Life Cycle Inventories for the Production of Detergent Ingredients

Nr. 244

EMPA-Bericht

Silvio Dall'Acqua
Dr. Matthias Fawer
Renato Fritschi
Caroline Allenspach

St. Gallen 1999

EMPA

Eidgenössische Materialprüfungs- und Forschungsanstalt
Laboratoire fédéral d'essai des matériaux et de recherche
Laboratorio federale di prova dei materiali e di ricerca
Institut federal da controlla da material e da retschertgas
Swiss Federal Laboratories for Materials Testing and Research

Lerchenfeldstrasse 5
Postfach 755
CH-9014 St. Gallen
Tel. +41-71-274 74 74
Fax +41-71-274 74 99

EMPA

Report No 244

ISSN 0258-9745
ISBN 3-905594-09-9

Life Cycle Inventories for the Production of Detergent Ingredients

Actualised an harmonised data and methodology

Commissioned by
the German Federal Environmental Agency (UBA), Berlin
and the Öko-Institut e.V., Freiburg i.Br.

Report by:

Silvio Dall'Acqua, dipl. math.
Matthias Fawer, Dr.sc.nat. ETH
Renato Fritschi, dipl. ing.
Caroline Allenspach,
eidg. dipl. Wirtschaftsinformatikerin

Section Ecology
EMPA St.Gallen

St.Gallen 1999

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ABBREVIATIONS

AE	Alcohol ethoxylates
AOX	Adsorbable organic halogenes
APME	Association of Plastics Manufacturers in Europe
AzB	Abfall zur Behandlung (Waste for treatment)
BOD	Biological oxygen demand
CAS	Chemical Abstract Service
CEES	Centre Européen d'Etude des Silicates
CEFIC	Conseil Européen de l'Industrie Chimique (European Chemical Industry Council)
CESIO	Comité Européen des Agents de Surface et leurs Intermédiaires Organiques
CMC	Carboxymethyl Cellulose
COD	Chemical oxygen demand
DOC	Dissolved organic carbon
DQI	Data quality indicator
EAA	European Aluminium Association
ECOSOL	European Centre of Studies on Linear Alkylbenzene
EDTA	Ethylenediaminotetraacetic acid
EMPA	Eidgenössische Materialprüfungs- und Forschungsanstalt (Swiss Federal Laboratories for Materials Testing and Research)
EO level	Ethoxylation level
ETH	Eidgenössische Technische Hochschule (Swiss Federal Institute of Technology)
FAS	Fatty alcohol sulphates
FWA	Fluorescent whitening agent
GJ	Gigajoule
H_l	lower heating value
H_u	upper heating value
ISO	International Standardisation Organisation
n.i.	no information
LAB	Linear alkylbenzene
LAS	Linear alkylbenzene sulphonate
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LPE	Federal Law relating to Protection of the Environment
MJ	Megajoule
NaOH	Sodium hydroxide
Nm^3	Standard cubic metre
NordEl	Organisation for Nordic Electric Power Generation

NTA	Nitrilotriacetate
RiL	Rohmaterial im Lager (Rawmaterial in stock)
SAEFL	Swiss Agency for the Environment, Forests and Landscape (Buwal)
SETAC	Society of Environmental Toxicology and Chemistry
SPOLD	The Society for Promotion of Life Cycle Assessment Development
SRU	Schriftenreihe Umwelt (Environmental Series of SAEFL)
STPP	Sodium tripolyphosphate
SWI	Verband der Schweizerischen Seifen- und Waschmittelindustrie (Association of Swiss Soap and Detergent Manufacturers)
TAED	Tetraacetylethylenediamine
TNO	Dutch abbreviation for Netherlands Organisation for Applied Scientific Research
TOC	Total organic carbon
UBA	Umweltbundesamt (German Federal Environmental Agency), Berlin
UCPTE	Union for the Coordination of Production and Transmission of Electricity
ZeoDet	Association of Detergent Zeolite Producers, CEFIC sector group

SUMMARY

This study presents basic data on the manufacture of the most important chemicals contained in detergents. These data have been harmonised and updated and are published as unevaluated life cycle inventories.

Two different groups are targeted. The first is the users of these LCI's from detergent industry. In order to carry out an investigation into detergents and washing, the industry relies on the relevant basic data. Applying the data published here eliminates concerns over whether the data are compatible with each other, and they can therefore be combined quickly and simply. Users can be sure that:

1. A uniform methodology has been applied in the life cycle inventory analyses;
2. Joint basic data on energy production, transport and basic chemicals have been used;
3. The LCI parameters are compatible with each other; and
4. The structure of the individual LCIs is constant.

It is thus possible for users to obtain reliable and meaningful results. Through the qualitative descriptions in the individual inventories, they can also quickly recognise whether the data are appropriate to their needs.

The second target group consists of the LCA experts. The problem of LCIs that are incompatible due to the use of varied methodologies and basic data is a common one. The effort needed to make these comparable should not be underestimated. This study can be helpful in demonstrating problems that arise and possible ways of proceeding. The steps to be carried out are therefore as detailed as possible and are described in such a way that they can be followed. The straightforward user of the LCIs is probably less interested in this detail.

So how is the harmonisation we strive for achieved? In this study two routes are taken. In one, we start from existing LCIs (on silicates, zeolite A, phosphate, perborate, hydrogen peroxide, tensides). For these, the methodology used previously is adapted as far as possible to the EMPA methodology described in chapter 3. Here, no new process data are collected from the manufacturers but available published figures are used. Alternatively, LCIs are freshly compiled for those component substances being investigated for the first time, on the basis of information provided by the manufacturers (SKS-6, polycarboxylates, percarbonates, whitening agents, cationic tensides, CMC). This procedure leads to an optimal harmonisation of the LCIs with justifiable effort and expense.

1. INTRODUCTION

Detergents and their ingredients have recently been the subject of public environmental interest <Giger 1994>. Individual chemicals have attracted various levels of attention because of their high level of environmental pollution. This has led to the industry making efforts towards ecological optimisation of detergents. Several research projects have been undertaken with this in mind, and have produced reliable basic information.

Several studies over the last ten years have recorded ecological data on the manufacture of many of the chemicals contained in detergents. These studies were carried out at various institutes using differing basic data. EMPA itself has also performed some Life Cycle Assessments, on the mandate of the SWI (Association of Swiss Soap and Detergent Manufacturers) and the relevant European manufacturers' associations (sector groups of CEFIC). Over the same period, the methodology of life cycle assessment has also developed further and is now an ISO Standard <ISO14040 1997>, <ISO14041 1998>.

This heterogeneity necessarily leads to very non-uniform LCIs. However, this does not mean we should give preference to one or other methodology; within the context of the goals set at the time, each of these studies fulfils its purpose. The situation becomes problematic when results from the various individual studies are combined or compared. For example, if the complete life cycle of a detergent application is calculated on the basis of one particular equation, the end result must be questioned critically. The result is much more credible if all data are available in a harmonised form.

The objective of this study, commissioned by the Federal Environmental Agency (UBA, Berlin) and the Öko-Institut e.V. Freiburg (Germany), is therefore to prepare LCIs of chemicals contained in detergents in a harmonised and updated form. The first two steps of a life cycle assessment, definition of goal and scope, and compilation of an inventory, are carried out according to ISO 14040/41. The steps of impact assessment and evaluation are omitted, since they are meaningful only within the total view of a detergent's application.

The procedure chosen for harmonising the individual ingredients and updating them is described in detail in chapter 4. In addition to the new determination of process data, in LCIs already published, basic data is replaced or supplemented by the appropriate modules from SRU 250 <SAEFL 1998>. This basic data includs data on energy production and consumption, transport data, and data on the manufacture of basic materials. Data related to energy are often the decisive quantities within an LCA, and therefore it is particularly important to calculate them using uniform data.

A further move towards harmonisation involves adapting the parameter lists, which sometimes differ. This is also described in detail in chapter 4.

Methodological differences which arise out of the particular circumstances cannot always be avoided. The effects on the individual LCIs are therefore described and impacts estimated as far as possible.

The actual inventories are printed in chapter 5. They are supplemented by a qualitative description of the data, which uses the format suggested in SPOLD 1997. These details also enhance the comparability of the individual LCIs.

The Life cycle inventories also can be found on the diskette as Excel 97 file.

2. DETERGENTS

This chapter gives a brief overview of the application of detergent ingredients and of detergent use in the household and in commercial laundries.

2.1. The washing process

Laundering and cleaning in aqueous wash liquors is a complex process in which numerous physical and chemical influences interact. A detailed description of the processes can be found in the literature <Frieser et al.>, <de Oede 1992>, <Ullmann 1989b>.

By "washing" we understand the removal of deposits which are difficult to dissolve in water and the sequestration of water-soluble soils. The wash result is influenced by factors such as textile characteristics, type of dirt, composition of the water, washing technique (mechanics, duration, temperature) and the composition of the detergents. These mutually influential factors can usually be altered only to a limited extent. The composition of the detergent is thus of major importance.

Water serves as a solvent for the detergent and for soluble salts in the dirt, and also as a transport medium for the dispersed or colloidal soil components. The composition of the water, in particular its natural salt content, can act negatively on the washing effect and the washing machine. The hardness of water caused by calcium and magnesium compounds can produce precipitates in the form of carbonate, or through a reaction with washing powder ingredients which may appear as irritating deposits. The sequestering agent and ion exchanger contained in detergent should bind these alkalis or heavy metal ions.

From the point of view of washing, the most important types of soil can be divided into groups. We can distinguish water-soluble substances (salts, sugar, urea, sweat), pigments (metals, carbonates, silicates, humus, soot), fats, proteins, carbohydrates and bleachable dyes. The removal of the dirt from the surface can be coupled to a transformation of the substance (i.e. a chemical reaction) or can take place without modification. Examples of the first case are redox reactions using whitening agents, where oxidisable substances (e.g. natural dyes) are broken down, and the breakdown of protein soiling by enzymes. In very many cases, however, the soil consists of substances that are not altered chemically and are therefore removed from the fibres by purely physical procedures. This is also reflected in the composition of the detergents, the most important components of which are the tensides, the water-soluble sequestering agent and the water-insoluble ion exchanger.

The ability to remove dirt also depends on the type of textile substrate. Textile fibres that have a high content of calcium on the surface (e.g. cotton) differ substantially from synthetic textile fibres with low calcium content. The wetting ability and ability to wash out are also influenced by the level of hydrophobicity and hydrophilicity.

After being dissolved away the dirt must be stabilised in the wash liquor and its redeposition prevented. This characteristic is described as a wash liquor's soil antiredeposition capability. The most important principle of effectiveness in this connection is dispersion.

Detergents are mixed products that contain different types of substance. These may be divided into larger groups: **tensides**, **builders**, **bleaches** and **auxiliary agents**. The individual components have quite distinct features within the washing process, although their effects sometimes influence each other synergistically. This means that only the sum of all effects can ensure successful washing under different conditions <Frieser et al.>, <de Oede 1992>, <Ullmann 1989b>.

2.2. Tensides

Tensides form the most important group of all detergent ingredients; they are contained in all types of detergent. They are surface-active substances (i.e. surfactants) and have a polar (=water-soluble, fat-insoluble) and a nonpolar (=water-insoluble, fat-soluble) part. They can therefore arrange themselves on the interface between polar and nonpolar substances and achieve thorough penetration of both phases. The structure of the water-insoluble moiety has a significant influence on the characteristics of the tensides. While tensides with relatively unbranched alkyl residues usually demonstrate good washing but less extensive wetting characteristics, comparably strongly branched tensides show good wetting but poorer washing effects.

Depending on the charge of the part of the molecule carrying the alkyl chain, we distinguish anion-active tensides (**anionic tensides**), **nonionic tensides**, **cationic tensides** and **amphoteric tensides**. Anionic tensides predominate in terms of quantity. Nonionic tensides have also achieved considerable significance. Cationic tensides are used almost exclusively in post-laundry treatment substances because of their incompatibility with anionic tensides. Amphoteric tensides have been of minor significance up to now.

Soap is one of the **anionic tensides**. It is no longer as significant in today's detergents as it was before synthetic tensides could be manufactured on a large scale. The disadvantage of sensitivity to water hardness is a further factor leading to reduced significance of soap in detergents. Today, soaps serve in detergents primarily as foam regulators. **Linear alkylbenzene sulphonate (LAS)** has largely replaced soap as an active component because of its economy and its advantageous properties. This is true not just for its washing but also its foaming properties. The foaming behaviour of a tenside is of great importance to its application. Although LAS is very foam-intensive, its behaviour can be kept under control through the addition of suitable foam regulators (e.g. soap). Because of its good solubility, LAS is also useful in the formulation of liquid products. **Fatty alcohol sulphates (FAS)** and sulphonates also possess a very favourable washing ability and are thus increasingly used today, in universal as well as specialised detergents.

A significant advantage of **nonionic tensides** over anionic tensides is that the hydrophobic and hydrophilic parts of the molecule can be better tailored to one another. Optimal properties of adsorption and washing effect, with the same hydrophobic residue, may be produced using an appropriate ethoxylation level (often shortened to EO level). The washing effect reaches a peak at a certain EO level and then decreases. The proportion of nonionic tensides in the whole tenside production has been increasing over the last few years. These are primarily **fatty alcohol ethoxylates (AE)**. The increased use is largely due to the favourable washing properties, especially for synthetics and at low temperatures.

Cationic tensides show antagonistic behaviour to anionic tensides in terms of their ability to attach to solid bodies. Equimolar mixtures of anionic and cationic tensides are almost unadsorbed onto surfaces and are also not washing-effective. However, mixtures of nonionic tensides and cationic tensides are largely compatible. Such mixtures are partly used in special detergents with an scrooping effect (softeners). The tenside class of distearyl-dimethyl-ammonium chlorides (**esterquats**) are particularly used as fabric softeners <Frieser et. al>, <de Oede 1992>, <Ullmann 1989b>.

2.3. Builders

Builders in detergents have central significance in the washing process. The function of these substances is primarily to bind the calcium and magnesium ions which stem partly from the water and partly from dirt or textiles; and to support the effect of the tenside. Builder substances include **alkalis** (such as sodium carbonate and sodium silicates), **sequestering agents** (sodium tripolyphosphate, EDTA, NTA), **ion exchangers** (zeolite A, SKS-6) and **co-builders** (Polycarboxylate)

As **wash alkalis** raise the pH value, dirt and textile fibres become more strongly negatively charged and thus their mutual electrostatic repulsion is increased. Apart from this, the hardness components of the water are removed. The builders currently in use no longer remove the hardness formers from the water, but eliminate them through complex formation.

As a rule, temperature and the concentration of the **sequestering agent** are decisive factors in the elimination of high-value metal ions. For most sequestering agents, the binding ability decreases as the temperature increases. An extensive ability to bind earth alkali ions is important because of their high concentrations in water, compared to other high-value ions. Heavy metal ions, which have a very negative effect on the washing process even in the smallest quantities, must also be removed. Selectively active sequestering agents in small concentrations are generally used for this. In addition to the elimination of disturbing cations and the existence of a good washing effect, the dispersal of dirt to prevent greying are of the greatest significance for the washing process. Because of their adsorption by charged soil pigments, sequestering agents often act as a means of dispersal for these pigments.

Like the low molecular weight sequestering agents, the removal of disturbing polyvalent metal ions can also be achieved by **ion exchangers**. The insoluble zeolite A, a sodium aluminium silicate, has proved particularly useful for the washing process and is also of economic interest. Ion exchange is dependent on the size of the ions and their level of hydration. Besides Ca and Mg ions, Pb, Cu, Ag, Cd, Zn and Hg ions are also exchanged. In addition, it is advantageous to use combinations with water-soluble sequestering agents. For example, the builder system sodium tripolyphosphate / zeolite A guarantees excellent washing results, and largely prevents incrustations due to the precipitation of calcium and magnesium phosphate <Ullmann 1989b>.

Co-builders (e.g. watersoluble polymeres like polycarboxylate), besides its function as sequestring agents, shows also a pronounced threshold effect. This means they have an adsorptive effect on amophous and crystaline particles and dirt also in low concentration. These polymeres therefore prevent greying of the laundry <Frieser et al.>.

2.4. Bleaches

In chemical bleaching, stains that have an affinity to fibre and cannot be washed out are decoloured oxidatively through degradation of the chromophore systems. The bleaching effect achieved is determined by the type of whitening agent, its concentration and the time it spends in the washing process, the washing temperature and the stains which are to be bleached. Bleachable stains are usually of vegetable origin.

Two processes of oxidative whitening have been successful: peroxide and hypochlorite bleaching. In peroxide bleaching, which is commonest in Europe, perhydroxyl anions arise as an active transition substance in the alkaline medium of hydrogen peroxide. Hydrogen peroxide is delivered by inorganic peroxides and peroxyhydrates, the most important representative of which is **sodium perborate**. This hydrolyses in water with the formation of hydrogen peroxide, but on the other hand in detergents it has excellent stability. **Sodium percarbonate** (actually peroxyhydrates) must be additionally stabilised in order to be stored.

To achieve a good whitening effect with sodium perborate at temperatures below 60 °C, bleach activators (TAED) are often used. These are chemicals which, with the whitening agent, form peracids. At low temperatures these have a greater ability to oxidise than hydrogen peroxide.

Traces of copper, manganese and iron ions may enter the wash liquor through the dirt on the laundry, and also through tap water. These heavy metals can cause the breakdown of the bleaching agent, and thus chemical damage to the fibres, in the washing process. Addition of bleach stabilisers (magnesium silicate) stop most of the catalytic breakdown of perborate. A further way to eliminate heavy metal traces is the addition of selectively active sequestering agents of the EDTA type or organic sequestering agents <Frieser et al.>, <de Oede 1992>, <Ullmann 1989b>.

