ESU-services

fair consulting in sustainability

Life Cycle Inventory of Sodium Acetate and Expanded Graphite

Short Report

Provider

Dr. Niels Jungbluth
ESU-services Ltd.
Kanzleistr. 4, CH - 8610 Uster
jungbluth@esu-services.ch
www.esu-services.ch
Tel. +41 44 940 61 32; Fax +41 44 940 61 94

Customer

Benoit Nguyen
HEIG-VD / LESBAT
Haute Ecole d'Ingénierie et de Gestion du canton de Vaud
Laboratoire d'Energétique Solaire et de Physique du BATiment
Route de Cheseaux 1
1401 Yverdon-les-Bains
0041 (0)24 55 76 352
benoit.nguyen@heig-vd.ch

Uster, 15. Januar 2008

1 Background and Objectives

The laboratory LESBAT of the HEIG-VD works at the moment on the solar energy storage issue. They found that the use of sodium acetate (Na(CH3COO)*3H2O), a phase change material (PCM), is a good way to optimize solar heating systems.

Actually, the customer uses sodium acetate mixed with expanded graphite (80 à 150 g/l), a chemical product produced by the following company: SGL Carbon located at Meitingen (Deutschland).

The product is not commercially available. A similar product, which uses paraffin instead of sodium acetate is marketed by the company SGL Carbon under the brand name Ecophit. This product has been included in the investigation in order to verify the data.

The goal of this study is to assess if the energy gain resulted from the use of sodium acetate is balanced or not by its embodied energy.

The ecoinvent data v2.0 do not yet investigate sodium acetate and expanded graphite (ecoinvent Centre 2007). Therefore the customer has asked ESU-services to conduct a life cycle inventory analysis of the two materials and to provide some aggregated key indicators for further analysis. The study should investigate sodium acetate with and without expanded graphite.

In general the ecoinvent methodology has been followed in order to achieve full consistency with the used background data (Frischknecht et al. 2007a).

2 Life cycle inventory of phase change material for solar energy storage

Author: Niels Jungbluth, ESU-services Ltd., Uster
Review: Sybille Büsser, ESU-services Ltd., Uster
Last changes: 15 January 2008

2.1 Sodium acetate

Sodium acetate is produced from acetic acid and sodium hydroxide. Therefore the following reaction takes place:

CH3COOH + NaOH + 2H2O = CH3COONa + 3H2O

Information about the technical production process was not available. Important issues could be:

- Is the product dried and how is this done?
- Which amounts of inputs are used and what is the efficiency of the process?
- Is there a heat release, how is this used and is cooling necessary?

The unit process raw data are based on literature references for similar chemical compounds of sodium salts (Hischier 2007) and own assumptions. These assumptions are described in the GeneralComment column of Tab. 2.1.

Tab. 2.1 Unit process raw data of sodium acetate production

	Name	Location	InfrastructureProcess	Unit	sodium acetate, trihydrate, at plant	UncertaintyType	StandardDeviation95%	GeneralComment
	Location				RER			
	InfrastructureProcess				0			
	Unit				kg			
product	sodium acetate, trihydrate, at plant	RER	0	kg	1			
technosphere	sodium hydroxide, 50% in H2O, production mix, at plant	RER	0	kg	5.13E-1	1	1.30	(4,na,1,1,1,5); Stoichiometric calculation with 95% yield
	acetic acid, 98% in H2O, at plant	RER	0	kg	7.72E-1	1	1.30	(4,na,1,1,1,5); Stoichiometric calculation with 95% yield
	transport, freight, rail	RER	0	tkm	7.71E-1	1	2.09	(4,5,na,na,na,na); Standard distance 600km
	transport, lorry >16t, fleet average	RER	0	tkm	1.28E-1	1	2.09	(4,5,na,na,na,na); Standard distance 100km
	heat, natural gas, at industrial furnace >100kW	RER	0	MJ	2.00E+0	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data for chemicals
	electricity, medium voltage, production UCTE, at grid	UCTE	0	kWh	3.33E-1	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data, range (.017-.33)
	chemical plant, organics	RER	1	unit	4.00E-10	1	3.09	(4,5,na,na,na,na); Standard assumption
	treatment, sewage, unpolluted, to wastewater treatment, class 3	CH	0	m3	1.20E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
resource, in water	Water, unspecified natural origin	-	-	m3	1.20E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
	Water, cooling, unspecified natural origin	-	-	m3	2.40E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
emission water, river	Sodium, ion	-	-	kg	1.40E-2	1	5.10	(4,na,1,1,1,5); Calculation 5%
	Ethyl acetate	-	-	kg	3.66E-3	1	3.09	(4,na,1,1,1,5); Calculation 5%
	BOD5, Biological Oxygen Demand	-	-	kg	6.39E-3	1	1.62	(4,na,1,1,1,5); Calculation, 90% removal in treatment
	COD, Chemical Oxygen Demand	-	-	kg	6.39E-3	1	1.62	(4,na,1,1,1,5); Calculation, 90% removal in treatment
	DOC, Dissolved Organic Carbon	-	-	kg	2.00E-3	1	1.62	(4,na,1,1,1,5); Calculation, 90% removal in treatment
	TOC, Total Organic Carbon	-	-	kg	2.00E-3	1	1.62	(4,na,1,1,1,5); Calculation, 90% removal in treatment
emission air, high population density	Heat, waste	-	-	MJ	1.20E+0	1	1.30	(4,na,1,1,1,5); Calculation with electricity use
	Carbon dioxide, fossil	-	-	kg	4.83E-2	1	1.30	(4,na,1,1,1,5); Calculation, 90% from waste water treatment

2.2 Graphite mining

Data for graphite in ecoinvent data v2.0 are a very rough assumption with the assumption that mining is the same as for lime (Hischier 2007). Thus, the inventory for this material has been updated.

The following information has been found on http://en.wikipedia.org.

