.02	mg
Nickel	0.09	mg	0.10	mg	0.08	mg
Selenium	0.09	mg	0.09	mg	0.09	mg
NOx	1997.64	mg	2144.39	mg	1368.71	mg
Radio nuclides (L)	431.85	kBq	431.85	kBq	431.85	kBq
Radio nuclides, total	431852	Bq	431852.39	Bq	431852.39	Bq
Sulfur dioxide	2729.63	mg	3253.10	mg	1706.05	mg
Hydrogen sulfide	0.18	mg	0.18	mg	0.18	mg
Hydrogen	1.56	mg	1.56	mg	0.65	mg
VOC (L)						
Methane	2420.85	mg	2748.18	mg	1533.88	mg

Continuation	Heating-mantle		Oil bath		Microwave	
Methane	2420.85	mg	2748.18	mg	1533.88	mg
NMVOC (L)						
Benzene	0.13	mg	0.17	mg	0.08	mg
NMVOC, aromatic, unspecified	4.39	mg	4.39	mg	0.75	mg
Hexane	0.12	mg	0.12	mg	0.12	mg
NMVOC, containing oxygen (L)	0.00	kg	0.00	kg	0.00	kg
Formaldehyde	0.08	mg	0.08	mg	0.08	mg
NMVOC, unspecified	175.02	mg	178.75	mg	169.95	mg
VOC (hydrocarbons)	108.74	mg	108.74	mg		
Emissions (Water)						
Emissions (W)						
Carbonate	13.72	mg	13.72	mg	2.01	mg
Chloride	120.24	mg	120.24	mg	67.86	mg
Solids, dissolved	10.78	mg	10.78	mg	3.57	mg
Solids, suspended	15.98	mg	15.98	mg	3.21	mg
Fluoride	0.13	mg	0.13	mg	0.13	mg
Acids as H(+)	4.05	mg	4.05	mg	0.62	mg
Ammonia	0.29	mg	0.29	mg	0.29	mg
Ammonium	1.42	mg	1.42	mg	1.16	mg
Nitrate	0.42	mg	0.42	mg	0.16	mg
Nitrogen compounds, unspecified	0.49	mg	0.49	mg	0.17	mg
Sulfate	628.11	mg	628.11	mg	609.93	mg
Compounds, inorganic (W)						
Chlorine	0.87	mg	0.87	mg	0.87	mg
Detergents, oil	4.01	mg	4.01	mg	0.43	mg
Hydrocarbons (W)						
Hydrocarbons, unspecified	3.03	mg	3.03	mg	0.42	mg
Hydrocarbons, unspecified	0.65	mg	0.65	mg	0.65	mg
Phenols	0.07	mg	0.07	mg	0.00	mg
Compounds, org., dissolved	1.17	mg	1.17	mg		
Compounds, org., unspecified	0.13	mg	0.13	mg		
Indicator parameters						
BSB-5	2.55	mg	2.55	mg	0.71	mg
CSB	15.76	mg	15.76	mg	4.03	mg
TOC	1.37	mg	1.37	mg	1.37	mg
Fine chemicals						

Continuation	Heating-mantle		Oil bath		Microwave	
1,3-Dioxolane	7800.00	mg	7800.00	mg	7800.00	mg
Minerals						
Gypsum (REA)	3125.44	mg	4666.75	mg	1032.30	mg
Sodium sulfate	43142.9	mg	43142.86	mg	43142.86	mg
Water	379.28	kg	388.15	kg	305.05	kg
kJ	20368.1	kJ	22362.69	kJ	13351.52	kJ
kg	382.32	kg	391.46	kg	307.62	kg