2.5. Auxiliary agents

Tensides, builders and whitening agents are the main components of modern detergents in terms of quantity, while the additives described below are used only in small quantities. However, they should not be overlooked in today's detergent formulations.

Enzymes:

Protein stains such as those from milk, cocoa, blood, egg yolk and grass are often as tough to remove from laundry as bleachable stains. Such impurities can usually be removed without difficulty in the washing process by protein-splitting enzymes. The effect of the enzymes rests on the enzymatic hydrolysis of peptide bonds. There are also fat-splitting enzymes.

Soil antiredeposition agents (Greying inhibitors):

Greying inhibitors act by attaching themselves to dirt particles and thus preventing soil and fibres re-attaching to one another. Classic greying inhibitors are **carboxymethyl celluloses (CMC)**. These substances however work only on cellulose fibres such as cotton. Certain tensides and special nonionic polymers are particularly suitable for synthetic fibres. Modern detergents usually contain mixtures of anionic and nonionic polymers.

Foam regulators:

Increased foam formation in drum washing machines leads to overfoaming of the wash liquor, often with substantial loss of wash-effective substances. In addition, the mechanical processing of the textiles to be washed is reduced. For this reason, additional foam regulators are used. However, only a few of the many regulators described in the patent literature have succeeded (e.g. **soap**).

Corrosion inhibitors:

The drum washing machines on the market today almost exclusively contain drums and laundry tubs made of corrosion-resistant stainless steel. Nevertheless, the fact that various machine components, particularly in older machines, are made of aluminium, has to be taken into account. To prevent the corrosive effect of the alkaline wash liquor on this metal, corrosion inhibitors in the form of **sodium silicates** are often mixed into washing powders.

Fluorescent whitening agents (FWAs):

FWAs are organic substances (fluorescent dyes) that are able to convert part of the invisible ultraviolet light contained in daylight into longer-wave blue light. The yellowish tone of a washed and bleached material is due to some of the blue wavelengths being absorbed from the white light falling on it, so that the reflected light lacks these blue wavelengths. The missing blue is added by the wavelengths emitted by the FWA, so that there is a higher level of whiteness and greater brightness. FWAs however have no actual washing action and are only effective when the laundry is clean.

Perfumes:

These substances are present not only to give the washing powder a pleasant smell, but more to cover the smell of the alkaline wash liquor that arises during the washing process. Furthermore, the washed laundry should be given a fresh and pleasant odour. The perfumes themselves are very complex mixtures.

Colorants:

Certain ingredients of washing powders are dyed for better recognition, so that the finished powder contains coloured particles as well as the basic white powder. Monochrome washing powders are also now available commercially. In liquid detergents the use of colorants is a general practice. Favourite colours are pink, blue and green.

Stabilisers and formulation additives:

Inorganic salts, especially sodium sulphates, are used as stabilisers for washing powders. They are intended to give the detergents good trickling ability, dosability and solubility. Clumping or dusting are also prevented.

<Frieser et al.>, <de Oede 1992>, <Ullmann 1989b>

2.6. Household detergents

The detergents found on the market can be divided according to type of use into **universal (all-purpose) detergents, special detergents, laundry aids** and **aftertreatment aids**

Under the term **universal detergent** we class detergents that are suitable for all washing procedures, and usually also at all washing temperatures. Previously, they were used in a somewhat different composition for whites up to 95 °C. Due to better-performing tenside combinations and enzymes, however, washing characteristics at temperatures between 30 °C and 60 °C have been significantly improved.

For certain kinds of textiles, such as woollens or synthetic fibres, **special detergents** were recommended for sensitive colours and when hand washing. They usually contain sodium perborate and no FWA. They are used if light-sensitive colours are present, or if there is a danger of dyes in pastel-coloured textiles running. Detergents for wool also contain no FWA. Many of these special detergents can be used for hand or machine washing. Greying inhibitors are added to detergents for net curtains, to prevent greying or yellowing. Strongly foaming hand-wash detergents are intended for occasional handwashing in basins.

Laundry aids of the pre-wash type assist in the removal of problematic stains, often only local, and are used in addition to detergents. Besides the classic fabric softeners, stain removers have also gained in significance. Fabric softeners are mostly strongly alkaline additives that loosen particularly tough soil, although pre-soaking plays a special role. Stain removers are tenside-rich products which are used to advantage on strong, localised fat stains. Water softeners are laundry aids that should also be mentioned. They usually contain sequestering agents and ion exchangers.

After the actual washing process, in which the main goal is the removal of dirt, the textiles are often submitted to **aftertreatment**. This attempts to restore certain characteristics to the laundry. Thus the textiles should be given elastic stiffness, a good sit, fullness, fatness, shine, softness, antistatic properties and so on as required. The main active substances of the soft rinses are cation tensides. Stiffness and fullness are obtained, on the other hand, with the use of stiffeners based on copolymers of vinyl acetate. The textiles treated with them are made firmer <Frieser et al.>, <Ullmann 1989b>.

2.7. Institutional detergents

Although the detergents used in the household and those used in commercial laundries act basically in the same way, the detergents used in laundries differ in that they must be tailored to the special conditions of institutional washing. In contrast to the home, soft water is often available in well-run laundries. It is usually obtained from softening plants by means of ion exchangers.

The development of continuously operating large-scale laundering plants, with rational use of water and energy, has made particular combinations of detergents necessary. This need has also arisen because of the desire to modify the procedure according to the type of washing and soiling, or to strengthen the effect of the detergent in a particular direction. Various partly tailored combinations are therefore used. The trend however is towards the simpler use of a single product, like the universal household detergents.

According to application, industrial laundries also work with special products. These include, for example, whitener-free detergents for coloureds and delicates, detergents for work clothes, and enzyme-containing products for particular protein-containing stains, or detergents with a disinfecting action.

3. METHODS USED BY EMPA ST GALLEN

3.1. General methodology

The methodology followed in this study is based on the work of ISO <ISO 14040/41>, SETAC <SETAC 1993>, and the ETH Zurich <Frischknecht et al. 1996>. This method has already been applied and published in the study SRU 250 by EMPA St.Gallen <SAEFL 1998>.

The method of life cycle assessment (LCA) can basically be divided into the steps **definition of goal and scope, inventory analysis, impact assessment** and **interpretation**. Although the field of planning measures is connected to life cycle assessment, it is not actually a component of an LCA.

In the goal definition step the purpose of the LCA and its target audience are established, the system under investigation is precisely defined and the functional unit is given. All conditions for the LCA, such geographical and temporal areas of validity, should be discussed and established in the goal definition. This step forms the basis for the procedure which follows.

After defining the goal and scope, the inventory is compiled. This step shows the environmental impacts over the defined area, establishes the impacts to be recorded (environmental parameters) and collects relevant data. The environmental impacts are recorded in inventories of substances and energy consumption. All values in the inventory are given in relation to the functional unit, and summarised in the life cycle inventory (LCI).

In the impact assessment of an LCA, the environmental damage caused by the individual impacts is assessed. For example, the damage caused by 1 kg CO_2 emitted into the air may be compared to 1 kg SO_2. There are various methods for this assessment, which differ in terms of practicability, basis for assessment and transparency <Buwal 1999>, <ISO/CD 14042 1998>.

The interpretation presents the results of the impact assessment and the information from the previous steps in such a way as to fulfil the purpose of the study and to give a basis for ecological decision-making. Methods of carrying out the evaluation phase are still being discussed and developed in professional circles. The literature is also of use here <SETAC 1993>; <SETAC 1996>, <ISO/CD 14043 1998>.

In undertaking a complete LCA, care should be taken that all the steps are connected and in harmony with one another.

The present study does not include all phases of an LCA. It contains only the first two, definition of goal and scope and compilation of the inventory. The impact assessment and interpretation phases are not undertaken in this study, since these steps are only meaningful for a complete detergent system, as is being carried out in the UBA project (see Chapter 1).

3.2. Methods of recording data

In life cycle assessment, input and output accounting is carried out via individual processes or modules. Input and output values are substances, forms of energy, or services that are assessed and that flow into or out of the appropriate processes. In this study, four levels are distinguished in the energetic and substance process outputs. The first is the so-called product level: products are intentional outputs. If several products arise in a process, the relevant product is described in the LCA as the **main product** and the others as **co-products** (or by-products).

Recoverable wastes appear on the second level. Those wastes that must be treated in special installations are classified at the third level (see Figure 3.1).

In addition to these outputs, emissions of substances into the air, water or possibly the soil are considered. These are unintentional, but arise through carrying out the process.

Emissions are principally recorded at the point at which they enter the environment, i.e. outside the human and technical sphere of influence. If purification steps are present, this means that emissions are shown not at the point of their first appearance but only after the cleaning steps have been taken.

Emissions of energy (e.g. waste heat) are not recorded in this study.

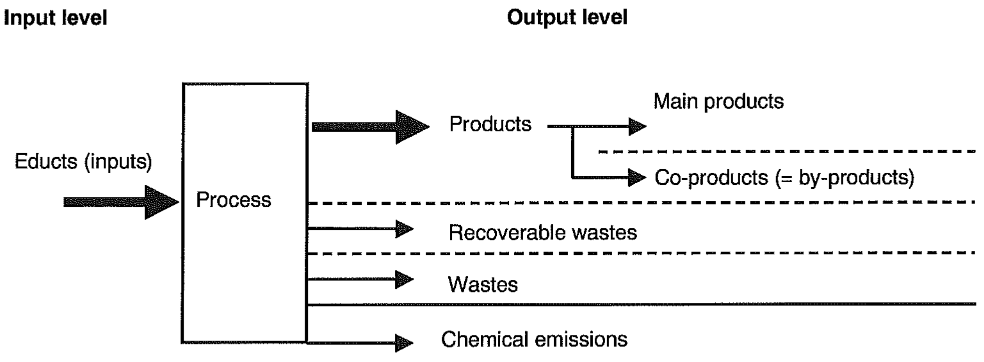


Fig. 3.1: The input and output levels of a process, as considered in this study <SAEFL 1998>.

All data are recorded according to these levels. If not already available in the literature, the data have been recorded using standard forms, as printed in Appendix F.

3.3. Definition of goal and scope

On the basis of life cycle assessments of detergent ingredients drawn up by several institutes at different times, different methods and parameters have been used. The goal of this study is to harmonise the existing LCAs of detergent ingredients or to draw up new ones (on SKS-6 and cationic tensides, polycarboxylates, percarbonate, FWA, CMC) according to ISO 14040/41, in order to reach a uniform list of parameters. The different fundamental data should also be comparable with one another. As far as possible, the same data modules were used for raw materials, heat and electricity production and transport, which sometimes required new calculations to be performed, even for existing LCIs. Where this was not possible, the differences are highlighted and their effects on the final result estimated. Table 4.1-4.4 (Chapter 4.1.) gives an overview of the studies carried out on the individual ingredients. The data should also give a picture of average European conditions.

The harmonised and newly compiled LCIs of the ingredients enable the product line analysis of washing and detergents carried out for the field of household detergents to be brought up to date (Produktlinienanalyse Waschen und Waschmittel <Griesshammer 1995>). In addition, institutional detergents will also be included in the substance flow analyses. These studies are carried out within the UBA project "Ökobilanzierung zu Wasch- und Reinigungsmittelrohstoffen und deren Anwendung in der gewerblichen Wäscherei" (Life cycle assessments of detergent ingredients and their use in commercial laundries) of the Öko-Institut e.V., Freiburg, Germany. This study's preparation of the harmonised fundamental data is part of that overall project.

3.4. Critical review

The critical review must ensure that

- the methods used to carry out the LCA are consistent with the ISO Standard 14040;
- the methods used to carry out the LCA are scientifically and technically valid;
- the data used are appropriate and reasonable in relation to the goal of the study;
- the interpretations reflect the limitations identified and the goal of the study;
- the study report is transparent and consistent.

<ISO 14040>

In this study the critical review was performed by Dr Rolf Bretz, Ciba S.C. Inc., Basel, based on the fourth draft of this report. In particular, the points detailed above should be guaranteed. Dr Bretz's report is given in Appendix A. The authors' statement and responses to the Critical Review can be found in Appendix B.

3.5. Functional unit

The functional unit establishes the unit of reference, to which all input and output details relate. It must be clearly defined and measurable.

The systems described end with the production of the relevant ingredient. All details in the inventory tables relate to the production of 1000 kg of the ingredient concerned in Europe. Precise details of water content, activity and other properties of the individual ingredients are given in the appropriate chapters.

3.6. System and system boundaries

The specific system boundaries of the individual detergent ingredients are presented in Chapter 4. The following principles also apply.

For most industrial systems, three main groups may be differentiated:

- **Main product line**
- **Additive production**
- **Energy production**

The main product line is the easiest to identify. It forms the actual subject of our interest.

The distinction between raw materials and additives is not established unequivocally. Additives are materials that are of significance for the system, but which are produced away from the main product line.

The third group covers energy production. Process and final energy represent all the energy needed for the processes. Their production, beginning with resources, should also be included. The following Figure 3.2 presents the relationships.

In the present study, in addition to the life cycle of the main product line, energy production and the production of additives are included in the calculations. Experience shows that the main product line and energy production cause the most environmental pollution. Construction and maintenance of infrastructure are not considered in any of these areas.

The infrastructure (manufacturing plants etc.) were not included in the calculations because recording them is extremely time- and labour-intensive, and because it can be assumed that many plants have already been in use for several years. The burdens resulting from the construction of plant, relative to 1000 t of the product, may therefore be regarded as insignificant. It can be assumed they are of the same order as the burdens produced by the infrastructure for energy production.

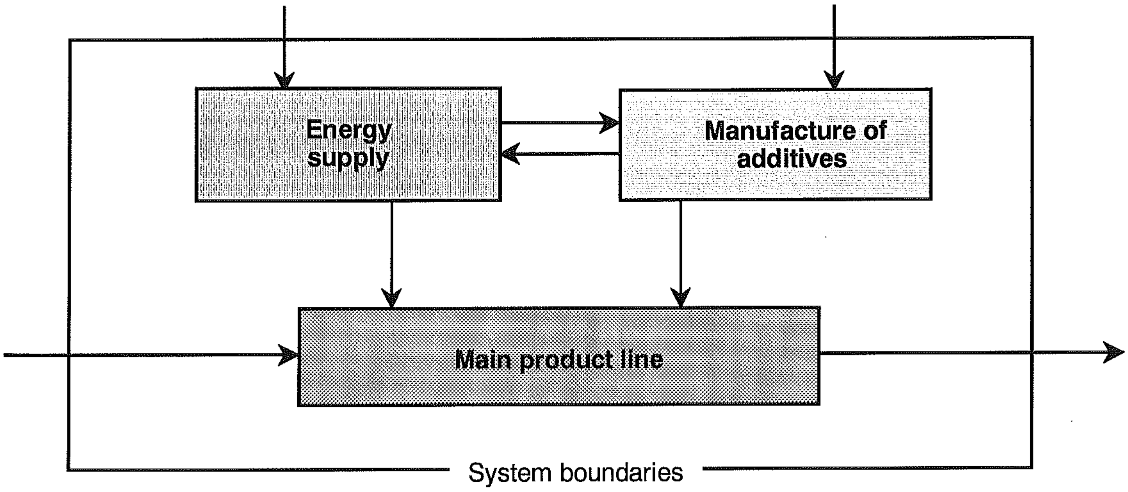


Fig. 3.2: Main product line, additive production and energy production, based on <Boustead 1992a> and <SETAC 1991>.

This study includes all processes for the production of chemicals contained in detergents as described by "cradle to factory gate". Consequently, the manufacture of the actual detergent and its use and disposal are not included.

Disposal processes for production wastes, e.g. incineration or landfill dumping, are considered in this study only when detailed routes of disposal and waste composition are known, or if meaningful assumptions can be made. Where this is not possible, the waste quantities are categorised according to Chapter 3.13.4 and shown in the inventory tables. An estimate of the environmental impacts these wastes have, based on an average composition, is not made as it would introduce errors.

3.7. Allocations

In LCAs, the distribution of environmental impacts to products, co-products and services is described as allocation. One example is the allocation of electricity consumption, and the environmental impacts connected with it, of an air liquefying plant to the products oxygen, nitrogen and argon.

The allocation of environmental impacts is carried out according to an allocation key, also known as an allocation rule. According to <TNO 1994> every allocation key must fulfil both the following requirements:

- the allocation takes place according to the polluter-pays principle, i.e. the environmental impacts of a process (e.g. emissions) are allocated to the products, co-products and services responsible for their creation. Here, it is important to recognise that there are no absolutely value-free criteria for determining the original responsibility.
- the sum total must add up ("100% rule"), i.e. in using the selected allocation key in a system, all the known inputs and outputs must be allocated to products, co-products and services.

In this study as far as possible allocation is prevented by dividing a process into sub-processes <ISO 14041 1998>. If not feasible the allocation is carried out according to the quantity relationships of main and co-products.

3.8. Data quality

The recording and processing of data quality has up to now been treated inadequately. This subject was first addressed by SETAC in a workshop in autumn 1992 <SETAC 1993>. In this study a **data quality indicator** (DQI) is recorded at the level of process data, and all the data are described at the level of the inventory table according to <SPOLD 1997> as precisely as possible.

Data quality at the process data level:

For the process data collected using the standard data recording forms (see Appendix F), data quality indicators have been required. These given information on the source, the creation and the type of the data. Table 3.1 explains the data quality indicators selected.

Origin of data	When data obtained	Type of data
B Company	I measured	e Single value
L Literature	II calculated	m Average of several single values
X Further	III estimated	x Other

Tab. 3.1: Data quality indicators (DQI) used for process data

At the level of the inventory table, no DQIs could be given as it is not possible to aggregate the DQIs of the individual environmental parameters of the modules into a higher indicator.