> Graphite is mined around the world by both open pit and underground methods. While flake graphite and amorphous graphite are both mined open pit and underground, lump (vein) graphite is only mined underground in Sri Lanka. The open pit mines usually employ equipment (i.e. bulldozers) to scoop up the ore, which is usually put in trucks and moved to the plant. Since the original rock is usually lateritized or weathered, this amounts to moving dirt with flecks or pieces of graphite in it from the pit (blasting is seldom required). The underground graphite mines employ drilling and blasting to break up the hard rock (ore), which is then moved by mine cars pulled by a locomotive, or moved by automotive vehicles, to the surface and then to the plant. In less-developed areas of the world, the ore can be mined by pick and shovel and transported by mine cars pushed by a laborer or by women carrying baskets of ore on their heads.
>
> Graphite usually needs beneficiation, although thick-bedded amorphous graphite and vein graphite is almost always beneficiated, if beneficiated at all, by laborers hand-picking out the pieces of gangue (rock) and hand-screening the product. The great majority of world flake graphite production is crushed and ground if necessary and beneficiated by flotation. Treating graphite by flotation encounters one big difficulty: graphite is very soft and "marks" (coats) the particles of gangue. This makes the "marked" gangue particles float off with the graphite to yield a very impure concentrate. There are two ways of obtaining a saleable concentrate or product: regrinding and floating it again and again (up to seven times) to obtain a purer and purer concentrate, or by leaching (dissolving) the gangue with hydrofluoric acid (for a silicate gangue) or hydrochloric acid (for a carbonate gangue).
>
> In the milling process, the incoming graphite products and concentrates can be ground before being classified (sized or screened), with the coarser flake size fractions (above 8 mesh, 8 mesh to 20 mesh, 20 mesh to 50 mesh) carefully preserved, and then the carbon contents are determined. Then some standard blends can be prepared from the different fractions, each with a certain flake size distribution and carbon content. Custom blends can also be made for individual customers who want a certain flake size distribution and carbon content. If flake size is unimportant, the concentrate can be ground more freely. Typical final products include a fine powder for use as a slurry in oil drilling; in zirconium silicate, sodium silicate and isopropyl alcohol coatings for foundry molds; and a carbon raiser in the steel industry (Synthetic graphite powder and powdered petroleum coke can also be used as carbon raiser). Rough

> graphite is typically classified, ground, and packaged at a graphite mill; often the more complex formulations are also mixed and packaged at the mill facility. Environmental impacts from graphite mills consist of air pollution including fine particulate exposure of workers and also soil contamination from powder spillages leading to heavy metals contaminations of soil. Dust masks are normally worn by workers during the production process to avoid worker exposure to the fine airborne graphite and zircon silicate.

The unit process raw data of graphite production in Tab. 2.2 are based on an LCA study (Pehnt 2002). Missing data have been assessed with data provided in the ecoinvent database for lime production (Hischier 2007).

Tab. 2.2 Unit process raw data of graphite production

	Name	Location	InfrastructurePro	Unit	graphite, natural, production Asia, at regional storage	UncertaintyType	StandardDeviation95%	GeneralComment	graphite, at plant (ecoinvent)	data Pehnt (2002)
	Location				RER				RER	
	InfrastructureProcess				0				0	
	Unit				kg				kg	kg
product	graphite, natural, production Asia, at regional storage	RER	0	kg	1					
technosphere	recultivation, limestone mine	CH	0	m2	6.52E-6	1	1.38	(4,3,1,3,3,5); approximation with data from lime production	6.52E-6	
	light fuel oil, burned in industrial furnace 1MW, non-modulating	RER	0	MJ	6.48E+0	1	1.31	(2,3,2,3,3,5); heating oil, energy, Pehnt 2002	3.59E-3	6.48E+0
	diesel, burned in building machine	GLO	0	MJ	6.66E+0	1	1.31	(2,3,2,3,3,5); heating oil, energy, Pehnt 2002	1.80E-2	6.66E+0
	electricity, medium voltage, production UCTE, at grid	UCTE	0	kWh	2.93E+0	1	1.31	(2,3,2,3,3,5); Pehnt 2002, mining	3.25E-2	2.93E+0
	electricity, medium voltage, at grid	CN	0	kWh	9.60E+0	1	1.31	(2,3,2,3,3,5); Pehnt 2002, preparation		9.60E+0
	mine, limestone	CH	1	unit	5.25E-11	1	3.14	(4,3,1,3,3,5); approximation with data from lime production	5.25E-11	
	industrial machine, heavy, unspecified, at plant	RER	1	kg	2.31E-4	1	3.14	(4,3,1,3,3,5); approximation with data from lime production	2.31E-4	
	conveyor belt, at plant	RER	1	m	2.78E-8	1	3.14	(4,3,1,3,3,5); approximation with data from lime production	2.78E-8	
	chemicals inorganic, at plant	GLO	0	kg	2.60E-1	1	1.31	(2,3,2,3,3,5); auxiliary materials, Pehnt 2002		2.60E-1
	lubricating oil, at plant	RER	0	kg	3.40E-3	1	1.31	(2,3,2,3,3,5); flotation oil, Pehnt 2002		3.40E-3
	hydrochloric acid, 30% in H2O, at plant	RER	0	kg	2.00E-1	1	1.31	(2,3,2,3,3,5); acids, Pehnt 2002		2.00E-1
	transport, transoceanic freight ship	OCE	0	tkm	1.00E+1	1	2.10	(2,3,2,3,3,5); transport from Asia		1.00E+1
	transport, freight, rail	RER	0	tkm	2.78E-1	1	2.10	(2,3,2,3,3,5); 600km for materials		2.78E-1
	transport, lorry >16t, fleet average	RER	0	tkm	1.00E+0	1	2.10	(2,3,2,3,3,5); transport from harbour		1.00E+0
resource, in water	Water, well, in ground	-	-	m3	2.93E-5	1	1.38	(4,3,1,3,3,5); approximation with data from lime production	2.93E-5	
resource, in ground	Metamorphous rock, graphite containing, in ground	-	-	kg	1.05E+0	1	1.38	(4,3,1,3,3,5); approximation with data from lime production	1.05E+0	
resource, land	Occupation, mineral extraction site	-	-	m2a	8.48E-5	1	1.68	(4,3,1,3,3,5); approximation with data from lime production	8.48E-5	
	Transformation, to mineral extraction site	-	-	m2	6.52E-6	1	2.15	(4,3,1,3,3,5); approximation with data from lime production	6.52E-6	
	Transformation, from forest	-	-	m2	6.52E-6	1	2.15	(4,3,1,3,3,5); approximation with data from lime production	6.52E-6	
emission air, low population density	Heat, waste	-	-	MJ	4.51E+1	1	1.31	(2,3,2,3,3,5); calculation	1.17E-1	4.51E+1
	Particulates, < 2.5 um	-	-	kg	8.87E-6	1	3.14	(4,3,1,3,3,5); approximation with data from lime production	8.87E-6	
	Particulates, > 10 um	-	-	kg	1.21E-4	1	1.68	(4,3,1,3,3,5); approximation with data from lime production	1.21E-4	
	Particulates, > 2.5 um, and < 10um	-	-	kg	4.78E-5	1	2.15	(4,3,1,3,3,5); approximation with data from lime production	4.78E-5	
	blasting	RER	0	kg		1	1.38	(4,3,1,3,3,5); approximation with data from lime production	7.73E-5	
	heat, light fuel oil, at industrial furnace 1MW	RER	0	MJ		1	1.38	(4,3,1,3,3,5); approximation with data from lime production	8.98E-2	

2.3 Expanded graphite

The following information has been found on http://en.wikipedia.org.

> Expanded graphite is made by immersing natural flake graphite in a bath of chromic acid, then concentrated sulfuric acid, which forces the crystal lattice planes apart, thus expanding the graphite. The expanded graphite can be used to make graphite foil or used directly as "hot top" compound to insulate molten metal in a ladle or red-hot steel ingots and decrease heat loss, or as firestops fitted around a firedoor (during a fire, the graphite expands and chars to resist fire penetration and spread), or to make high-performance gasket material for high-temperature use. After being made into graphite foil, the foil is machined and assembled into the bipolar plates in fuel cells. The foil is made into heat sinks for laptop computers which keeps them cool while saving weight, and is made into a foil laminate that can be used in valve packings or made into gaskets. Old-style packings are now a minor member of this grouping: fine flake graphite in oils or greases for uses requiring heat resistance. A GAN estimate of current U.S. natural graphite consumption in this end use is 7'500 tonnes.

So far no data were available. The unit process raw data in Tab. 2.3 are roughly estimated based on data for similar expanded materials, e.g. expanded vermiculite, clay and perlite (Hischier 2007). The column GeneralComment provides further information about the estimations.

Tab. 2.3 Unit process raw data of expanded graphite production

	Name	Location	InfrastructureProcess	Unit	graphite, expanded, at plant	UncertaintyType	StandardDeviation95%	GeneralComment
	Location				RER			
	InfrastructureProcess				0			
	Unit				kg			
product	graphite, expanded, at plant	RER	0	kg	1			
technosphere	graphite, natural, production Asia, at regional storage	RER	0	kg	1.10E+0	1	1.30	(4,na,1,1,1,5); Rough assumption, 10% losses
	sulphuric acid, liquid, at plant	RER	0	kg	1.00E-1	1	1.30	(4,na,1,1,1,5); Used, but no data, own estimation
	nitric acid, 50% in H2O, at plant	RER	0	kg	1.00E-1	1	1.30	(4,na,1,1,1,5); Used, but no data, own estimation
	chromium oxide, flakes, at plant	RER	0	kg	1.00E-1	1	1.30	(4,na,1,1,1,5); Used, but no data, own estimation
	packaging film, LDPE, at plant	RER	0	kg	4.81E-4	1	1.30	(4,na,1,1,1,5); Packaging standard data
	corrugated board base paper, kraftliner, at plant	RER	0	kg	2.00E-3	1	1.30	(4,na,1,1,1,5); Packaging standard data
	transport, freight, rail	RER	0	tkm	8.41E-1	1	2.09	(4,5,na,na,na,na); Standard distance 600km
	transport, lorry >16t, fleet average	RER	0	tkm	1.40E-1	1	2.09	(4,5,na,na,na,na); Standard distance 100km
	light fuel oil, burned in industrial furnace 1MW, non-modulating	CH	0	MJ	8.50E+0	1	1.30	(4,na,1,1,1,5); Rough estimation with maximum literature data
	electricity, medium voltage, production UCTE, at grid	UCTE	0	kWh	6.50E-2	1	1.30	(4,na,1,1,1,5); maximum other expanded materials
	tap water, at user	RER	0	kg	6.60E-1	1	1.30	(4,na,1,1,1,5); Rough estimation, thoroughly rinsed with water
	chemical plant, organics	RER	1	unit	4.00E-10	1	3.09	(4,5,na,na,na,na); Standard
	disposal, inert material, 0% water, to sanitary landfill	CH	0	kg	1.00E-3	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
	treatment, sewage, unpolluted, to wastewater treatment, class 3	CH	0	m3	6.60E-4	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
resource, in water	Water, cooling, unspecified natural origin	-	-	m3	2.40E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
emission water, river	Sulfate	-	-	kg	5.00E-4	1	1.62	(4,na,1,1,1,5); Calculation 0.5%
	Nitrate	-	-	kg	5.00E-4	1	1.62	(4,na,1,1,1,5); Calculation 0.5%
	Chromium, ion	-	-	kg	5.00E-4	1	3.09	(4,na,1,1,1,5); Calculation 0.5%
emission air, high population density	Heat, waste	-	-	MJ	2.34E-1	1	1.30	(4,na,1,1,1,5); Calculation

2.4 Composite material of sodium acetate and expanded graphite

PCM's (phase change materials) are materials whose latent heat (heat of fusion) at the solid-liquid phase transition point is used in technical applications, e.g. energy storage. Because of their high storage density, PCM's allow the construction of compact energy storage systems. Here we investigate as an example the ECOPHIT material produced by SGL Carbon.

On the homepage of SGL Carbon,[1] the share of materials in the Ecophit product is given with 10% vol. of expanded graphite and 85% vol. of sodium paraffin. In a personal communication the composition has been defined 15 weight.-% Graphite and 85 weight.-% Natriumacetat-Trihydrat. For the calculation from the volume shares the porosity of the material has to be considered. This might be quite dependent how the materials are pressed together.[2]

The company has been asked for further information about this process and possible relevant inputs and outputs. No data were provided, as the process is proprietary.[3] Also it was not possible to find independent information on this process.

For the paraffin the following information was available.

> Paraffin wax (C25H52) is an excellent material to store heat, having a specific heat capacity of 2.14–2.9 J g–1 K–1 and a heat of fusion of 200–220 J/g. This property is exploited in modified sheetrock for home building material: it is infused in the sheetrock during manufacture so as, when installed, it melts during the day, absorbing heat, and solidifies again at night, releasing the heat. Wax expands considerably when it melts and this allows its use in thermostats for industrial, domestic and, particularly, automobile purposes.[4]

Thus the whole modelling can only be done as a very rough assumption as described in Tab. 2.4.

---

1 www.sglcarbon.de, Retrieved on 5.12.2007.