Data quality at the inventory table level:

A good data quality of the present Life Cycle Inventories is achieved by the highest possible transparency. This is done through a description of the data, which contains details of the data sources, the relative time period or the assumptions and simplifications made, relying on the SPOLD data format <SPOLD 1997>. For each inventory table the data explained in Table 3.2 are included.

Field	SPOLD field	Meaning
Type	201: DataSetInformation.Type	(Non-)terminated system or process. For a terminated system there are no input or output flows from or to the technosphere. Cradle-to-gate inventories are therefore always non-terminated. Wastes for disposal also belong in this study under "output to the technosphere" (see Chapter3.6)
Version	202: DataSetInformation.Version	Version of the data module. Every LCI (published or internal) of the concerning ingredient conducted by the data generator counts as version.
Time period	601: TimePeriod.StartDate 602: TimePeriod.EndDate	Indicates the period from which the data used originate.
Energy values	203: DataSetInformation.EnergyValues	Indicates whether upper or lower heating values have been used.
Timestamp	200: DataSetInfomation.Timestamp	The date on which the data were produced.
Geography	662: Geography.CountryCodes 663: Geography.Text	Indicates the geographical area for which the data are valid.
Technology	692: Technology.Text	Indicates the technology to which the data relate. State-of-the-art technology refers to the industrial procedures in use at the time of data collection.
Representativeness	722: Representativeness.Text	Indicates the representativeness of the data in relation to the total quantity of the ingredient produced in the relevant geographical area. In addition, the number of firms that produce the ingredient and contributed to the data are given, as far as is known.

Tab. 3.2 Headers for the qualitative data description of LCIs.

Field	SPOLD field	Meaning
In percent	723: Representativeness.Percent	Indicates the approximate representativeness of the data in percent in relation to the total quantity of ingredient produced in the relevant geographical area.
Data entered by	302: DataEntryBy.Name	Names the person who produced the data in its present form.
Original data generator	751: DataGeneratorAndPublication.Name	Names the person who originally generated or researched the data.
Data published in	756: DataGeneratorAndPublication.DataPublishedIn	Publication of the data by the original data generator.
Data sources	802: PrimarySources.SourceType 1002: SecondarySources.FirstAuthor	Data sources used for compiling the present data. This includes both primary data, as recorded using data recording forms and also data from the literature.
Name	401: ReferenceFunction.Name	Describes the chemical and physical properties of the product in the greatest possible detail.
German name	-	Describes the product in German.
Amount	404: ReferenceFunction.Amount	Together with the Name field this forms the functional unit of the product.
CAS No.	502: ReferenceFunction.CASNumber	CAS number of the product, if available.
Infrastructure	-	States whether the use of infrastructure is included in the system boundaries or not.

Tab. 3.2 Headers for the qualitative data description of LCIs. (continued)

3.9. Raw materials and thermal energy

Energy can be added to a system as electricity, as heat or as a material input. The energy contained in material does not always have to be used energetically in the system.

To determine energy consumption within a system, this study considers both types of energy input, used energetically and non-energetically. Here, the non-energetically used energy input, contained in material, is given as “Feedstock energy” and labelled as “**Feedstock**” in the inventory.

To calculate the inventories, the energy input must be calculated from its total environmental impact, i.e. resources (used as energy), emissions and wastes.

The combustion energy of fuels is as a rule determined experimentally and described as heating value. The upper heating value here is the maximum energy that could theoretically be obtained (including steam). For this reason it is a value for the total energy that could be used for a process.

In the present study, the upper heating value (H_u) is included in the calculations. This is because the actual quantity of heat released is more important, and not the quantity that could technically be used.

	Quantity	Supply [MJ]	H_u [MJ]	Total [MJ]
Heating oil EL	1 kg	8.0	45.4	53.4
Heating oil H	1 kg	14.9	42.3	57.2
Diesel	1 kg	7.3	45.4	52.7
Natural gas	1 m^3	5.3	40.2	45.5
Brown coal	1 kg	10.9	9.9	20.8
Coal	1 kg	5.2	30.3	35.5
Others	1 kg	50.0	0	50.0

Tab. 3.3: Heating values and supply energies used <SAEFL 1998>

Materials used in small quantities (<1% regarding to the functional unit) with unknown data on production are weighted with a flat 50 MJ/kg (see table 3.3.).

Where the ingredient manufacturers delivered differing heating values, the variation has been taken into account. This especially affects the values for natural gas (see Chapter 5).

Furthermore, the modules on heat production from SRU 250 <SAEFL 1998> have been used as far as possible. Differences from this procedure are described in Chapter 4 for the individual ingredients.

3.10. Electricity

In order to take the different volume of electricity production in the different countries into account, country-specific production mixes are calculated according to the following formula:

Country mix = Country consumption = Own production - Export + Import

The net trading balances are not considered, but the actual imports and exports. To calculate a country's mix, it is assumed that the imported electricity is used in that country and not exported further.

The country-specific data are used wherever a process under investigation can be allocated unequivocally to a country.

If the source of a substance or the location cannot be localised, as is the case for many additives, for example, the electricity associations of economic regions are used (UCPTE, Nordel).

Even with low European representation in the available process data, individual processes are calculated using the UCPTE model. Here, this procedure gives a better European average than country-specific data. The processes treated thus are given in Chapter 4.

Producing country	Hard coal	Brown coal	Oil	Natural gas	Nuclear power	Hydroelectric power	Others	Efficiency	Data source of production mix	Data source import/export
	[%]	[%]	[%]	[%]	[%]	[%]	[%]	[%]		
Belgium	22.8	0.0	2.2	14.2	58.4	2.4	0.0	28.7	UN	UCPTE
West Germany	28.9	18.8	1.2	4.5	39.3	6.3	1.0	28.6	National statistics	UCPTE, National statistics
Denmark	73.8	0.1	3.7	2.1	5.2	12.7	2.4	31.5	UN	UCPTE
France	7.3	0.4	2.1	1.5	72.9	15.7	0.1	30.4	UN	UCPTE
Great Britain	59.0	0.0	8.2	3.2	26.4	2.9	0.3	28.7	UN	UN
Italy	8.6	0.5	43.4	14.5	8.2	23.5	1.3	33.6	UN	UCPTE
Luxembourg	25.7	14.7	1.7	10.3	37.2	9.7	0.7	29.7	UN	UCPTE
The Netherlands	30.4	3.1	3.6	48.9	12.8	0.9	0.3	30.9	UN	UCPTE
Portugal	36.3	0.7	43.4	0.4	2.6	16.6	0.0	31.0	UN	UCPTE
Spain	30.5	9.9	9.2	1.7	35.4	13.3	0.0	30.0	UN	UCPTE

Tab. 3.4: Electricity models used <SAEFL 1998>, <Landbank 1994>, <WEC 1995>

Producing country	Hard coal	Brown coal	Oil	Natural gas	Nuclear power	Hydroelectric power	Others	Efficiency	Data source of production mix	Data source import/export
	[%]	[%]	[%]	[%]	[%]	[%]	[%]	[%]		
Switzerland	4.7	1.4	2.5	1.2	50.0	40.1	0.1	36.8	National statistics	UCPTE, National statistics
Austria	7.1	8.8	2.8	9.9	6.3	65.0	0.1	48.1	National statistics	UCPTE, National statistics
Norway	0.1	0.0	0.2	0.2	0.3	99.2	0.0	75.6	Nordel	Nordel
Sweden	0.9	0.0	5.9	0.1	39.5	53.6	0.0	41.6	Nordel	Nordel
Finland	21.1	0.0	14.4	9.1	31.2	24.2	0.0	33.2	Nordel	Nordel
Iceland	0.0	0.0	0.0	0.1	0.0	94.5	5.4	76.4	Nordel	Nordel
Slovenia	16.3	15.7	3.0	3.2	28.6	33.1	0.1	34.5	UN	UCPTE
UCPTE	17.4	7.8	10.7	7.4	40.3	16.4	0.0	31.0	UCPTE	
Nordel	11.8	0.0	5.3	1.5	21.8	59.2	0.4	44.7	Nordel	
Morocco	0.0	0.0	87.0	0.0	0.0	13.0	0.0		Landbank	Not considered
Malaysia	44.0	0.0	9.0	18.0	0.0	29.0	0.0	35.9	World Energy Council	No Imports
Philippines	7.0	0.0	56.0	0.0	0.0	15.0	22.0	35.8	World Energy Council	No Imports

Tab. 3.4: Electricity models used <SAEFL 1998>, <Landbank 1994>, <WEC 1995> (continued)

3.11. Transports

All transports between different production locations are considered.

Table 3.5 gives information on the energy consumption of the standard transports used. The details originate from SRU 250 <SAEFL 1998>. For transports with electricity consumption, an electricity model must also be chosen.

	Unit	Capacity	Heating oil H [kg]	Diesel [kg]	Petrol [kg]	Electricity [kWh]
Freighter overseas	tkm	60%	0.0022			
Freighter inland waterways	tkm	70%		0.011		
Private car western Europe	km			0.012	0.051	
Van 3.5 t	tkm	50%		0.0263	0.111	
Lorry 16 t	tkm	50%		0.0635		
Lorry 28 t	tkm	50%		0.0423		
Lorry 40 t	tkm	50%		0.0259		
Rail electric	tkm			0.0011		0.058
Rail electric/diesel mixed	tkm			0.0033		0.042

Tab. 3.5: Energy requirement of standard transports <SAEFL 1998>

Where exact transport distances are not known, a standard distance of 300 km is assumed (road, rail or combination).

3.12. Calculation of average values

It should be possible to use LCAs generally and not just in individual cases, thus the data they contain should be broadly based. The representative average value is sought. For the processes considered, several possible energy systems in various possible locations are considered. From this plethora of process data, there are several possible ways of calculating average values:

- at the energy level
- at the process level
- at the inventory level

If the creation of an average value takes place at the inventory level, the results obtained are least sensitive to changes in energy supply or location. We proceed according to the principle of "aggregation as late as possible". Figure 3.3 clarifies the procedure.

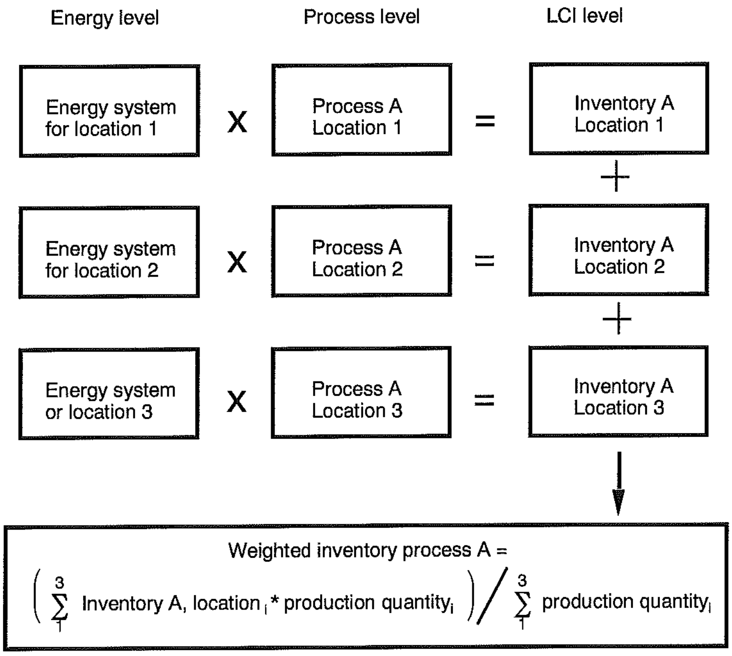


Fig. 3.3: Calculation of weighted average values

3.13. Composition of inventory and parameter list

The results table of an LCI contains a listing of:

- the qualitative description of the data (see Chapter 3.8):
  - headers
  - reference function
- the actual environmental impacts:
  - resources used as energy
  - resources used as raw material
  - recoverable wastes
  - disposal
  - air pollutants
  - water pollutants
  - water consumption
- separate details of energy consumption:
  - final energy requirement.

3.13.1. Resources used as energy

Under the heading “Resources used as energy” (commercial fuels), the non-renewable and then the renewable energies are presented, in the units in which they are measured (mass, volume). Finally, the potential energy of water used as a resource is given in MJ because details on quantity of water and height of drop are missing.

3.13.2. Resources used as raw materials

Under resources used as raw materials, the actual resources are given alphabetically and in their usual units of measurement (sizes, volumes). Energy resources that are not used energetically but as material input are labelled as Feedstock.

An asterisk (*) marks input materials, the production of which has not been inventoried due to a lack of information or minor relevance. They act as substitutes for the resources originally used for their production, and are debited with a flat amount of 50 MJ/kg. Emissions are not added together.

3.13.3. Recoverable wastes

Recoverable wastes do not have to undergo waste treatment, but can be used as inputs for other systems. The difference between this and co-production is the methodological procedure of compiling the inventory. No multipurpose allocation is carried out for recoverable wastes, but the environmental impacts are no longer considered in the calculated system because of their re-use.

3.13.4. Disposal

Waste category	Notes
Mineral wastes	Mining slag; dumped at place of excavation
Industrial wastes	Wastes for incineration or dumping (depending on country)
Inert wastes	Mineral and inert wastes to be dumped on a landfill.
Slag	Incineration residues for controlled dumping.
Special wastes	Wastes which will undergo special treatment.

Tab. 3.6: Waste categories used

The production wastes for which no detailed disposal routes or compositions are known, and where no useful assumptions can be made, are listed here. The production wastes are given according to quantity and divided into categories according to type of waste treatment (table 3.6.). An assessment of the environmental impacts of these wastes based on an average composition is not made, as this would lead to errors.

3.13.5. Air pollutants and water pollutants

Air and water pollutants are to be found in separate lists (Table 3.7.). They are based on the emission list in SRU 250 <SAEFL 1998> and represent the Standard used in this study. Chapter 4 explains how the parameters of the individual detergent ingredients are allocated to this list.

Note that fossil and geogenic CO_2 are shown among the air pollutants under “carbon dioxide fossil”.

The list of water pollutants includes the quantity of waste water. Multiple entries (recording the same emission under different parameters) have largely been avoided. Exceptions: in the energy modules based on the LCAs of energy systems <Frischknecht et al. 1996> the emissions of organic substances into water in refining, regional distribution and crude oil extraction and oil products, have been recorded partly as a single substance and also as COD. However, in the cases identified so far, they have had negligible if any influence on the results of the impact assessment <öbu 1998>. The resulting weightings for the various inventory parameters are thus summable. (See Appendix C on the problem of multiple entries in the TOC/DOC and COD/BOD fields.)

Emission parameters into air:	**Emission parameters into water:**
Ammonia (NH_3)	Waste water quantity
Aromatic HC	Aluminium (Al)
Benzene (C_6H_6)	Ammonium (NH_4^+)
Cadmium (Cd)	Antimony (Sb)
Carbon dioxide fossil (CO_2)	AOX as Cl^-
Carbon dioxide non-fossil (CO_2)	Aromatic HC
Carbon monoxide (CO)	Arsenic (As)
Chlorinated HC	Barium (Ba)
Chlorine (Cl_2)	BOD
Dust/particulates	Boron (B)
Fluorine (F_2)	Cadmium (Cd)
Halogenated HC	Chlorate (ClO_3^-)
Halon H1301	Chloride (Cl^-)
Hydrochloric acid (HCl)	Chlorinated HC
Hydrogen (H_2)	Chromium (Cr)
Hydrogen fluoride (HF)	COD
Lead (Pb)	Copper (Cu)
Manganese (Mn)	Cyanide (CN^-)
Mercaptans	DOC
Mercury (Hg)	Fats/oils
Metals	Fluoride (F^-)
Metals (Energy modules SRU 250)	H_2O_2
Methane (CH_4)	Inorganic salts and acids
Nickel (Ni)	Iron (Fe)
Nitrogen oxides (NO_x) as NO_2	Lead (Pb)
Nitrous oxide (N_2O)	Mercury (Hg)
NMVOC non-methane hydrocarbons	Metals
PAH polycyclic aromatic HC	Nickel (Ni)
Radioactive substances	Nitrate (NO_3^-)
Sulphur oxides (SO_x) as SO_2	Nitrogen organically bound
Zinc (Zn)	Nitrogen total
	PAH polycyclic aromatic HC
	Phenols
	Phosphate (PO_4^{3-})
	Radioactive substances
	Silicates
	Sulphate (SO_4^{2-})
	Sulphide (S^{2-})
	Suspended substances
	TOC
	Toluene (C_7H_8)
	Zinc (Zn)

Tab. 3.7 List of emission parameters used

The parameter for non-specific metal emissions into air deserve special mention. Where these originate in the basic data for energy production, they are quantitatively primarily non-heavy metals <SAEFL 1998, Chapter 16>. In the case of an impact assessment (e.g. using Eco-indicator 95) of the inventory data, therefore, no assessment should be made of the non-specific metal emissions from energy production. This procedure is also recommended by <öbu 1998>. In the inventories in Chapter 5 these non-specific metal emissions from energy production are shown separately from the other metal emissions, and labelled "Metals (Energy modules SRU 250)".

3.13.7. Water consumption

Water consumption is divided into process water, cooling water and washing water. Process water is actually a consumption of a raw material resource. This water should be considered as having been consumed, in contrast to cooling or washing water, which can leave the system again.

3.13.8. Final energy requirement

The total energy consumption is represented on the basis of the final energy carriers used. The consumption of final energy carriers "from cradle to gate" is given in energy units [MJ]. The energy is coupled, through the appropriate energy system and its level of effect, with the quantity of final energy carriers employed. For final energy, the expenditure in supply of final energy carriers (=supply energy) is given in MJ. This is not split further into energy carriers which explicitly deliver the supply energy. Materials that cannot be followed back to their resources are debited with a flat amount of 50 MJ/kg. Feedstock energy results from the energy resource input, and not used as energy, into the system. It is given in MJ under the heading of "Feedstock". The total energy consumption results from the sum of all these energies and is given in MJ under "Grand Total". Table 3.8 shows the format used.

The final energy requirement should be understood as a subtotal within the system boundaries, i.e. all resources required when using final energy, and emitted substances, are already contained in the appropriate inventory.

Final energy requirement (as additional information within the system boundaries)	Explanation
Electricity	Consumption of electrical final energy.
Biomass	Consumption of thermal final energy (wood, fruit of the oil palm, coconuts).
Diesel	Consumption of thermal final energy from diesel.
Natural gas	Consumption of thermal final energy from natural gas.
Heating oil EL	Consumption of thermal final energy from heating oil extra light.
Heating oil H	Consumption of thermal final energy from heating oil heavy.
Oil fuels	Consumption of thermal final energy from unknown final energy sources from oil.
Coal	Consumption of thermal final energy from coal.
Energy unspecified	Consumption of thermal final energy from unknown final energy sources.
Total final energy	Total consumption of final energy.
Energy production & delivery	Energy used to produce electrical and thermal final energy.
Auxiliary material (50MJ/kg)	Flat rate debit for materials not traced back to their resources.
Feedstock	Material inputs not used as energy, which could be used as energy.
Recovered energy	Energy recovered from processes, which can be used in the same system.
Total primary energy	Sum from sub-total to recovered energy.

Tab. 3.8 Final energy table

4. DESCRIPTION OF THE INDIVIDUAL DETERGENT INGREDIENTS

4.1. Overview

The following four tables give an overview of the chemicals contained in detergents investigated in this harmonisation and updating. For those substances for which no new data have been determined, the study used for the harmonisation is also given. Details of the individual data sources are also to be found in the relevant flow diagrams and in the headers of the inventory tables (Chapter 5).

Tensides	**Detergent ingredients considered**	**Studies carried out towards updating and harmonisation**	**Original study used for harmonisation**
Anionic tensides *Chap. 4.2.*	• LAS: Linear alkylbenzene sulphonate from petrochemical raw materials • FAS: alcohol sulphates from palm kernel oil • Soap: mixture with short-chain fats from coconut or palm oil	• Adaptation of the parameter list • New compilation using energy data from SAEFL SRU 250 <SAEFL 1998>	<Berna 1995> <Hirsiger and Schick 1995> <Postlethwaite 1995>
Nonionic tensides *Chap. 4.2.*	• AE: Alcohol ethoxylate with 7 EO chains from petrochemical raw materials	• Adaptation of the parameter list • New compilation using energy data from SAEFL SRU 250 <SAEFL 1998>	<Schul 1995>
Cationic tensides *Chap. 4.3.*	• Esterquat from coconut/palm kernel oil • Esterquat from tallow	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	-

Tab. 4.1 Overview of the tensides investigated

Builders	**Detergent ingredients considered**	**Studies carried out towards updating and harmonisation**	**Original study used for harmonisation**
Alkalies *Chap. 4.4.*	• Sodium silicate solution, hydrothermal • Sodium silicate spray powder • Sodium silicate, pieces • Sodium silicate solution, Furnace process • Sodium metasilicate	• Adaptation of the parameter list	<Fawer 1997>
Complexing agents *Chap. 4.5.*	• Sodium tripolyphosphate	• New compilation using energy and basic data from SAEFL SRU 250 <SAEFL 1998> • Adaptation of the parameter list	<Landbank 1994>
Ion exchangers *Chap. 4.6.*	• Zeolite A powder • Zeolite A slurry	• Adaptation of the parameter list	<Fawer 1996>
Chap. 4.4.	• Layered sodium silicate	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	-
Co-Builder *Chap. 4.7.*	• Polycarboxylates	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	<Fawer and Fecker 1993>

Tab. 4.2 Overview of the builders investigated

Bleaches	**Detergent ingredients considered**	**Studies carried out towards updating and harmonisation**	**Original study used for harmonisation**
Oxidising bleaches *Chap. 4.8..*	• Hydrogen peroxide • Perborate (tetrahydrate) • Perborate (monohydrate)	• New compilation using energy data from SAEFL SRU 250 <SAEFL 1998> • Adaptation of the parameter list	<Boustead and Fawer 1998 a,b>
Chap. 4.9.	• Sodium percarbonate	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	-

Tab. 4.3 Overview of the bleaching agents investigated

Auxiliary agents	**Detergent ingredients considered**	**Studies carried out towards updating and harmonisation**	**Original study used for harmonisation**
Fluorescent whitening agents *Chap. 4.10.*	• DAS-1 Triazinylaminostilbene-Type	• Actualisation and completion of the existing Life Cycle Inventories	<CIBA 1994>
Chap. 4.10.	• DSBP Distyrylbiphenyl-Type	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	-
Soil antiredeposition agents *Chap. 4.11.*	• Carboxymethyl cellulose (CMC)	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>	-

Tab. 4.4 Overview of the auxiliary agents investigated

Note on the flow diagram system:

The modules given in the flow diagrams with multiple boxes are not presented at a more detailed resolution, to retain the clarity of the overview . They are however traced back to the resources according to the general methodology. These modules are generally used as ready-calculated inventories, so that further division is not essential. The origin of the data used is given in italics in the individual modules. More precise details of these modules can be found in the references.

4.2. Anionic and nonionic tensides

Four classes of tensides were considered: linear alkylbenzene sulphonates made from petrochemical raw materials (**LAS**), fatty alcohol sulphonates from palm kernel oil (**FAS**), alcohol ethoxylates with 7 EO chains from petrochemical raw materials (**AE**), and **soap** as a mixture of short-chain fatty acids on the basis of coconut or palm oil. The descriptions used in <Ecosol 1995> for the modules are LAS, AS-PKO, AE7Pc and Soap CNO/PO.

4.2.1. Flow diagram

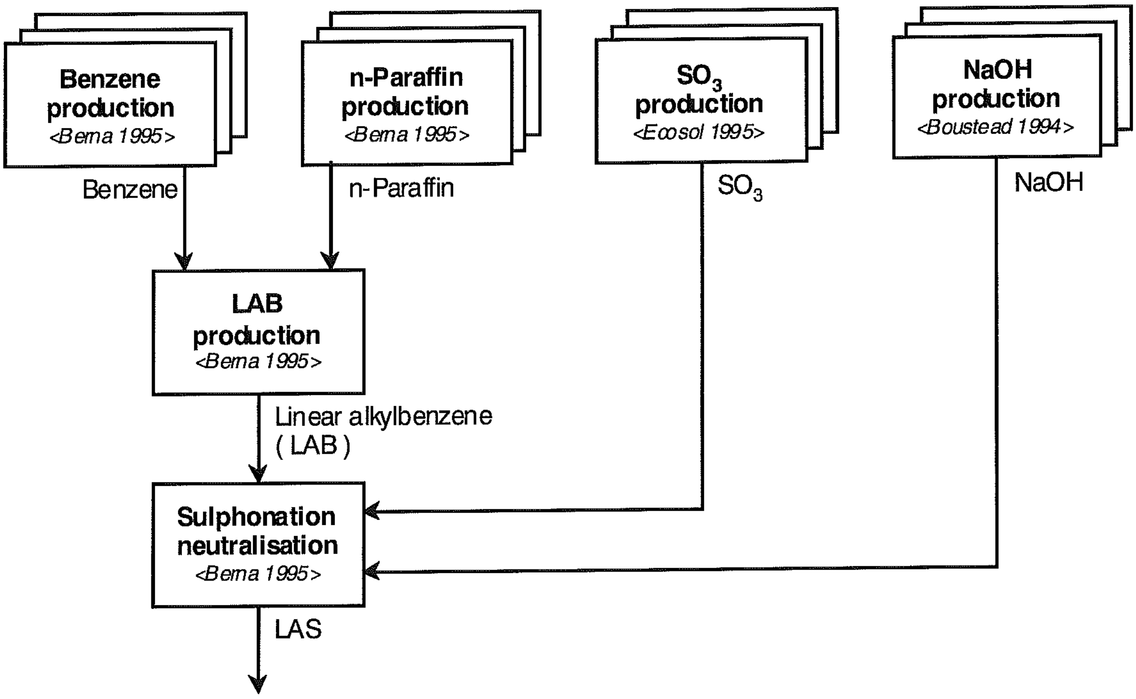


Fig. 4.1 Flow diagram of the manufacture of linear alkylbenzene sulphonates (LAS) from petrochemical raw materials; transport modules not included.

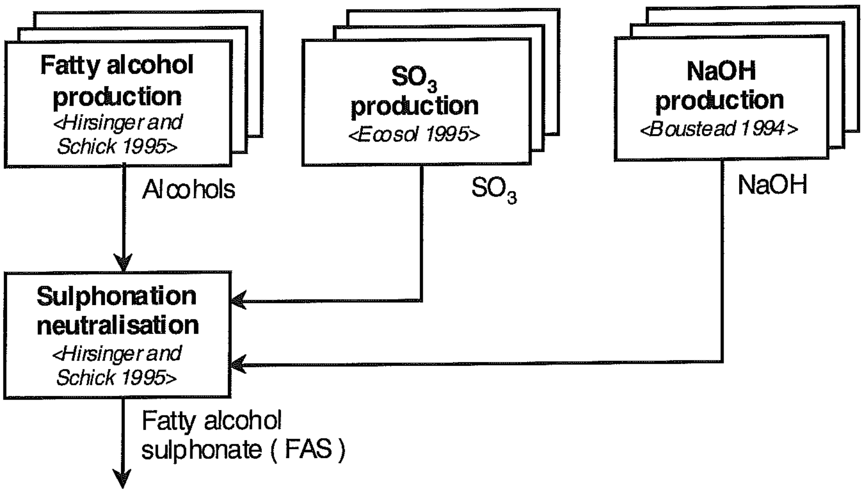


Fig. 4.2 Flow diagram of the production of fatty alcohol sulphonate: transport modules not included

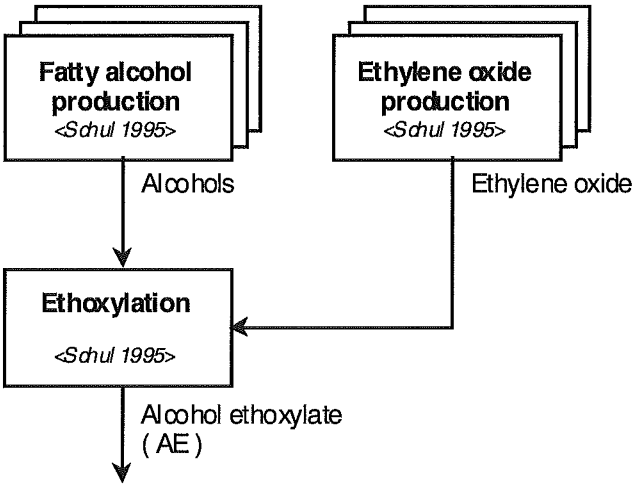


Fig. 4.3 Flow diagram of the production of alcohol ethoxylate: transport modules not included

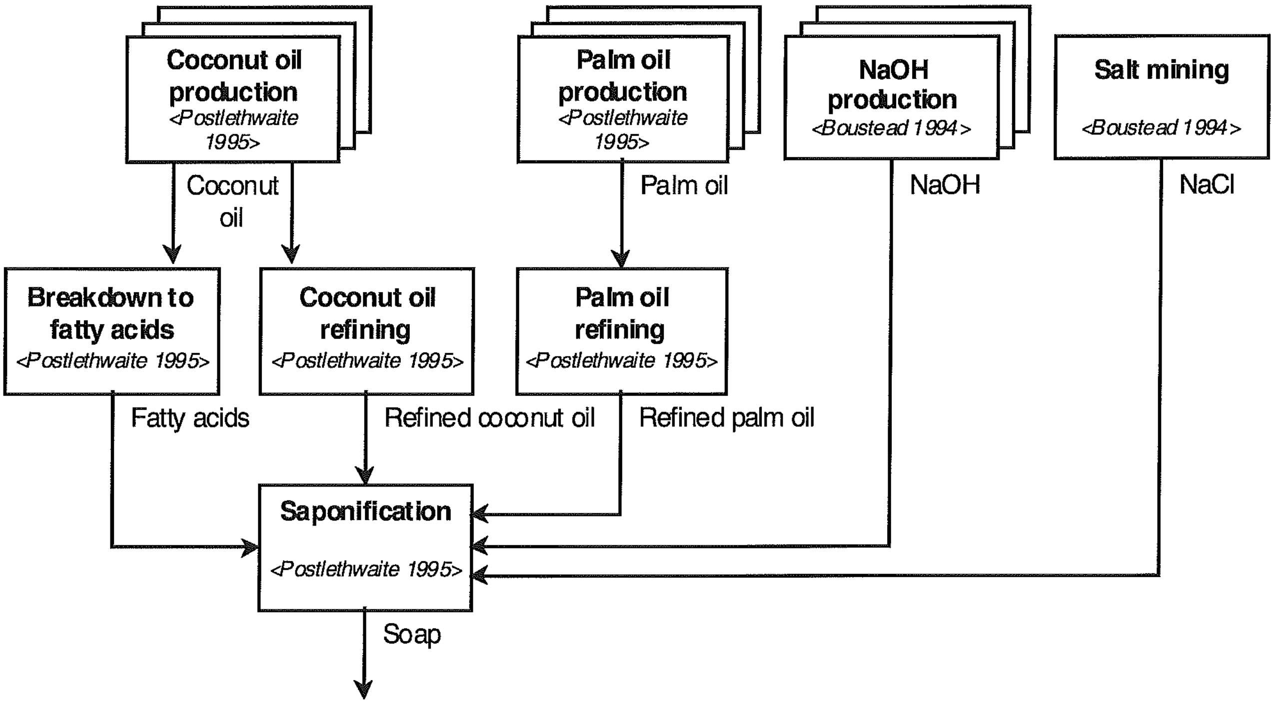


Fig. 4.4 Flow diagram of the manufacture of soap from a mixture of coconut oil and palm oil; transport modules not included

4.2.2. Summary of the production procedure

Linear alkylbenzene sulphonates (LAS) from petrochemical raw materials: R-C_6H_4-SO_3-Na

LAB (linear alkylbenzene) is the starting point for sulphonation. The manufacture of LAB can take place in two different ways: using the aluminium chloride ($AlCl_3$) process or the hydrofluoric acid (HF) process. In the HF process, benzene is alkylated directly with n-olefins, using HF as a catalyst. The n-olefins themselves are produced by catalytic dehydrogenation of n-paraffins. In the $AlCl_3$ process the benzene is alkylated with chloro-paraffins and /or n-olefins with the help of an $AlCl_3$ catalyst. In this process part of the n-paraffins are chlorinated, the remainder are used to produce n-olefins. The n-paraffins are responsible for the linearity of the alkyl chain in both processes. Sulphonation of LAB is then carried out, usually with SO_3. Here, an SO_3 group is added to the aromatic ring of the LAB molecule. The reaction is exothermic and requires careful control of the temperature. Finally, sodium hydroxide is used to neutralise the acid that has been produced <Berna 1995>.

Fatty alcohol sulphonates from palm kernel oil (FAS): $R\text{-}CH_2\text{-}O\text{-}SO_3\text{-}Na$

Fatty alcohols ($R\text{-}CH_2OH$) are the starting product for the manufacture of FAS. They can be produced from palm kernel oil, palm oil, coconut oil (C_{16} – C_{18}) or petrochemically (C_{12} – C_{15} chains). FAS is obtained by sulphonation of the alcohols. Here, a thin film of alcohol is brought together with a mixture of SO_3 and dry air inside a vertical tube. The heat produced by the reaction is removed using coolants outside the tube. SO_3 itself is produced through the catalytic oxidisation of SO_2, which derives from the combustion of sulphur or as a secondary product. After sulphonation, sodium hydroxide is used to neutralise the acid that has formed <Hirsiger and Schick 1995>.

Alcohol ethoxylates with 7 EO chains from petroch. raw materials (AE): $R\text{-}CH_2\text{-}O\text{-}(CH_2CH_2\text{-}O)_7H$

AE (fatty alcohol-polyglycol-ether) is produced by ethoxylation of fatty alcohols (C_{12} – C_{15} chains from petrochemical raw materials) using ethylene oxide ($RCH_2OH + n\ O\text{-}CH_2CH_2 \rightarrow R\text{-}CH_2\text{-}O\text{-}(CH_2CH_2\text{-}O)_nH$, here n=7). The reaction takes place at temperatures between 150 °C and 200 °C and under pressure. The deposition of a defined quantity of ethylene oxide on the fatty alcohol can be influenced in particular by the choice of catalyst. Usually, alkaline catalysts are used <Schul 1995>.

Soap from short-chain fatty acids from coconut or palm oil: $R\text{-}CH_2\text{-}CO_2Na$

What we call soaps are mixtures of solid or semi-solid alkaline salts (usually sodium salts) of higher fatty acids ($>C_8$). The most significant ingredients for their manufacture are, besides sodium hydroxide, natural oils and fats. The most important fats are ox tallow and coconut oil; palm oil and palm kernel oil also play important roles. Soap is obtained from these fats mainly in two ways: neutral oil saponification (approx. 90%) and fatty acid saponification (approx. 10%).