2 Personal communication, Dr. Martin Christ, SGL CARBON GmbH, 11.1.2008.

3 Personal communication, Axel Winkler, SGL CARBON GmbH, 11.1.2008.

4 http://en.wikipedia.org/wiki/Paraffin

Tab. 2.4 Unit process raw data of composite materials

	Name	Location	InfrastructureProcess	Unit	composite material, sodium acetate+graphite, at plant	composite material, paraffin+graphite, at plant	UncertaintyType	StandardDeviation95%	GeneralComment
	Location				RER	RER			
	InfrastructureProcess				0	0			
	Unit				kg	kg			
product	composite material, sodium acetate+graphite, at plant	RER	0	kg	1	0			
	composite material, paraffin+graphite, at plant	RER	0	kg	0	1			
technosphere	graphite, natural, production Asia, at regional storage	RER	0	kg	1.50E-1	1.50E-1	1	1.24	(3,1,1,1,1,5); Producer information about share
	sodium acetate, trihydrate, at plant	RER	0	kg	8.50E-1	0	1	1.24	(3,1,1,1,1,5); Producer information about share
	paraffin, at plant	RER	0	kg	0	8.50E-1	1	1.24	(3,1,1,1,1,5); Producer information about share
	transport, freight, rail	RER	0	tkm	5.10E-1	5.10E-1	1	2.09	(4,5,na,na,na,na); Standard distance 600km
	transport, lorry >16t, fleet average	RER	0	tkm	8.50E-2	8.50E-2	1	2.09	(4,5,na,na,na,na); Standard distance 100km
	transport, lorry 20-28t, fleet average	CH	0	tkm	5.20E-1	5.20E-1	1	2.06	(4,4,1,1,1,na); Transport to Yverdon, 520 km
	heat, natural gas, at industrial furnace >100kW	RER	0	MJ	2.00E+0	2.00E+0	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
	electricity, medium voltage, production UCTE, at grid	UCTE	0	kWh	3.33E-1	3.33E-1	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data, range (.017-.33)
	chemical plant, organics	RER	1	unit	4.00E-10	4.00E-10	1	3.09	(4,5,na,na,na,na); Standard
	treatment, sewage, unpolluted, to wastewater treatment, class 3	CH	0	m3	1.20E-2	1.20E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
resource, in water	Water, unspecified natural origin	-	-	m3	1.20E-2	1.20E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
	Water, cooling, unspecified natural origin	-	-	m3	2.40E-2	2.40E-2	1	1.30	(4,na,1,1,1,5); Rough estimation with literature data
emission air, high population density	Heat, waste	-	-	MJ	1.20E+0	1.20E+0	1	1.30	(4,na,1,1,1,5); Calculation
	Carbon dioxide, fossil	-	-	kg			1	1.30	(4,na,1,1,1,5); Calculation, 90% from waste water treatment

2.5 Waste management

Generally for the use of the PCM material about 30% up to 50% volume of the tank storage is filled with PCM. The PCM is stored in a cylindrical aluminium bottle. About 150 kg to 300 kg of PCM are used for a tank storage with a capacity is between 400 to 1000 litres. It can be assumed that at the end of the life cycle of the solar system, PCM can be easily collected by emptying the aluminium bottles. The PCM should lose its thermal performances at the end of life span of the solar system. Giving this assumption, recycling this PCM is quite unlikely, unless it could be used for other purposes than thermal storage.

The PCM is not an inert material as it has, with the graphite, a carbon content of about 30%. According to the legal regulations in Switzerland it would not be possible to dispose it in an inert material landfill, because therefore the carbon content should be near zero.

Other types of landfills are phasing out in Switzerland. Thus, it seems to be not so likely that in future this will be a possible disposal route.

Recycling of the PCM seems to be difficult because the close compound of the two materials and the low value of the sodium acetate. In the moment it seems not be possible to separate the materials and to win back the valuable expanded graphite for further uses.

Thus, in conclusion it is assumed that the solar storage is demounted and the PCM is incinerated after separation in a municipal waste incineration.

The demounting is not included in the present inventory, because it depends on the whole installation. Thus, only incineration is calculated for the inventory. The disposal in a residual material landfill is calculated with the same model.

The life cycle inventory for the disposal has been calculated with the model developed for ecoinvent (Doka 2007). The basic assumptions for the composition of PCM with sodium acetate has been calculated from the chemical formula of the materials as shown in Tab. 2.5. For PCM with paraffin in Tab. 2.6, the paraffin type has been assumed as $C_{25}H_{52}$.

The production of the solar storage as a whole, including the mounting and demounting must be calculated separately. Therefore a recycling of the aluminium seems to be easily possible.

Tab. 2.5 Waste composition and quality for the disposal of composite material of sodium acetate and expanded graphite

Enter name for waste		**composite material, sodium acetate+graphite**
Water content	kg/kg waste	33.7587%
Oxygen (without O from H2O)	kg/kg waste	19.9875%
Hydrogen (without H from H2O)	kg/kg waste	1.8888%
Carbon (enter share of biogenic C below)	kg/kg waste	30.0049%
Sodium	kg/kg waste	14.3601%
sum wet mass	**kg/kg waste**	**100.0000%**
Degradability of waste in a municipal landfill within 100 years		50.0%
extrapolated upper heating value (Michel 1938)		1.12
extrapolated lower heating value (Michel 1938)	-	1.12
theoretic upper heating value (Michel 1938)		10.59
theoretic lower heating value (Michel 1938)		3.86

Tab. 2.6 Waste composition and quality for the disposal of composite material of paraffin and expanded graphite

Enter name for waste		**composite material, paraffin+graphite**
Hydrogen (without H from H2O)	kg/kg waste	12.6318%
Carbon (enter share of biogenic C below)	kg/kg waste	87.3682%
sum wet mass	**kg/kg waste**	**100.0000%**
Degradability of waste in a municipal landfill within 100 years		100.0%
autotext comment: waste fractions		
autotext comment: waste fractions degradability		
extrapolated upper heating value (Michel 1938)		2.50
extrapolated lower heating value (Michel 1938)	-	2.50
theoretic upper heating value (Michel 1938)		45.42
theoretic lower heating value (Michel 1938)		45.14

2.6 Meta Information

Tab. 2.7 shows the meta information of all investigated processes. This information helps to better understand the depth of analysis, the included processes and the reliability of the data.

Tab. 2.7 Meta information for all materials investigated for the production of phase change composite materials