In neutral oil saponification, suitable fats and oils are saponified directly by sodium hydroxide:

$(CH_2\text{-}O\text{-}CO\text{-}R)_2(CH\text{-}O\text{-}CO\text{-}R) + 3\ NaOH \rightarrow 3\ R\text{-}COO\ Na + (CH_2\text{-}OH)_2(CH\text{-}OH)$,

In fatty acid saponification, distilled fatty acids are neutralised by sodium hydroxide:

$(CH_2\text{-}O\text{-}CO\text{-}R)_2(CH\text{-}O\text{-}CO\text{-}R) + 3\ H_2O \rightarrow 3\ R\text{-}COOH + (CH_2\text{-}OH)_2(CH\text{-}OH)$ und

$R\text{-}COOH + NaOH \rightarrow R\text{-}COO\ Na + H_2O$.

Glycerine is a by-product in both cases. Which route is the more favourable must be investigated on case by case basis. The expense of splitting the fats and the distillation of the fatty acids is not inconsiderable; however, fatty acid saponification is quite simple using modern techniques. Both types of saponification can be performed discontinuously or continuously. However, the discontinuous sieving process in open vats is expensive and not trivial. Closed, continuous plants are easier to operate.

During saponification, a certain electrolyte content is mandatory, which can be achieved by adding sodium chloride. The basic liquid soap produced, with a fatty acid content of approx. 60%, must finally be brought to a higher fatty acid content through drying, and then serves as a starting material for the manufacture of fine soaps <Ullmann 1993>.

4.2.3. Calculations performed and methodological variation

Original study used for the harmonisation:	• European Life-Cycle Inventory for Detergent Surfactant Production <Ecosol 1995>; in particular data for LAS, AS-PKO, AE7Pc and Soap CNO / PO
Studies carried out towards updating and harmonisation:	• New compilation of the inventories using energy data from SAEFL 1998 • Adaptation of parameter lists

New compilation of inventory tables:

Energy data are often a decisive component of LCAs. To improve harmonisation, it is therefore sensible to use the same basic data for the calculations. In <Ecosol 1995> there are no details of the final energy required. The final energy consumption therefore had to be estimated from the figures available. The new energy-derived emissions are calculated from this. To these can be added the process emissions published in <Ecosol 1995> in order to arrive at a complete LCI. The estimates made are described in detail in the following tables. Explanations of the individual columns can be found in the text below.

LAS	Primary energy [GJ], Total without Feedstock	Primary energy, electrical [GJ]	Primary energy, thermal [GJ]	Heating value [MJ/ kg]	Primary energy, thermal [kg]	Conversion factors	Final energy, thermal
Nuclear power	2.29	2.29 (40 %)	0	-	-	-	-
Hydroelectric power	0.43	0.43 (8 %)	0	-	-	-	-
Coal	4.60	1.95 (34 %)	2.65	27.1	97.92	1.66	58.99 kg
Gas	8.52	0.46 (8 %)	8.06	52.6	153.27	1.05 * 0.80	182.46 m3
Oil	8.10	0.57 (10 %)	7.53	43.9	171.47	1.10	155.88 kg
Total	23.94	5.73 (100 %) = 493 kWh	18.22				

Tab. 4.5 Determination of thermal and electrical final energy consumption for LAS from <Berna et al. 1995>

FAS	Primary energy [GJ], Total without Feedstock	Primary energy, electrical [GJ]	Primary energy, thermal [GJ]	Heating value [MJ/ kg]	Primary energy, thermal [kg]	Conversion factors	Final energy, thermal
Nuclear power	1.95	1.95 (40 %)	0	-	-	-	-
Hydroelectric power	0.88	0.88 (18 %)	0	-	-	-	-
Coal	5.05	1.22 (25 %)	3.83	27.2	140.85	1.66	84.85 kg
Gas	7.10	0.34 (7 %)	6.76	52.8	128.01	1.05 * 0.80	152.39 m3
Oil	8.22	0.49 (10 %)	7.73	45.2	171.07	1.10	155.52 kg
Total	23.20	4.88 (100 %) = 420 kWh	18.32				

Tab. 4.6 Determination of thermal and electrical final energy consumption for LAS from <Hirsiger and Schick 1995>

AE	Primary energy [GJ], Total without Feedstock	Primary energy, electrical [GJ]	Primary energy, thermal [GJ]	Heating value [MJ/ kg]	Primary energy, thermal [kg]	Conversion factors	Final energy, thermal
Nuclear power	2.86	2.86 (40 %)	0	-	-	-	-
Hydroelectric power	0.34	0.34 (5 %)	0	-	-	-	-
Coal	4.82	2.86 (40 %)	1.96	29.4	66.67	1.66	40.16 kg
Gas	16.90	0.72 (10 %)	16.19	53.1	304.80	1.05 * 0.80	362.86 m3
Oil	4.00	0.36 (5 %)	3.64	43.9	82.97	1.10	75.43 kg
Total	28.92	7.15 (100 %) = 616 kWh	21.79				

Tab. 4.7 Determination of thermal and electrical final energy consumption for AE from <Schul 1995>

Soap	Primary energy [GJ], Total without Feedstock	Primary energy, electrical [GJ]	Primary energy, thermal [GJ]	Heating value [MJ/ kg]	Primary energy, thermal [kg]	Conversion factors	Final energy, thermal
Nuclear power	0.58	0.58 (40 %)	0	-	-	-	-
Hydroelectric power	0.20	0.20 (14 %)	0	-	-	-	-
Coal	1.15	0.39 (27 %)	0.76	25.4	29.86	1.66	17.99 kg
Gas	1.44	0.12 (8 %)	1.32	45.0	29.42	1.05 * 0.80	35.02 m3
Oil	7.66	0.16 (11 %)	7.50	42.1	178.16	1.10	161.96 kg
Total	11.03	1.45 (100 %) = 125 kWh	9.58				

Tab. 4.8 Determination of thermal and electrical final energy consumption for soap from <Postlethwaite 1995>

Primary energy [GJ], Total without Feedstock:

This column lists the quantities of primary energy given in <Ecosol 1995>, minus the proportion of Feedstock energy

Primary energy, electrical [GJ]:

The fraction of nuclear energy from <Ecosol 1995> is used as a guide. The estimate is based on the assumption that nuclear energy accounts for 40% of the total electrical primary energy consumption of the processes localised to Europe. This figure accords with the UCPTE mode (see Chap. 3.10.). The total electrical primary energy consumption is calculated from this. The fractions of other energy carriers for electricity production are subsequently brought closer to the UCPTE model. The percentages used are given in brackets. From the electrical primary energy consumption in GJ we can calculate the electricity consumption required in kWh with the efficacy of the UCPTE model ($\eta = 0.31$; a differentiation in the level of efficacy according to tenside has not been made) using the equation:

$$E[kWh] = \frac{1000}{3.6} \times \eta \times E[GJ]$$

Primary energy, thermal [GJ]:

The difference between total and electrical primary energy gives the fraction of thermal primary energy. In determining the difference it should be noted that the total primary energy in <Ecosol 1995> also contains a fraction of Feedstock energy that therefore has already been subtracted.

Heating value [MJ/kg]:

The heating values used in <Ecosol 1995> are calculated from the relationship between the energy used in GJ and the quantity used in kg. The values vary for different tensides. One reason for this is the variable fuel qualities. Another is the use of data sources with different origins.

Primary energy, thermal [kg]:

Using the heating values given, the primary energy consumption is converted from GJ to kg.

Conversion factors:

The factors given in this column are used to convert the thermal primary energy consumption into thermal final energy consumption. Here it is assumed that 1.10 kg crude oil are required to produce 1 kg heating oil heavy. Similarly, 1 kg natural gas require 1.05 kg crude gas and 1 kg coal 1.66 kg raw hard coal. These factors have been obtained with the help of <Boustead 1992b>, <Boustead 1993a> and <SAEFL 1998>. In addition, natural gas is calculated at a density of 0.80 kg/m^3 <SAEFL 1998>.

Final energy, thermal:

This column contains the quantities of final energy used to calculate the LCIs anew.

Comparison between data in <Ecosol 1995> and this study:

Table 4.9 compares the energy totals and CO_2 emissions of the original data in <Ecosol 1995> and the newly calculated data of this study. From this it can be seen that the original values have been reasonable well reproduced. CO_2 emissions can usually be determined precisely, so that good agreement of these values indicates a good criterion for a new calculation.

Per 1000 kg	Total energy <Ecosol 1995>	Total energy this study	Fossil CO_2 <Ecosol 1995>	Fossil CO_2 This study
LAS	60.9 GJ	63.4 GJ	1613 kg	1666 kg
AS-PKO	55.8 GJ	56.3 GJ	1410 kg	1375 kg
AE-7Pc	78.8 GJ	78.7 GJ	2210 kg	2193 kg
Soap CNO / PO	47.3 GJ	49.3 GJ	675 kg	793 kg

Tab. 4.9 Comparison of the data in <Ecosol 1995> with the newly calculated data.

Evaluated comparison of the data from <Ecosol 1995> and this study:

Total energy and CO_2 emissions are not in themselves amounts that affect the environment. A comparison of the evaluated data (model: Eco-Indicator 95) from <Ecosol 1995> and the newly calculated data of this study is shown in Figure 4.5. A clear increase in impact through heavy metals is compensated by a reduction in potentials for acidification and summer smog. The heavy metal emissions stem from the energy supply chain and reflect the improved state of the data for this field. On the other hand, the emissions of nitrogen and sulphur oxides are lower in the energy systems from SAEFL 1998. This may be explained by the fact that these are European averages, which tend to be rather smaller than certain country-specific emission values for energy systems.

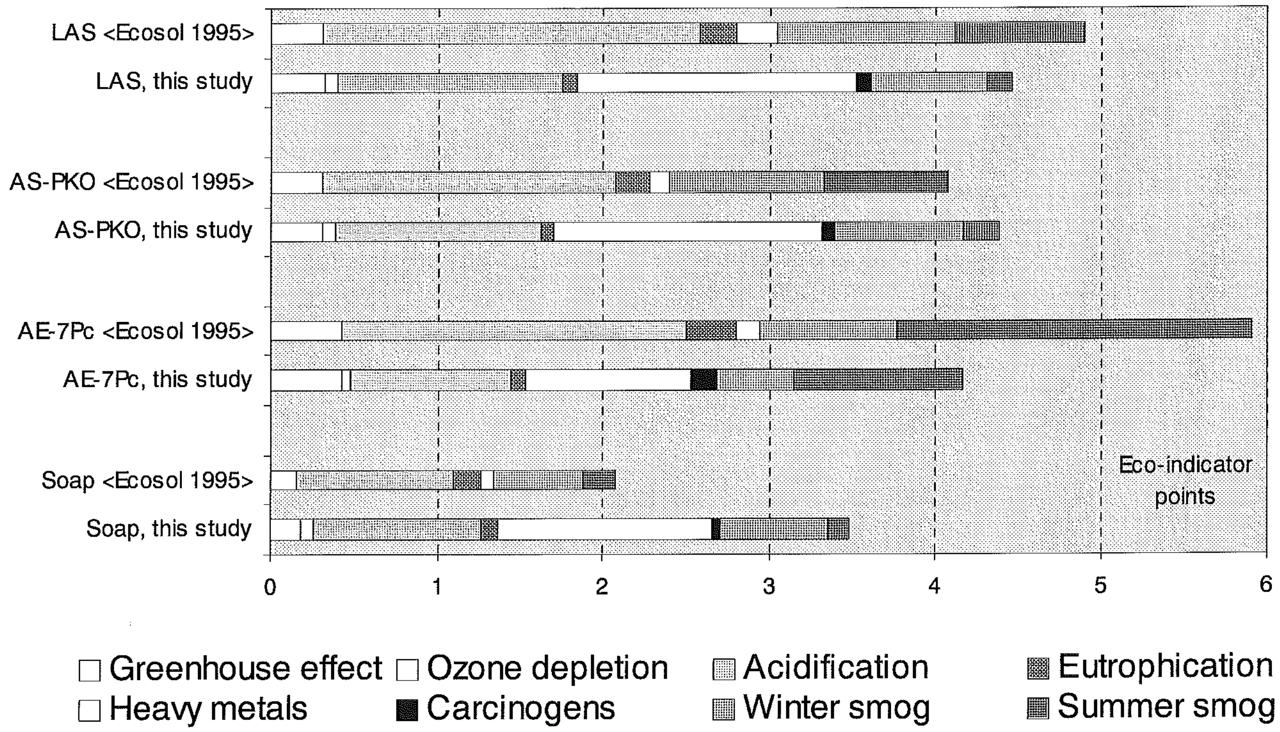


Fig. 4.5. Emission profile of tensides from <Ecosol 1995> and the newly calculated inventories, evaluated using Eco-indicator 95.

Adapting the parameter lists:

The parameter lists of LAS, FAS, AE and soap in <Ecosol 1995> have been adapted to the structure used in this study. All changes were made analogously to the procedure used in SRU 250 <SAEFL 1998>.

Table 4.10 gives an overview of how and with what conversion factors, the parameters from <Ecosol 1995> have been used. The conversion factors result from the relationship between the atomic weights. All parameters not given in Table 4.10 have been taken directly.

Parameters in <Ecosol 1995>	**Conversion factors**	**Parameters in this study**
Atmospheric emissions		
Hydrocarbons Other organic compounds Aldehydes	-	Non-methane VOCs (NMVOC)
Water emissions		
Acid as H+ Dissolved solids	- -	Inorganic salts and acids
Hydrocarbons	0.85	TOC
Fluorides (NB: sodium fluoride)	0.452	Fluoride (F^-)
Phosphate as P_2O_5	1.338	Phosphate (PO_4^{3-})
Ammonia as NH_3	1.06	Ammonium (NH^{4+})
Nitrogen	-	Nitrogen total
Wastes		
Total solid waste	-	Industrial wastes

Tab. 4.10 Arrangement of the parameters from <Ecosol 1995>

Under resource consumption, the values for crude oil and raw hard coal could be applied directly; crude gas was converted with a density of 0.8 kg/m^3 from kg to cubic metres. Uranium from ore has been calculated from "Nuclear" with an energy content of 451 MJ/g.

Variations in methodology from standard procedures:

Chlorine, which is needed to manufacture LAS, does not itself appear as a component of LAB. For this reason, its production was not considered in <Ecosol 1995>. The total burden of chlorine production is assigned to the co-product hydrochloric acid.

Since the data in <Ecosol 1995> are presented only cumulatively, it is not possible to use the standard modules for the basic materials and transports from <SAEFL 1998> in the calculations. Therefore, the modules used in <Ecosol 1995> are contained in the LCIs published here.

4.3. Cationic tensides (fabric softeners)

4.3.1. Flow diagram

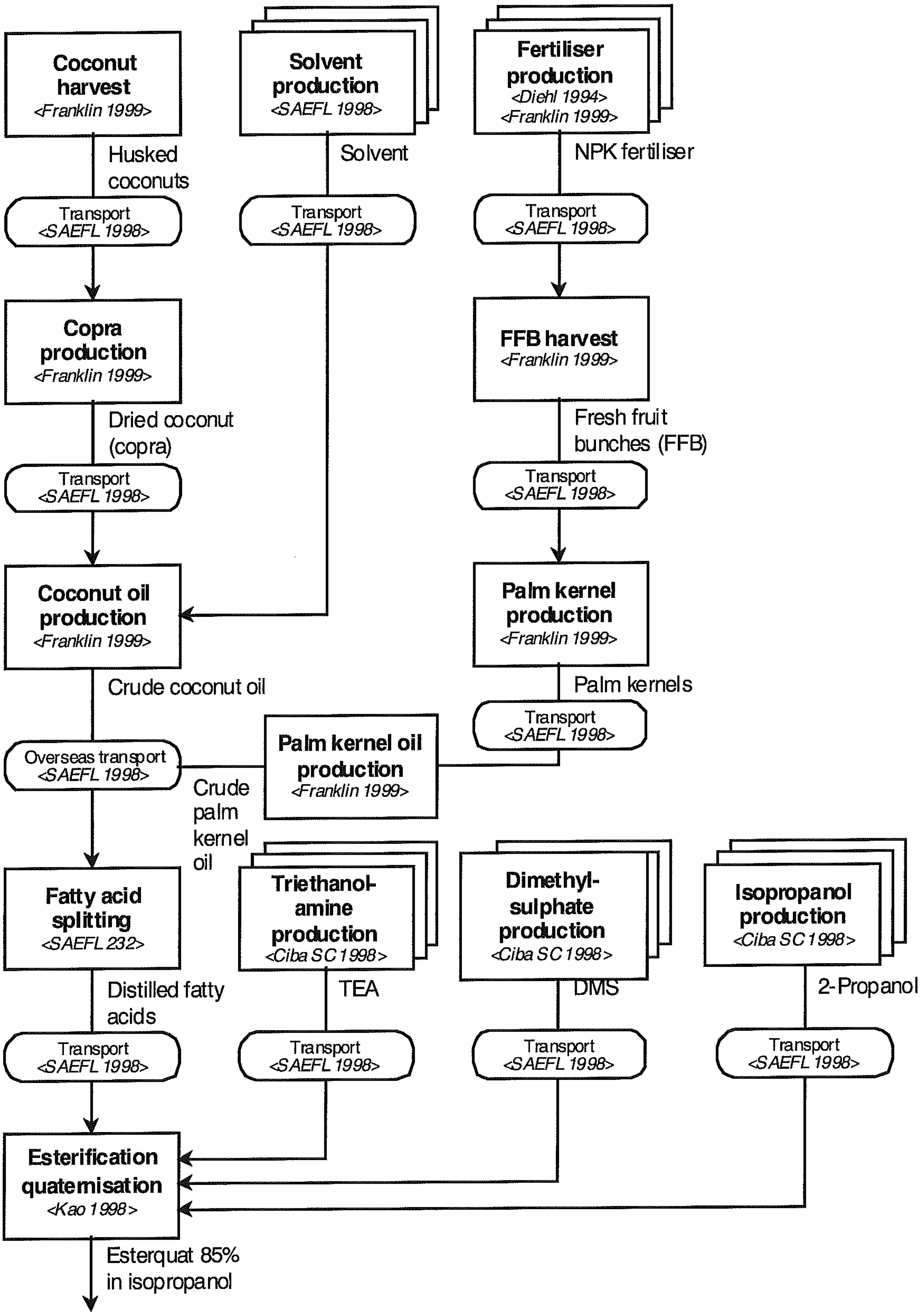


Fig. 4.6 Flow diagram of the manufacture of esterquat from coconut oil / palm kernel oil

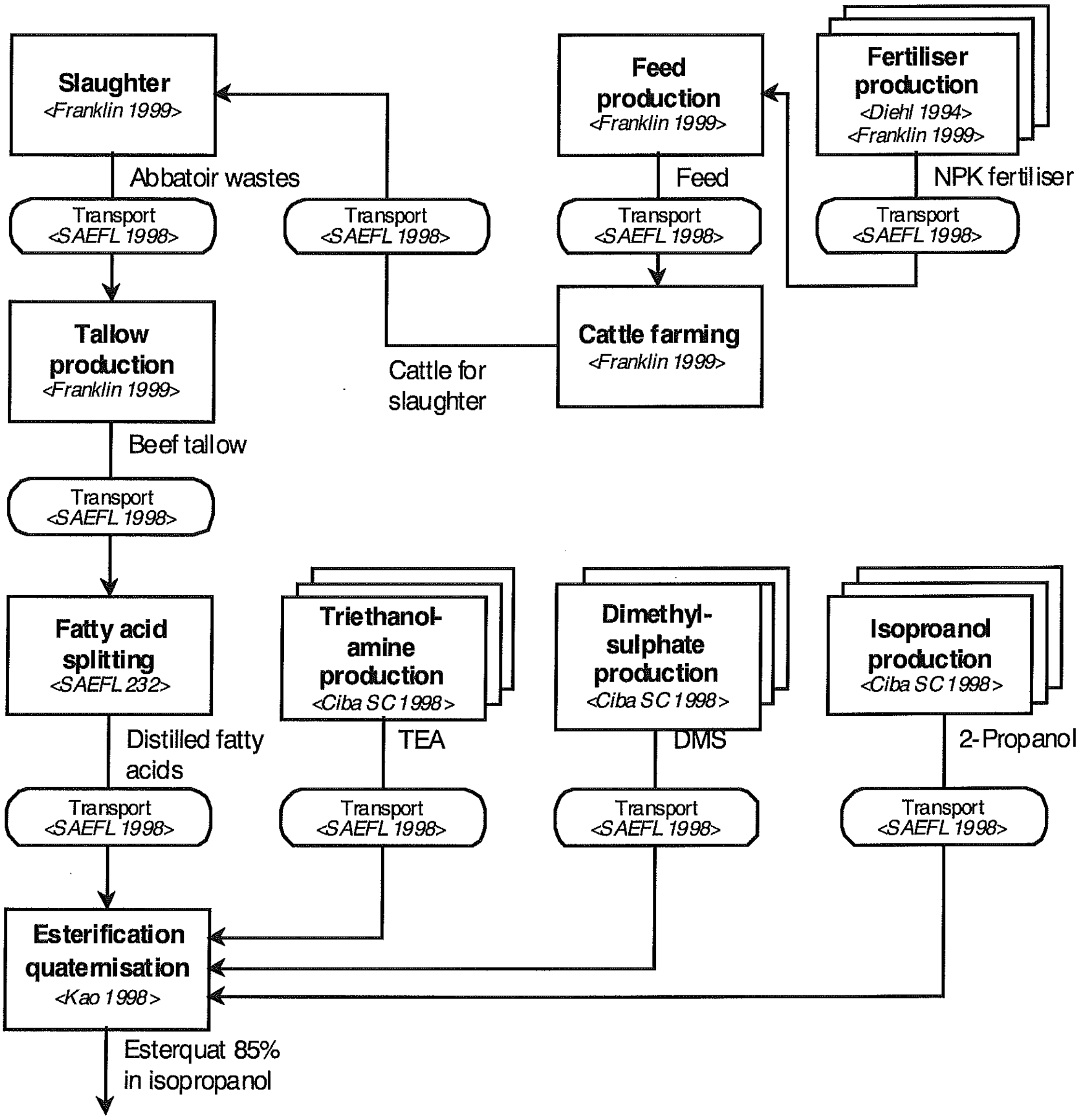


Fig. 4.7 Flow diagram of the manufacture of esterquat from beef tallow

4.3.2. Summary of the production procedure

Chemical equation for esterification: $2\ RCOOH + N(CH_2CH_2OH)_3$ (= triethanolamine) $\rightarrow N(CH_2CH_2OCOR)_2\ (CH_2CH_2OH)$

Chemical equation for quaternisation: $N(CH_2CH_2OCOR)_2\ (CH_2CH_2OH) + (CH_3)_2SO_4$ (=dimethylsulphate) $\rightarrow [N(CH_3)\ (CH_2CH_2OCOR)_2\ (CH_2CH_2OH)]^+$ (=esterquat) + $(CH_3SO_4)^-$

The most important cationic tensides are the quaternary nitrogen compounds, in particular tetra-alkyl ammonium salts, N,N–dialkylimidazolines, and the N-alkylpyridinium salts. The positive electrical charge of the hydrophilic moiety gives the cationic tensides properties that open up applications which are unsuitable or barely suitable for anionic or nonionic tensides. Important applications for these cationic tensides are as microbicides, herbicides, inhibitors of corrosion or of oxidation, as fabric softeners, dispersants and so on. The cationic fabric softeners investigated in this study attach well to textiles thanks to their affinity for fibres. They give the washed textiles a soft feel and thus improve their wearability.

Quaternary ammonium compounds are obtained by alkylisation of tertiary amines. At least one of the alkyl residues must be longer. In general, we start from tertiary amines with one or two long alkyl residues (fatty amines), reacted with shorter alkyl residues in the form of methyl chloride, ethyl chloride or bromide, or dimethyl sulphate. This then gives the relevant ammonium chloride or bromide or methyl sulphate. The addition requires a polar solvent, e.g. alcohol. for alkyl chlorides, which are primarily used for alkylisation, several hours of reaction time at higher temperatures of 50 °C to 100 °C are required. The procedure may be simplified by carrying out the reaction in surplus alkylisation solution, e.g. using methylene chloride as a solvent, under pressure, and obtaining the finished product after completion of the reaction through relaxation and evaporation of the unconverted alkyl chloride <Ullmann 1982>.

Quaternary ammonium compounds are not only obtained from fatty amines. The compounds examined here are obtained by esterification of triethanolamines and subsequent quaternation with dimethylsulphate. Isopropanol is used as a solvent. Fatty acids can be obtained from vegetable oils as well as from tallow.

In addition to quaternary ammonium compounds, imidazoline derivatives are also significant as a starting product for the manufacture of cationic tensides.

4.3.3. Calculations performed and methodological variation

Original study used for the harmonisation:	• none
Studies carried out towards updating and harmonisation:	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>

The data for the production of coconut oil, palm kernel oil and beef tallow derive from <Franklin 1999>. These also served as the basis for the Ecosol study <Ecosol 1995>. The data are already allocated but not aggregated. Allocations were made on the basis of mass in each case. The data resolution goes down to the level of single processes.

Palm kernel oil is produced in Malaysia, coconut oil in the Philippines. A mixture of 75% coconut oil and 25% palm kernel oil has been used for the calculations. The modules for heat and energy production, basic materials and transport were taken from SRU 250 <SAEFL 1998> according to the goal definition (Chap. 3.3). In addition, the electricity models for Malaysia and the Philippines according to <WEC 1995> were used. For the subsequent transport of the oils to Europe, distances of 15,000 km (from Malaysia) and 18,000 km (from the Philippines) were used. Beef tallow is produced all over Europe. Here we have performed the calculations using the UCPTE model.

The production of coconut oil, palm kernel oil and beef tallow is associated with a considerable number of co-products, leading to substantial uncertainty in allocating environmental impacts. This situation needs to be considered more precisely by a larger-scale study. This study has used the modelling in <Franklin 1999>.

The actual manufacture of esterquat was modelled according to information from a European producer and calculated using the UCPTE electricity model. Although it would have been possible to use a country-specific electricity model, we decided against this so that the data module would become more "European". In Europe there are various producers of cationic tensides, and thus this procedure gives a better average than a country-specific one (see Chap. 3.10.).

Methodological variation from standard procedure:

none

4.4. Sodium silicates (water glass)

4.4.1. Flow diagram

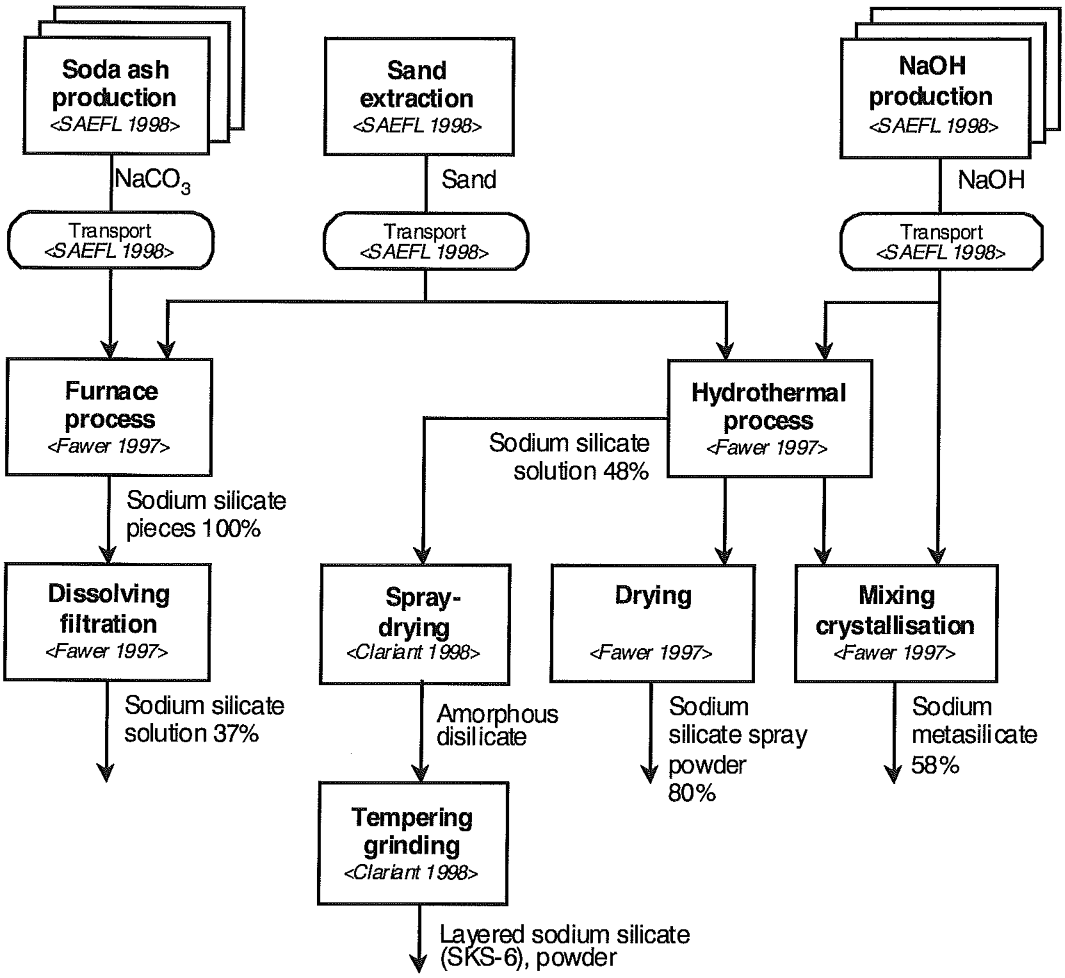


Fig. 4.8 Flow diagram of the production of sodium silicates

4.4.2. Summary of the production procedure

Chemical structure of sodium silicates: x SiO_2 * Na_2O

There are currently three principal areas of use for sodium silicates: as a raw material in detergents, as a starting material for the chemical industry, and as an adhesive in various fields. In detergents it serves as a builder, corrosion inhibitor and additive.

Two main processes, furnace and hydrothermal, are used to produce sodium silicate.

In the furnace process, water glass is produced directly by melting pure silicon sand and soda. Temperatures of approx. 1400 °C are required for this. The sodium silicate produced can then be used directly in a solid form, but is usually in aqueous solution (37%).

In the hydrothermal procedure, sand is dissolved in sodium hydroxide. This process is carried out under temperature and pressure in an autoclave. After filtration, sodium silicate is obtained in a 48% solution. By spray-drying the liquid, a solid content of 80% is obtained. The sodium silicate solution can be reacted again with sodium hydroxide. Metasilicate crystallises out of this, which can be treated in a solid form.

Layered sodium silicate (SKS-6):

A newer development in the sector of detergent ingredients is crystalline layered sodium silicate (SKS-6). The hydrothermal 48% sodium silicate solution is dehydrated and crystallised at high temperature to the δ-modification of the disilicate. SKS-6 can subsequently be milled and turned into granulate if desired.

Layered sodium silicates (as zeolites) also occur naturally. In its stoichiometric composition, SKS-6 is equivalent to $Na_2Si_2O_5$ and its crystalline layer structure is closest to the mineral natrosilite. The crystal structure is built in layers.

SKS-6 can remove the hardness of water by ion exchange. Besides calcium ions, it also binds magnesium ions. SKS-6 also provides the alkalinity necessary for the washing process, and stabilises the pH value over the whole procedure.

4.4.3. Calculations performed and methodological variation

Original study used for the harmonisation:	• Life Cycle Inventories for the Production of Sodium Silicates <Fawer 1997>
Studies carried out towards updating and harmonisation:	• Sodium silicates: Adaptation of the parameter list • Layered silicate (SKS-6): Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>

The LCIs in <Fawer 1997> were to a great extent compiled using the methodology and basic data used in this study. The parameter lists, in particular, are in agreement. To ensure that the inventory presentation conforms in this study, the waste parameter “filter residues” was assigned to industrial wastes. In using the data, only the total of the columns “Processes”, “Transport” and “Energy” were used.

The LCI for layered sodium silicate (SKS-6) was freshly compiled. The data for production were obtained from the main producer. For the precursor product “sodium silicate 48%” we resorted to the module “Sodium silicate (hydrothermal liquor)” of this study.

Methodological variation from standard procedures:

In contrast to the upper heating value of natural gas given in Table 3.9 (40.2 MJ/kg) the value given by the producer (36 MJ/kg) was used for calculating the production of SKS-6.

4.5. Sodium tripolyphosphate (STPP)

4.5.1. Flow diagram

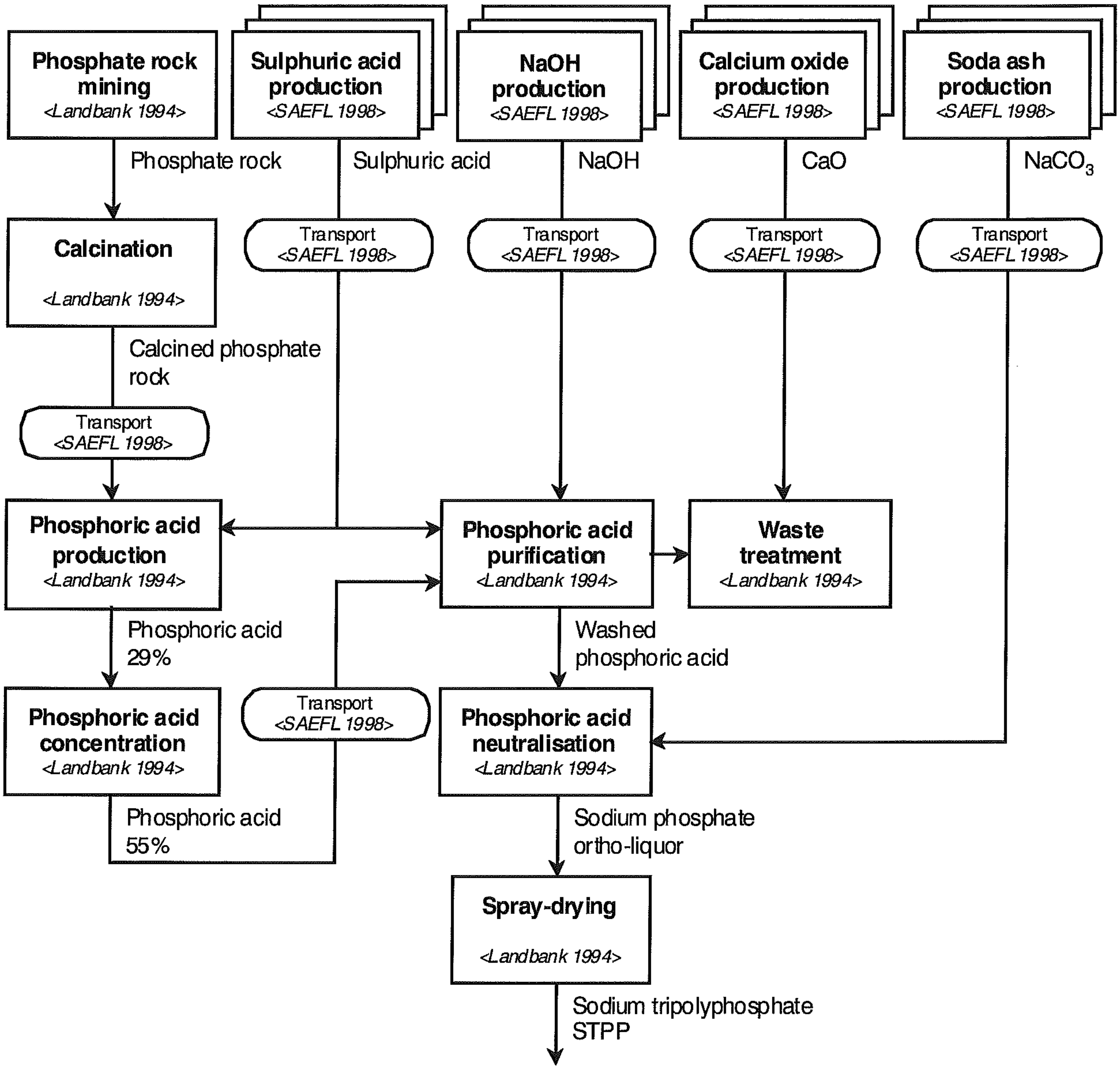


Fig. 4.9 Flow diagram of the production of tripolyphosphate (STPP)

4.5.2. Summary of the production procedure

Chemical structure of sodium tripolyphosphate: $Na_5P_3O_{10}$

The principle raw material for the production of STPP is phosphate rock, which is extracted in Morocco, among other places. In a first step, this is calcined at temperatures of approx. 750 °C. It is subsequently reacted exothermically with sulphuric acid in the dihydrate process. The phosphoric acid produced is filtered and washed. It has a concentration of 29% and is concentrated to 55% by vaporisation. In the subsequent purification step, the phosphoric acid is dissolved in an organic solvent. The residues that occur are treated with a mixture of solvents and sulphuric acid. The waste produced by this is reacted with calcium carbonate, which produces a stable material (raffinate solidification process). This is deposited. The phosphoric acid solution itself is purified in a counter-current with small quantities of the final product and separated again from the solvent, which is re-used. The purified phosphoric acid is neutralised with sodium carbonate, and the so called ortho-liquor of dissolved sodium phosphate is produced. This is dried to obtain sodium tripolyphosphate.