ReferenceFunction	Name	sodium acetate, trihydrate, at plant	graphite, natural, production Asia, at regional storage	graphite, expanded, at plant	composite material, sodium acetate+graphite, at plant	composite material, paraffin+graphite, at plant
Geography	Location	RER	RER	RER	RER	RER
ReferenceFunctic	InfrastructureProcess	0	0	0	0	0
ReferenceFunctic	Unit	kg	kg	kg	kg	kg
	IncludedProcesses	Raw materials and chemicals used for production, transport of materials to manufacturing plant, estimated emissions to air and water from production (incomplete), estimation of energy demand and infrastructure of the plant (approximation). Solid wastes omitted.	Raw materials, machineries and energy consumption for production, estimated emissions to air from production and infrastructure of the site (approximation). No water emissions.	Raw materials, machineries and energy consumption for production, estimated emissions to air from production and infrastructure of the site (approximation). Estimated water emissions.	Raw materials including expanded graphite, machineries and energy consumption for production, estimated emissions to air from production and infrastructure of the site (rough approximation). Estimated water emissions.	Raw materials including expanded graphite, machineries and energy consumption for production, estimated emissions to air from production and infrastructure of the site (rough approximation). Estimated water emissions.
	LocalName	Natriumacetat, Trihydrat, ab Werk	Graphit, natürlich, Produktion Asien, ab Regionallager	Graphit, expandiert, ab Werk	Verbundmaterial, Natriumacetat+Graphit, ab Werk	Verbundmaterial, Paraffin+Graphit, ab Werk
	Synonyms	0			ECOPHIT//PCM//phase change material	ECOPHIT//PCM//phase change material
	GeneralComment	The functional unit represent 1 kg. Large uncertainty of the process data due to weak data on the production process.	The functional unit represent 1 kg of milled graphite. Density: 2.09–2.23 g/cm³. Large uncertainty of the process data due to weak data on the production process.	The functional unit represent 1 kg of expanded graphite. Vermicular expanded graphite is a low bulk density, (usually between 0.002 and 0.02 gram per cubic centimetre). Large uncertainty of the process data due to weak data on the production process.	The functional unit represent 1 kg of PCM material. Density is 0.5-1.5 g/cm3. Large uncertainty of the process data due to weak data on the production process. Only the share of graphite and second material is known. Other data were not available as the process is proprietary.	The functional unit represent 1 kg of PCM material. Density is 0.5-1.5 g/cm3. Large uncertainty of the process data due to weak data on the production process. Only the share of graphite and second material is known. Other data were not available as the process is proprietary.
	InfrastructureIncluded	1	1	1	1	1
	Category	chemicals	chemicals	chemicals	chemicals	chemicals
	SubCategory	inorganics	inorganics	inorganics	inorganics	inorganics
	LocalCategory	Chemikalien	Chemikalien	Chemikalien	Chemikalien	Chemikalien
	LocalSubCategory	Anorganika	Anorganika	Anorganika	Anorganika	Anorganika
	Formula	C2H3NaO2	C	C		
	StatisticalClassification					
	CASNumber	6131-90-4	7782-42-5	7782-42-5		
TimePeriod	StartDate	2007	2000	2007	2000	2000
	EndDate	2007	2007	2007	2007	2007
	DataValidForEntirePeriod	1	1	1	1	1
	OtherPeriodText					
Geography	Text	Data estimated for European production	Data estimated for European production	Data estimated for European production	Data estimated for European production	Data estimated for European production
Technology	Text	Not known	Mining	Expanded graphite is made by immersing natural flake graphite in a bath of chromic acid, then concentrated sulphuric acid, which forces the crystal lattice planes apart, thus expanding the graphite.	Technology for production not known.	Technology for production not known.
Representativene	Percent	0	0	0	0	0
	ProductionVolume	unknown	worldwide 873 kt in 2001	7500t in US	7500t in US	7500t in US
	SamplingProcedure	unknown	approximation with data from literature	approximation with data from literature	approximation with data from literature	approximation with data from literature
	Extrapolations	none	Data approximated with data from lime mining, crushing and milling. Literature data for mining in Zimbabwe.	Data approximated with data from other expanded building materials.	Data approximated with data from other building materials.	Data approximated with data from other building materials.
	UncertaintyAdjustments	none	none	none	none	none
	Details	11.01.2008	11.01.2008	11.01.2008	11.01.2008	11.01.2008

Tab. 2.8 Meta information for the disposal of composite material with sodium acetate and graphite

ReferenceFunction	Name	disposal, composite material, sodium acetate+graphite, to residual material landfill	disposal, composite material, sodium acetate+graphite, to municipal incineration
Geography	Location	CH	CH
ReferenceFunction	InfrastructureProcess	0	0
ReferenceFunction	Unit	kg	kg
ReferenceFunction	IncludedProcesses	Waste-specific short-term emissions to water from leachate. Long-term emissions from landfill to ground water.	waste-specific air and water emisions from incineration, auxiliary material consumption for flue gas cleaning. Short-term emissions to river water and long-term emisisons to ground water from slag compartment (from bottom slag) and residual material landfill (from solidified fly ashes and scrubber sludge). Process energy demands for MSWI.
ReferenceFunction	LocalName	Entsorgung, Verbundmaterial, Natriumacetat+Graphit, in Reststoffdeponie	Entsorgung, Verbundmaterial, Natriumacetat+Graphit, in Kehrichtverbrennung
ReferenceFunction	Synonyms		
ReferenceFunction	GeneralComment	Inventoried waste contains . waste composition (wet, in ppm): H2O 337590; O 199870; H 18888; C 300050; S n.a.; N n.a.; P n.a.; B n.a.; Cl n.a.; Br n.a.; F n.a.; I n.a.; Ag n.a.; As n.a.; Ba n.a.; Cd n.a.; Co n.a.; Cr n.a.; Cu n.a.; Hg n.a.; Mn n.a.; Mo n.a.; Ni n.a.; Pb n.a.; Sb n.a.; Se n.a.; Sn n.a.; V n.a.; Zn n.a.; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si n.a.; Fe n.a.; Ca n.a.; Al n.a.; K n.a.; Mg n.a.; Na 143600; Share of carbon in waste that is biogenic 0%. Additional solidification with 0.02955 kg of cement.	Inventoried waste contains . waste composition (wet, in ppm): H2O 337590; O 199870; H 18888; C 300050; S n.a.; N n.a.; P n.a.; B n.a.; Cl n.a.; Br n.a.; F n.a.; I n.a.; Ag n.a.; As n.a.; Ba n.a.; Cd n.a.; Co n.a.; Cr n.a.; Cu n.a.; Hg n.a.; Mn n.a.; Mo n.a.; Ni n.a.; Pb n.a.; Sb n.a.; Se n.a.; Sn n.a.; V n.a.; Zn n.a.; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si n.a.; Fe n.a.; Ca n.a.; Al n.a.; K n.a.; Mg n.a.; Na 143600; Share of carbon in waste that is biogenic 0%. Share of iron in waste that is metallic/recyclable 0%. Net energy produced in MSWI: 0MJ/kg waste electric energy and 0MJ/kg waste thermal energy Allocation of energy production: no substitution or expansion. Total burden allocated to waste disposal function of MSWI. One kg of this waste produces 0.1212 kg of slag and 0.07388 kg of residues, which are landfilled. Additional solidification with 0.02955 kg of cement.
ReferenceFunction	Category	waste management	waste management
ReferenceFunction	SubCategory	residual material landfill	municipal incineration
ReferenceFunction	Formula		
ReferenceFunction	StatisticalClassification		
ReferenceFunction	CASNumber		
TimePeriod	StartDate	1994-01	1994-01
TimePeriod	EndDate	2000-12	2000-12
TimePeriod	OtherPeriodText	Waste composition as given in literature reference, theoretical data or other source. Transfer coefficients from prospective model.	Waste composition as given in literature reference, theoretical data or other source. Transfer coefficients for modern Swiss MSWI. Emission speciation based on early 90ies data.
Geography	Text	Technology encountered in Switzerland in 2000. Landfill includes base seal and leachate collection system.	Specific to the technology mix encountered in Switzerland in 2000. Well applicable to modern incineration practices in Europe, North America or Japan.
Technology	Text	Swiss residual material landfill for polluted, inorganic waste. With base seal and leachate collection system. Recultivation after closure.	average Swiss MSWI plants in 2000 (grate incinerators) with electrostatic precipitator for fly ash (ESP), wet flue gas scrubber and 29.4% SNCR , 32.2% SCR-high dust , 24.6% SCR-low dust -DeNOx facilities and 13.8% without Denox (by burnt waste, according to Swiss average). Share of waste incinerated in plants with magnetic scrap separation from slag : 50%. Gross electric efficiency technology mix 12.997% and Gross thermal efficiency technology mix 25.57%
Representativeness	ProductionVolume		
Representativeness	SamplingProcedure	Landfill model based on observed leachate concentrations in literature. Extrapolated to 60'000 years heeding chemical characteristics. Initial waste composition from various literature sources.	waste-specific calculation based on literature data
Representativeness	Extrapolations		Typical elemental transfer coefficients from current studies for modern MSWI, completed with data from coal power plants and estimates, adapted for inert/burnable waste.
Representativeness	UncertaintyAdjustments	uncertainty of waste input composition data derived from generic formula GSD(c) = N*ln(c)+1. Minimal long-term emissions are the emissions until the carbonate buffer in the landfill is used up. Mean long-term emissions are the emissions until the next ice age.	uncertainty of waste input composition data derived from generic formula GSD(c) = N*ln(c)+1