4.5.3. Calculations performed and methodological variation

Original study used for the harmonisation:	• The phosphate report <Landbank 1994>
Studies carried out towards updating and harmonisation:	• New compilation using the energy and basic data from SRU 250 <SAEFL 1998> • Adaptation of parameter lists

The data for phosphate production could be harmonised well as one of the goals of this study. A degree of uncertainty exists in relation to the process data used, since not much is known about their current quality. In contrast to the Landbank Report, the method chosen has been able to produce data on the resources used as energy and detailed emission parameters. Data on the consumption of final energy are now also available. Energy supply is also considered. The methodological characteristics of the Landbank Report have been described in <Fawer 1996>.

The Landbank Report considered gives detailed and verifiable details of phosphate production. The data are subdivided down to the level of single processes. This permits phosphate production to be newly modelled and calculated. The process tree is the same as that described in the Landbank Report and can be found there in Chapter 4.3.2. For the process whose data source is given in the flow diagram as *Landbank*, data from the Landbank Report have been used. The substances have been replaced and newly grouped according to the parameter lists in Chapter 3.13.5. Details of this can be found in Table 4.11.

The modules for heat and electricity production, raw materials and transports were taken from SRU 250 <SAEFL 1998>, according to the goal definition (Chap. 3.3). In addition to these, the energy details from the Landbank Report (MJ) have been divided according to Table 7.4 (Landbank Report) and converted with the upper heating values from Chapter 3.9 into the appropriate mass or volume units. Electricity consumption in MJ was converted to kWh (factor 3.6) and linked to the modules for Morocco or the UCPTE. The quantity of the raw materials sulphuric acid, sodium hydroxide, lime and soda consumed were linked directly to the relevant modules from SRU 250 <SAEFL 1998>. Details from the Landbank Report were used for transport distances of raw materials and intermediate products. This linkage was also carried out for the relevant transport modules from SRU 250 <SAEFL 1998>.

One difference between the newly calculated inventory and the result of the Landbank Report is the energy total, which is about three times greater (Landbank: 9.5 MJ/tonne STTP; this study: 31.2 MJ/tonne STTP). This difference may be explained as follows:

- The Landbank Report does not consider expenditure for energy supply.
- The Landbank Report gives energy credits (and sometimes emission credits) for exothermic reactions.
- The data for the production of sulphuric acid, sodium hydroxide, lime and soda from SRU 250 also contain energy supply and therefore introduce higher energy values into the system.
- The energy consumption to be included from the transport modules does not appear to be included in the Landbank Report's energy total of 9.5 MJ/tonne STTP.

In the field of emissions there are also certain differences. These may be explained in part the chosen classification of emissions (see Table 4.11). They may also be explained by the use of different data modules for heat and electricity production, raw materials and transport. The "classical" combustion emissions (CO_2, SO_x, NO_x,..) of energy consumption, however, agree relatively well. Furthermore, in the Landbank Report's energy credits in sulphuric acid production (exothermic reaction), additional credits are given for energy savings. The methodology of this study avoids this.

The data on resources used as raw materials agree well with those of the Landbank Report.

Process	Treatment of inputs and outputs documented in the Landbank Report
Phosphate rock extraction	• Electricity model Morocco • *Oversize* is recorded as *Mineral wastes*.
Calcination	• *Heat*: 80% heating oil H, 20% natural gas • Electricity model Morocco • *Waste rock* is recorded as *Mineral waste*. • *Waste air* and *Water vapour* are not recorded.
Phosphoric acid production	• Electricity model Morocco • *Gypsum* is recorded as *Suspended solids*. • *Fluorides* are viewed as sodium fluoride. The fluoride fraction is calculated using the factor 0.452 and is recorded as *Fluoride* (F^-) . • *Cake water* is recorded under Waste water quantity. • *Cd* and *Zn* are not given together under Metals or Heavy metals (in contrast to the Landbank Report) but recorded separately. • *Fluorides* into the air and U_3O_8 are not recorded (as in the Landbank Report) • *Water vapour* is not recorded.
Concentration	• *Heat*: 80% heating oil H, 20% natural gas • Electricity model Morocco • *Sea water* is recorded as *Cooling water*. • *Waste water* is recorded as Waste water quantity. • *Fluorides* are viewed as sodium fluoride. The fluoride fraction is calculated using the factor 0.452 and is recorded as *Fluoride* (F^-) . • Waste heat is not recorded; no energy credits are made.
Purification	• It is assumed that *Steam* is produced according to the model 40% heating oil H, 40% natural gas, 20% coal and an impact level of 0.8. • *Water for steam* is recorded as *Process water*. • *Waste water* is recorded as *waste water quantity*. • *Fluorides* are viewed as sodium fluoride. The fluoride fraction is calculated using the factor 0.452 and is recorded as *Fluoride* (F^-) . • Electricity consumption is not considered, since a surplus of electricity is produced in this process. It is assumed that the rest of this surplus is used in the process Spray drying. • Water vapour is not recorded.
Neutralisation	• *Heat*: 40% heating oil H, 40% natural gas, 20% coal • *Waste water* is recorded as *waste water quantity*. • *Water vapour* is not recorded.
Spray-drying	• *Heat*: 100% natural gas • Electricity model UCPTE • The electricity consumption is reduced by the rest of the surplus from the process Purification. • *STPP* as emissions are recorded as *Dust/particulates*. • *Water vapour* is not recorded.
Solidification of waste	• Electricity model UCPTE • *Solidified raffinate waste* is recorded as *Industrial waste*. • *Water vapour* is not recorded.

Tab. 4.11 Treatment in this study of the data documented in the Landbank Report

The processes not localised to Morocco have been calculated using the UCPTE electricity model. It would not have been possible to use the production-specific electricity model, so to make the data more "European" we have not done so. In Europe there are various producers of phosphate, and this procedure thus gives a better average than a country-specific view (see Chap. 3.10).

Methodological variation from standard procedures:

The electricity model used and documented in the Landbank Report for Morocco (87% oil, 13% hydroelectric power) does not consider trade in electricity with other countries. A simulated calculation of the system using the UCPTE model instead of the Morocco model, however, shows only negligible differences (total energy 31.1 MJ/tonne STPP instead of 31.2 MJ/tonne STPP). The slightly different emission profile does not vary in any parameter by more than 50% of the quantities emitted. In an impact assessment using the models Eco-indicator 95 <NOH 1995> and UBP 97 <SAEFL 1997> the total points are reduced in both models by only 5% each.

4.6. Zeolite A

4.6.1. Flow diagram

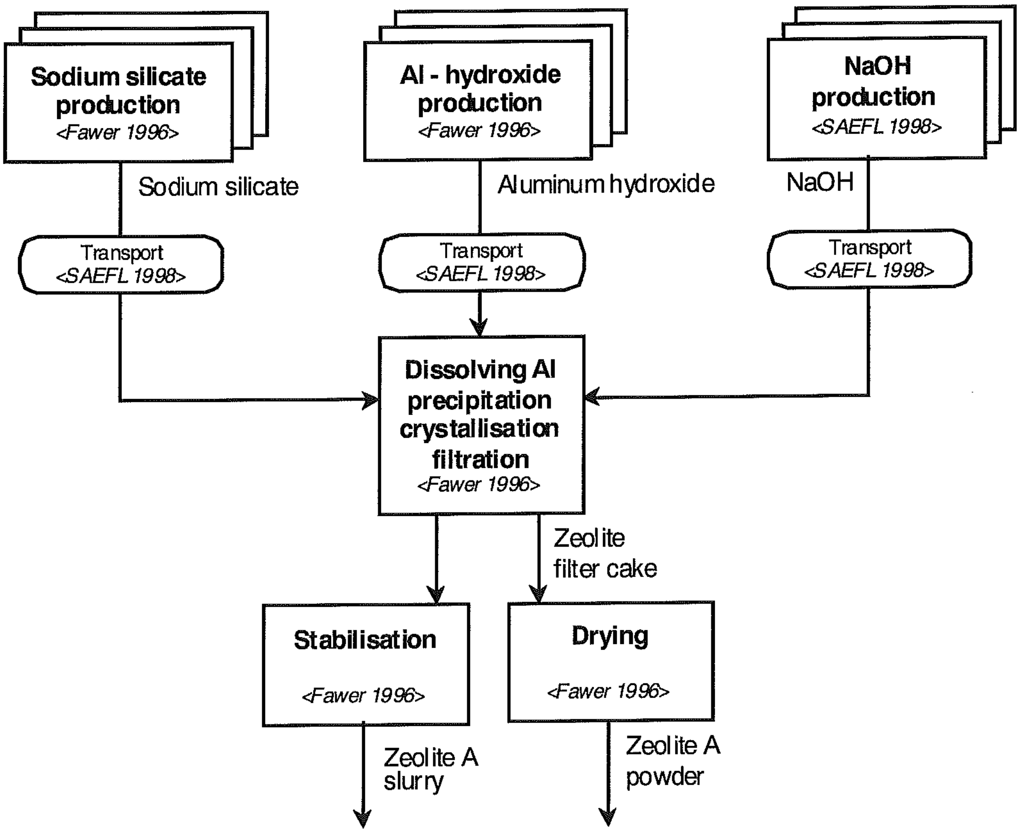


Fig. 4.10 Flow diagram of the production of zeolite

4.6.2. Summary of the production procedure

Chemical structure of zeolite A: $Na_{12}(AlO_2)_{12}(SiO_2)_{12} * 27\ H_2O$

Zeolite A, a synthetic zeolite, was developed as a builder for washing powders. Furthermore, it is used in many other fields, e.g. as an additive in animal feeds, cleaning fluid, drying substances or as a catalyst. There are two commercially used production routes: the aluminosilicate procedure (hydrogel) and the crystallisation of calcined kaolin clay. The hydrogel process has the greatest worldwide significance and is therefore described here. Solutions of aluminium hydroxide and sodium silicate are mixed. The amorphous sodium aluminium silicate produced is crystallised hydrothermally and filtered to give zeolite A. A portion (38%) is then used directly as slurry. Slurry is a watery suspension of zeolite A (approx. 50% water content) which is stabilised with surfactant substances (tensides) to prevent sedimentation. These surfactants are the same as those normally used in a finished detergent. The other portion of zeolite A filter cake (62%) is dried (to approx. 20% water content) and used as powder.

4.6.3. Calculations performed and methodological variations

Original study used for the harmonisation:	• Life Cycle Inventory for the Production of Zeolite A for Detergents <Fawer 1996>
Studies carried out towards updating and harmonisation:	• Adaptation of the parameter list

The LCIs in <Fawer 1996> were largely compiled using the methodology and basic data used in this study. In particular, the parameter lists are the same. For the adaptation of the inventory presentation, the waste parameter "red mud" was assigned to mineral wastes. In using the data, only the totals of the columns "Processes", "Transport" and "Energy" were used.

Methodological variation from standard procedure:

In contrast to the upper heating value of natural gas given in Table 3.9 (40.2 MJ/kg) we have calculated the production of zeolite using the values provided by the manufacturer (31.8 – 40.8 MJ/kg).

4.7. Polycarboxylates

4.7.1. Flow diagram

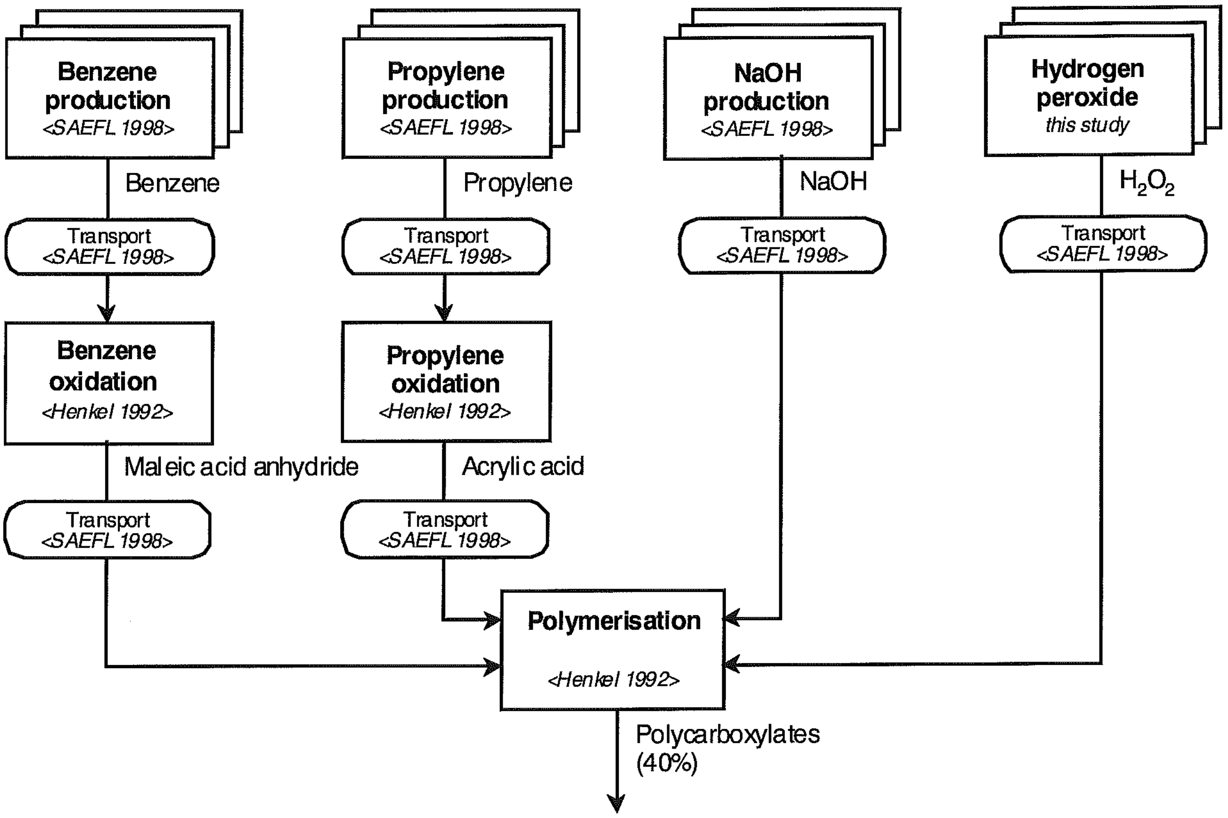


Fig. 4.11 Flow diagram of the production of polycarboxylates

4.7.2. Summary of the production procedure

Chemical structure of polycarboxylates: $[(\text{-CH}_2\text{-CH-})_x\text{-COOH HOOC-(-CH-CH-)}_y\text{-COOH}]_n$

Polycarboxylates have established themselves in connection with builders as water-soluble, linear polymers with numerous carboxy groups. In today's detergents only homopolymers of acrylic acid and copolymers of acrylic and maleic acid are used. This study considers only these copolymers. They are used in detergents as dispersion agents.

Benzene and propylene are starting materials for the manufacture of polycarboxylates. Benzene is mixed with air and oxidised to maleic acid anhydride at approx. 450 °C using a catalyst. Maleic acid is produced as a co-product. This reaction is strongly exothermic. In the one-step direct oxidation, propylene and air or O_2 are partially diluted using steam and, depending on the catalyst, converted at temperatures of between 200-400 °C and pressure of up to 10 bars. The catalyst contains heavy metal molybdates and tellurium compounds. Acroleine and acrylic acid are produced together. Acroleine is traced back to oxidation.