Tab. 2.9 Meta information for the disposal of composite material with paraffin and graphite

ReferenceFunction	Name	disposal, composite material, paraffin+graphite, to residual material landfill	disposal, composite material, paraffin+graphite, to municipal incineration
Geography	Location	CH	CH
ReferenceFunction	InfrastructureProcess	0	0
ReferenceFunction	Unit	kg	kg
ReferenceFunction	IncludedProcesses	Waste-specific short-term emissions to water from leachate. Long-term emissions from landfill to ground water.	waste-specific air and water emisions from incineration, auxiliary material consumption for flue gas cleaning. Short-term emissions to river water and long-term emisisons to ground water from slag compartment (from bottom slag) and residual material landfill (from solidified fly ashes and scrubber slugde). Process energy demands for MSWI.
ReferenceFunction	LocalName	Entsorgung, Verbundmaterial, Paraffin+Graphit, in Reststoffdeponie	Entsorgung, Verbundmaterial, Paraffin+Graphit, in Kehrichtverbrennung
ReferenceFunction	Synonyms		
ReferenceFunction	GeneralComment	Inventoried waste contains . waste composition (wet, in ppm): H2O n.a.; O n.a.; H 126320; C 873680; S n.a.; N n.a.; P n.a.; B n.a.; Cl n.a.; Br n.a.; F n.a.; I n.a.; Ag n.a.; As n.a.; Ba n.a.; Cd n.a.; Co n.a.; Cr n.a.; Cu n.a.; Hg n.a.; Mn n.a.; Mo n.a.; Ni n.a.; Pb n.a.; Sb n.a.; Se n.a.; Sn n.a.; V n.a.; Zn n.a.; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si n.a.; Fe n.a.; Ca n.a.; Al n.a.; K n.a.; Mg n.a.; Na n.a.; Share of carbon in waste that is biogenic 0%. Additional solidification with 0.001206 kg of cement.	Inventoried waste contains . waste composition (wet, in ppm): H2O n.a.; O n.a.; H 126320; C 873680; S n.a.; N n.a.; P n.a.; B n.a.; Cl n.a.; Br n.a.; F n.a.; I n.a.; Ag n.a.; As n.a.; Ba n.a.; Cd n.a.; Co n.a.; Cr n.a.; Cu n.a.; Hg n.a.; Mn n.a.; Mo n.a.; Ni n.a.; Pb n.a.; Sb n.a.; Se n.a.; Sn n.a.; V n.a.; Zn n.a.; Be n.a.; Sc n.a.; Sr n.a.; Ti n.a.; Tl n.a.; W n.a.; Si n.a.; Fe n.a.; Ca n.a.; Al n.a.; K n.a.; Mg n.a.; Na n.a.; Share of carbon in waste that is biogenic 0%. Share of iron in waste that is metallic/recyclable 0%. Net energy produced in MSWI: 0MJ/kg waste electric energy and 0MJ/kg waste thermal energy Allocation of energy production: no substitution or expansion. Total burden allocated to waste disposal function of MSWI. One kg of this waste produces 0.006595 kg of slag and 0.003014 kg of residues, which are landfilled. Additional solidification with 0.001206 kg of cement.
ReferenceFunction	Category	waste management	waste management
ReferenceFunction	SubCategory	residual material landfill	municipal incineration
ReferenceFunction	Formula		
ReferenceFunction	StatisticalClassification		
ReferenceFunction	CASNumber		
TimePeriod	StartDate	1994-01	1994-01
TimePeriod	EndDate	2000-12	2000-12
TimePeriod	OtherPeriodText	Waste composition as given in literature reference, theoretical data or other source. Transfer coefficients from prospective model.	Waste composition as given in literature reference, theoretical data or other source. Transfer coefficients for modern Swiss MSWI. Emission speciation based on early 90ies data.
Geography	Text	Technology encountered in Switzerland in 2000. Landfill includes base seal and leachate collection system.	Specific to the technology mix encountered in Switzerland in 2000. Well applicable to modern incineration practices in Europe, North America or Japan.
Technology	Text	Swiss residual material landfill for polluted, inorganic waste. With base seal and leachate collection system. Recultivation after closure.	average Swiss MSWI plants in 2000 (grate incinerators) with electrostatic precipitator for fly ash (ESP), wet flue gas scrubber and 29.4% SNCR , 32.2% SCR-high dust , 24.6% SCR-low dust -DeNOx facilities and 13.8% without Denox (by burnt waste, according to Swiss average). Share of waste incinerated in plants with magnetic scrap separation from slag : 50%. Gross electric efficiency technology mix 12.997% and Gross thermal efficiency technology mix 25.57%
Representativeness	ProductionVolume		
Representativeness	SamplingProcedure	Landfill model based on observed leachate concentrations in literature. Extrapolated to 60'000 years heeding chemical characteristics. Initial waste composition from various literature sources.	waste-specific calculation based on literature data
Representativeness	Extrapolations		Typical elemental transfer coefficients from current studies for modern MSWI, completed with data from coal power plants and estimates, adapted for inert/burnable waste.
Representativeness	UncertaintyAdjustments	uncertainty of waste input composition data derived from generic formula GSD(c) = N*ln(c)+1. Minimal long-term emissions are the emissions until the carbonate buffer in the landfill is used up. Mean long-term emissions are the emissions until the next ice age.	uncertainty of waste input composition data derived from generic formula GSD(c) = N*ln(c)+1

2.7 Data quality

The data for graphite are considered to be quite good for the purpose of this modelling. Also data for the expanded graphite and sodium acetate are assumed to be a good approximation for the intended purpose. The quality of the data for the production of the composite materials is not satisfactory as no real information for the necessary production process was available. The quality of the data for the disposal is good as the composition of the materials is well known.

3 Category indicators in the Life Cycle Impact Assessment

3.1 Life cycle inventory analysis

The LCA software SimaPro is used as the best suited for the purpose of this project (PRé Consultants 2007). The ecoinvent data v2.0 is used as background data (ecoinvent Centre 2007).

3.2 Impact assessment

The following impact categories are evaluated in the LCIA. The results for the materials investigated will be provided in an EXCEL table:

- Global warming potential
- Environmental scarcity 1997 (and if published 2006) (Brand et al. 1998; Frischknecht et al. 2007b)
- Cumulative energy demand

Fig. 3.1 shows the global warming potential of the investigated materials. The production of the expanded graphite causes much higher environmental impacts than the second materials sodium acetate or paraffin. But, for the final PCM material only a smaller share of graphite is used. This is why the results for this final material are lower than for the graphite.

The total greenhouse gas emissions for the PCM with sodium acetate are about 5 kg/kg. The incineration of the material after use is quite significant and adds 1.1 kg CO_2-eq/kg to this amount. The paraffin based material shows lower impacts during production that are more than outweigh by higher impacts during incineration. In the model for landfill it is assumed that carbon is partly leached with effluents, but not decomposed and directly emitted as CO_2.

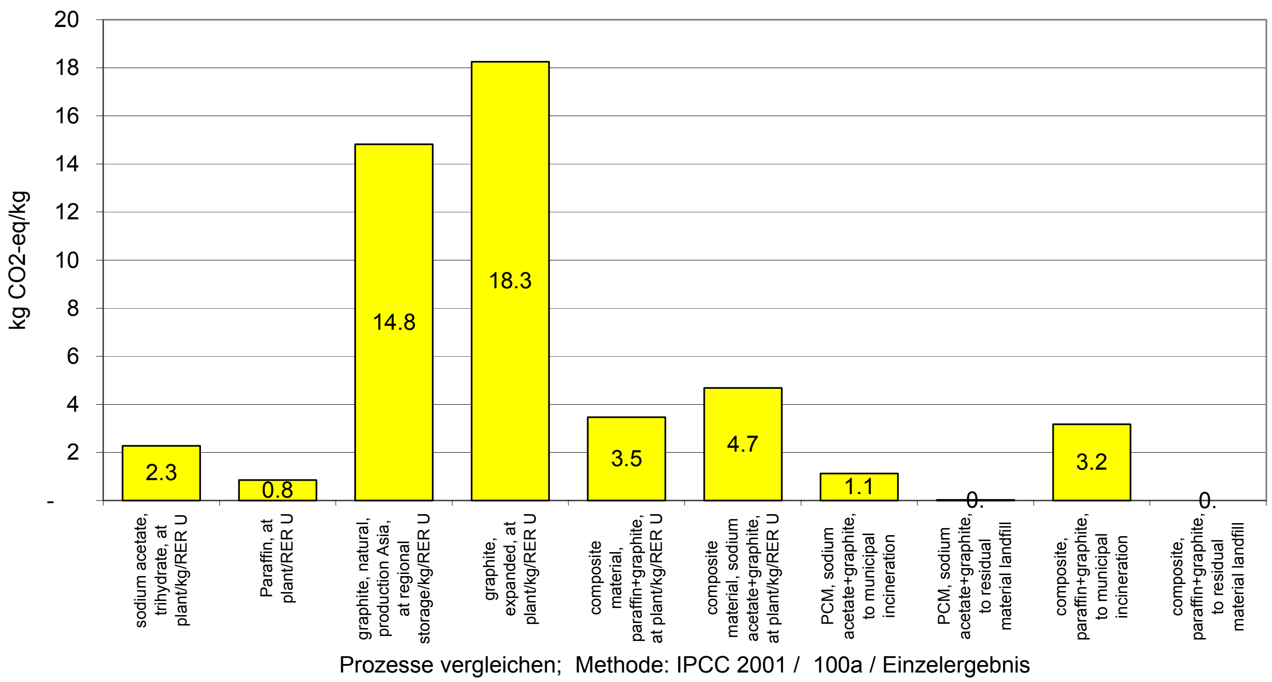

Fig. 3.1 Global warming potential of the materials investigated (kg CO_2-eq/kg)

Fig. 3.2 shows the non-renewable cumulative energy demand of all investigated materials.

The energy content of graphite is included in the calculation. Graphite is similar to coal and thus assumed to be a non-renewable resource. A second way of producing it would be from coke. This would also result in an energy content of the product. The higher heating value of graphite is 32.8 MJ/kg. This has been recalculated to the amount per kg Metamorphous Rock with (32.8/1.0526 =) 31.161 MJ-eq CED, fossil per kg Metamorphous Rock. This factor has to be introduced in the LCIA weighting of SimaPro.

The non-renewable cumulative energy demand of the PCM material is about 100 MJ/kg. There is no significant impact from the waste disposal for this indicator.

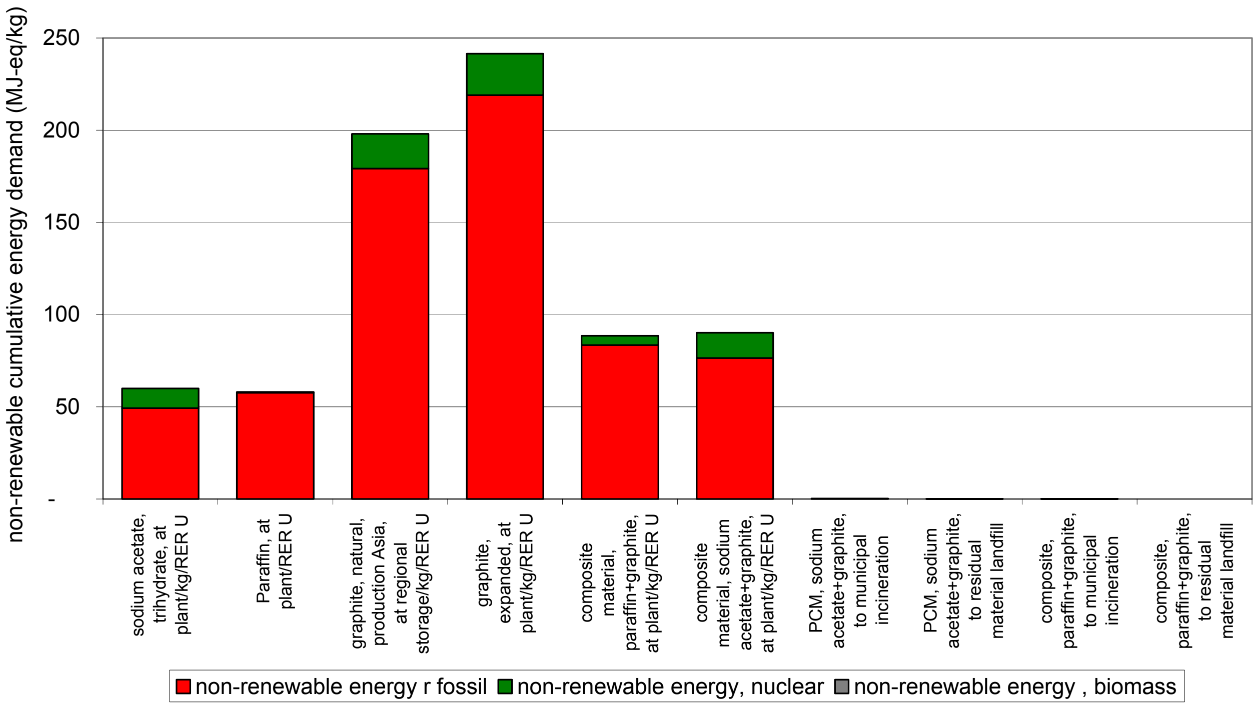

Fig. 3.2 Non renewable cumulative energy demand of the materials investigated (MJ-eq/kg)

Fig. 3.3 shows the Eco-points of all investigated materials. Also here a weighting factor for the energy content of graphite has been applied. The disposal of the materials is not very important compared to their production.

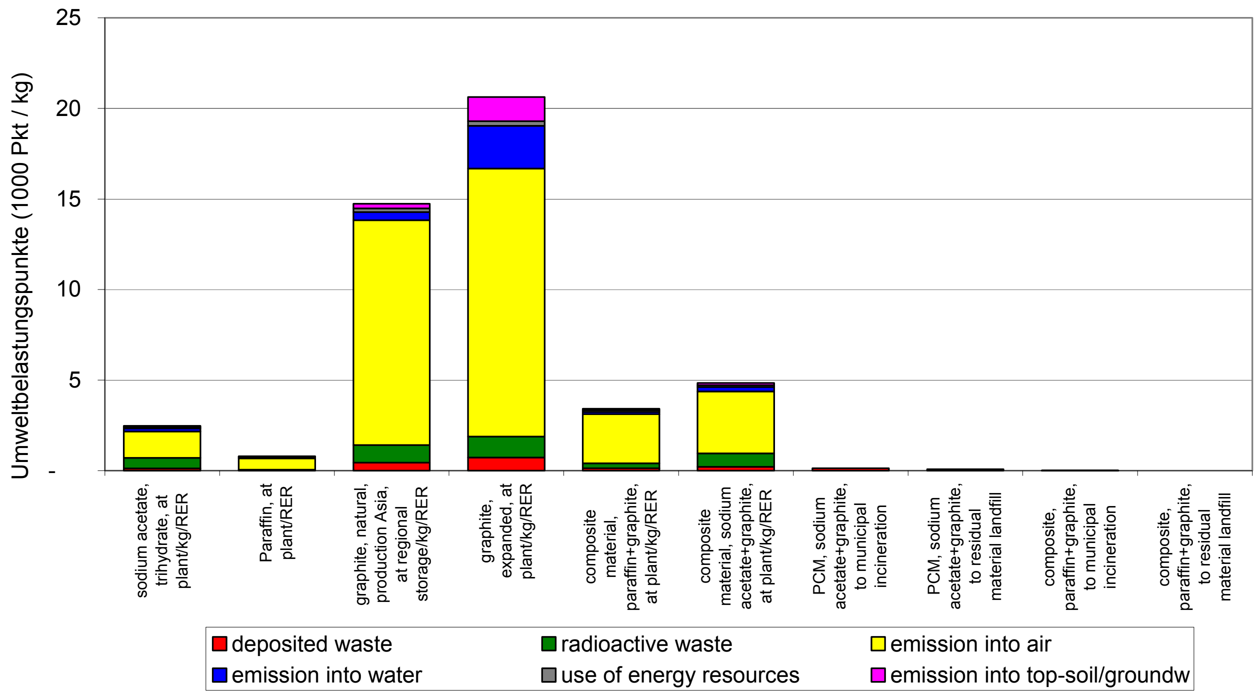

Fig. 3.3 Eco-points of the materials investigated (1000 Umweltbelastungspunkte 1997/kg)

4 Literature

Brand et al. 1998 Brand G., Scheidegger A., Schwank O. and Braunschweig A. (1998) Bewertung in Ökobilanzen mit der Methode der ökologischen Knappheit - Ökofaktoren 1997. Schriftenreihe Umwelt 297. Bundesamt für Umwelt, Wald und Landschaft (BUWAL), Bern.

Doka 2007 Doka G. (2007) Life Cycle Inventories of Waste Treatment Services. ecoinvent report No. 13, v2.0. EMPA St. Gallen, Swiss Centre for Life Cycle Inventories, Dübendorf, CH, retrieved from: www.ecoinvent.org.

ecoinvent Centre 2007 ecoinvent Centre (2007) ecoinvent data v2.0, ecoinvent reports No. 1-25. Swiss Centre for Life Cycle Inventories, Duebendorf, Switzerland, retrieved from: www.ecoinvent.org.

Frischknecht et al. 2007a Frischknecht R., Jungbluth N., Althaus H.-J., Doka G., Dones R., Heck T., Hellweg S., Hischier R., Nemecek T., Rebitzer G. and Spielmann M. (2007a) Overview and Methodology. ecoinvent report No. 1, v2.0. Swiss Centre for Life Cycle Inventories, Dübendorf, CH, retrieved from: www.ecoinvent.org.

Frischknecht et al. 2007b Frischknecht R., Steiner R. and Jungbluth N. (2007b) Methode der ökologischen Knappheit - Ökofaktoren 2006. Schriftenreihe Umwelt (noch im Entwurf). Bundesamt für Umwelt (BAFU), ÖBU Schweizerische Vereinigung für ökologisch bewusste Unternehmungsführung, Bern.

Hischier 2007 Hischier R. (2007) Life Cycle Inventories of Packaging and Graphical Paper. ecoinvent report No. 11, v2.0. EMPA St. Gallen, Swiss Centre for Life Cycle Inventories, Dübendorf, CH, retrieved from: www.ecoinvent.org.

Pehnt 2002 Pehnt M. (2002) Ganzheitliche Bilanzierung von Brennstoffzellen als zukünftige Energiesysteme. Dissertation. Universität Stuttgart, Fakultät Energietechnik, Düsseldorf.

PRé Consultants 2007 PRé Consultants (2007) SimaPro 7.1, Amersfoort, NL, retrieved from: www.pre.nl.