Maleic acid anhydride and acrylic acid are copolymerised using hydrogen peroxide as an initiator, and the salts produced using sodium hydroxide. The manufacture takes place in a batch reactor at approx. 100 °C. The plants are usually multifunctional polymerisation plants, in which a multiplicity of products can be made.

4.7.3. Calculations performed and methodological variation

Original study used for the harmonisation:	• LCAs of detergent ingredients <Fawer and Fecker 1993>
Studies carried out towards updating and harmonisation:	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>

The LCI for polycarboxylates was newly compiled, using data collected by an earlier study <Fawer and Fecker 1993>. However, detailed data on emissions in the processes of benzene oxidation, propylene oxidation and polymerisation are missing in that study. For propylene oxidation, the emissions could be estimated with the help of a similar procedure (production of acetic acid by oxidising with liquid butane) <SAEFL 1995>. Furthermore, the state of the data on the production of benzene, propylene, sodium hydroxide <SAEFL 1998> and hydrogen peroxide (this study) has also improved significantly, so that the data for polycarboxylates published in this study represent a substantial updating.

The processes “propylene oxidation”, “benzene oxidation” and “polymerisation” were calculated using the UCPTE electricity model. Although it would have been possible to use a country-specific electricity model we decided against this, in order to make the data module more “European” (see Chap. 3.10). There are various producers of polycarboxylates in Europe, and this method thus gives a better average than a country-specific one.

Methodological variation from standard procedures:

None

4.8. Perborates and hydrogen peroxide

The LCIs for perborates and hydrogen peroxide were newly calculated in a similar way, and are thus discussed here in the same chapter.

4.8.1. Flow diagram

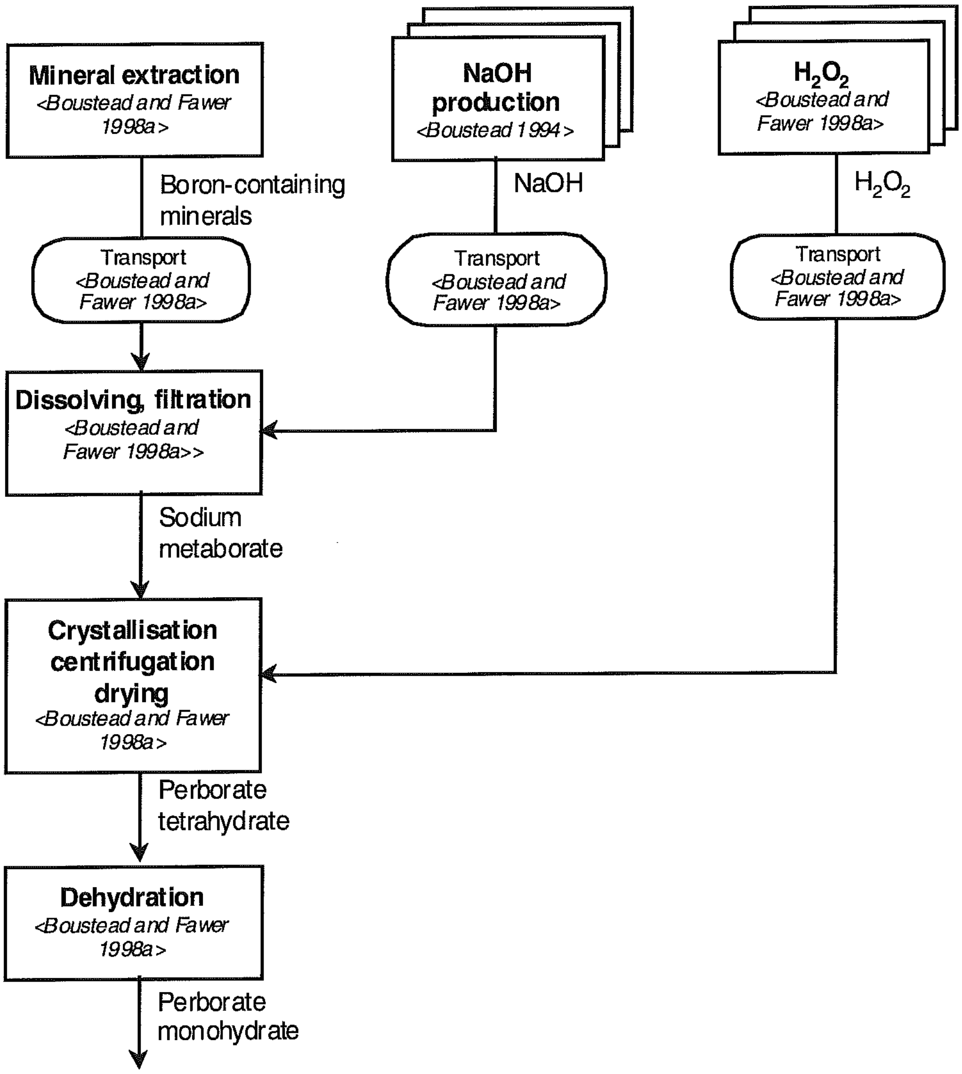


Fig. 4.12 Flow diagram of the production of hydrogen peroxide (H_2O_2)

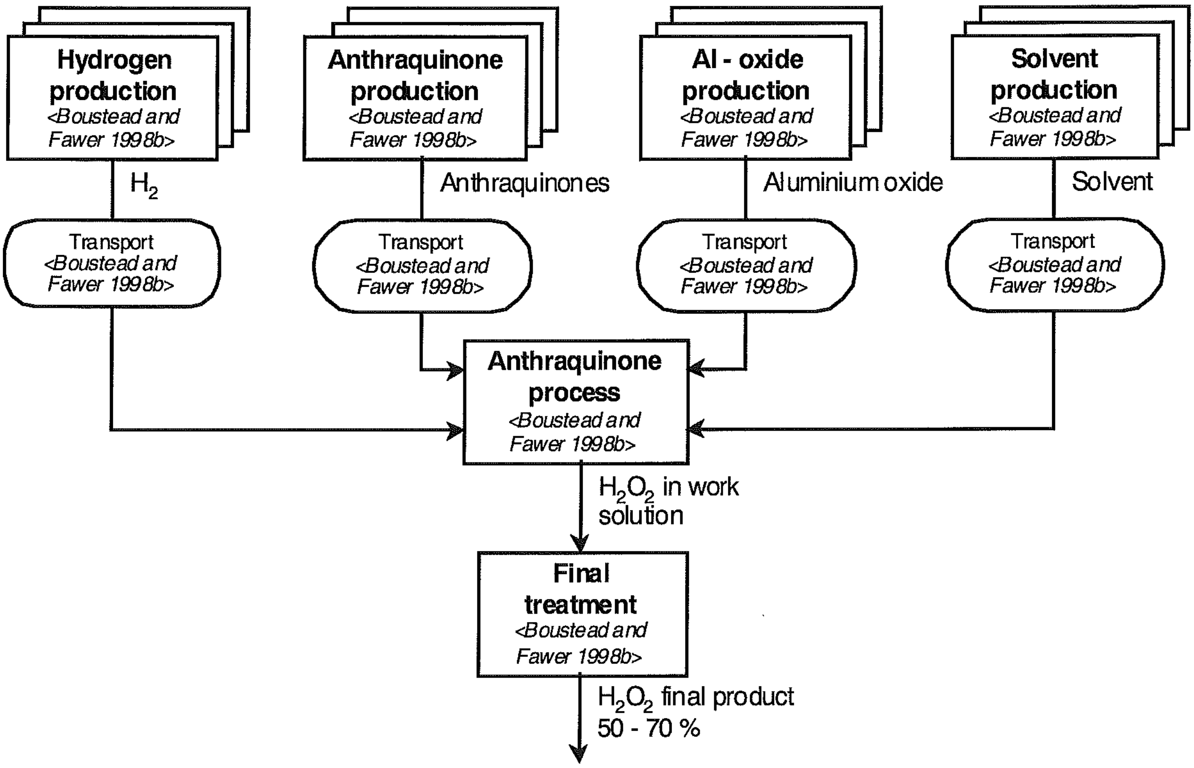


Fig. 4.13 Flow diagram of the production of hydrogen peroxide (H_2O_2)

4.8.2. Summary of the production procedure

Chemical structure of perborates: $NaBO_3 * 4H_2O$ (tetrahydrate), $NaBO_3 * H_2O$ (monohydrate)

Perborates are used in detergents as oxidisers and bleaches. In the washing process they serve as providers of hydrogen peroxide, which achieves the bleaching effect. Perborates are also used in cleaning, cosmetics and pharmaceuticals.

The main sources of the boron present in perborates are the minerals kernite and tincal. These boron-containing minerals are first dissolved in sodium hydroxide. The concentrated solution is filtered and thinned. The solution is then reacted with hydrogen peroxide, which causes the tetrahydrate to crystallise out. Monohydrate is produced by drying in warm air.

Chemical structure of hydrogen peroxide: H_2O_2

Hydrogen peroxide itself is not used as a raw material in detergents, but arises during the washing process. As a precursor and initiator of various processes, however, it is of great significance, and is therefore considered in this study. The most common method of hydrogen peroxide production is the anthraquinone process. Here, anthraquinones are converted to the respective hydroquinones using hydrogen in the presence of a catalyst. After removal of the catalyst, which would otherwise degrade the H_2O_2 that forms, the hydroquinones are oxidised by oxygen (air) to quinones, and H_2O_2 is simultaneously formed. The quinones are then re-hydrolysed. The whole process takes place in a working solution, which consists of a mixture of various solutions, some aromatic. The process is exothermic. Hydrogen peroxide is finally extracted from the working solution and concentrated.

4.8.3. Calculations performed and methodological variations

Original study used for the harmonisation:	• Ecoprofile of perborates <Boustead and Fawer 1998a> • Ecoprofile of hydrogen peroxide <Boustead and Fawer 1998b>
Studies carried out towards updating and harmonisation:	• New compilation using the energy data from SRU 250 <SAEFL 1998> • Adaptation of parameter lists

The data for perborates and hydrogen peroxide published in <Boustead and Fawer 1998a,b> were collected for the "sector group peroxygen" of the European Chemical Industry Council (CEFIC) and had very broad support from the industry. The data are accordingly representative and of high quality. In order to harmonise data from various sources, it is however important to calculate using the same energy and basic data. Experience has shown that the energy-related data dominates.

Here, we proceed in a similar way to the new calculation of the LCI on STPP (Chap. 4.5). In <Boustead and Fawer 1998a,b> the process- and energy-related emissions are shown separately. This makes it possible to use the energy data from <SAEFL 1998> in place of those used in <Boustead and Fawer 1998a,b>. In contrast to STPP, however, reduction down to the unit process is not possible. so that we work directly with the cumulative process emissions. The energy quantities for "Delivered energy" and "Transport energy" given in the tables "Gross energy" are used to determine the total consumption of final energy required. "Oil fuels" are interpreted here as heating oil H, and "other fuels" as natural gas. The data in MJ are converted using the upper heating values of 42.3 MJ/kg and 40.2 MJ/m^3 (Chap 3.9) in kilograms or cubic metres. They can then be linked with the energy data from <SAEFL 1998>. This method guarantees that the final energy required for processes and transport is still the same at the end.

Linkage to the data for electricity production is carried out using the UCPTE model (Chap. 3.9), since the data from <Boustead and Fawer 1998a,b> also stem from various European countries.

It is apparent that the necessary supply energy in the new data is somewhat greater than before. Energy consumption itself remains the same, as mentioned previously. The energy totals also rise slightly, as can be seen in Table 4.12.

	Total energy <Boustead and Fawer 1998a,b>	Total energy in this study
Perborate tetrahydrate	14.83 MJ/kg	15.71 MJ/kg
Perborate monohydrate	34.46 MJ/kg	36.98 MJ/kg
Hydrogen peroxide	23.00 MJ/kg	24.20 MJ/kg

Tab. 4.12 Comparison of energy totals from <Boustead and Fawer 1998a,b> and this study

Adaptation of the parameter list:

Table 4.13 gives an overview of how and with what conversion factors the parameter lists from Boustead and Fawer 1998a,b have been used. The conversion factors result from the relationship between atomic weights. All parameters not mentioned in Table 4.13 were used directly.

Parameters in <Boustead and Fawer 1998a,b>	Conversion factors	Parameters in this study
Atmospheric emissions		
Hydrocarbons	-	Non-methane VOCs (NMVOC)
Water emissions		
Acid as H+ Dissolved solids Ca++ Na++		Inorganic salts and acids
Hydrocarbons Dissolved organic compounds Other organic compounds	0.85 0.85 0.85	TOC
Phosphate as P_2O_5	1.338	Phosphate (PO_4^{3-})
Wastes		
Mixed industrial Paper/board Plastics To incinerator	-	Industrial waste
Regulated chemical Metals	-	Special waste

Tab. 4.13 Classification of parameters from <Boustead and Fawer 1998a,b>

The values of the emissions parameters in this study differ as expected, sometimes considerably, from those in Boustead and Fawer 1998a,b. This shows once more how important it is to use the same energy and basic data where possible, and to compare only harmonised inventories. The values for the typical combustion emissions CO_2, NO_x, SO_x, and so on are nevertheless in very good agreement.

Methodological variation from standard procedures:

Since the data in <Boustead and Fawer 1998a,b> are available only cumulatively, it is not possible to perform calculations using the standard modules for raw materials and transport from SAEFL 1998. In the LCIs published here the modules used by <Boustead and Fawer 1998a,b> are therefore used. However, this situation is unproblematic for the following reasons:

- The module for sodium hydroxide production from <SAEFL 1998> was taken from <Boustead 1994>. Detailed information on this can be found in <SAEFL 1998>.
- Transport modules are essentially characterised by their energy consumptions. This has been linked to the energy modules in <SAEFL 1998>, as described above.
- The remaining precursors (hydrogen, anthraquinones,..) are not used in any of the data published here, so that no conflicts arise.

4.9. Percarbonate

4.9.1. Flow diagram

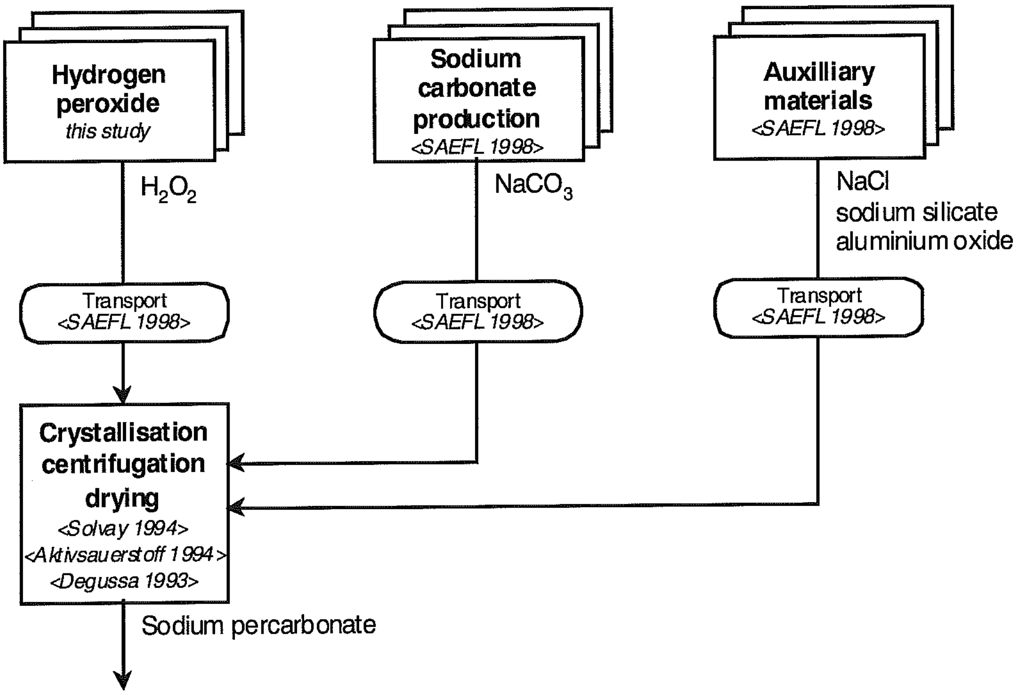


Fig. 4.14 Flow diagram of the production of percarbonate

4.9.2. Summary of the production procedure

Chemical structure of sodium percarbonate: $2Na_2CO_3 * 3H_2O_2$

Sodium percarbonate is a term used unspecifically for sodium carbonate peroxyhydrate. Sodium percarbonate forms a white, water-soluble powder which readily decomposes to sodium carbonate and bleaching oxygen, and is therefore used in detergents as a whitening agent.

Sodium percarbonate is preferably produced from an aqueous solution (crystallisation process). Crystalline sodium percarbonate is obtained by the conversion of aqueous solutions of sodium carbonate and hydrogen peroxide at 10-20 °C in the presence of sodium chloride and possibly aluminium ions. The centrifuged crystallised salt contains approx. 10% mother liquor and is dried in a fluidised-bed dryer at an air temperature of 90 °C. The centrifuged mother liquor is then reused.

Stabilisation during the manufacturing procedure is not adequate for the storage stability required. The percarbonate is thus ideally given additional stabilisation. This may be achieved, for example, by coating with sodium silicate.

4.9.3. Calculations performed and methodological variations

Original study used for the harmonisation:	• none
Studies carried out towards updating and harmonisation:	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>

The LCI for percarbonate was entirely recalculated on the basis of details from four manufacturers. The data for salt and aluminium oxide production have been taken from SRU 250 <SAEFL 1998>; for sodium silicate production and hydrogen peroxide, the data in this study were used.

Methodological variation from standard procedures:

Because details on quantities produced are missing, the four inventories of percarbonate have been weighted equally. A separate evaluation of the four LCIs using the Eco-indicator 95 model shows greater variation in some impact categories (up to 40%) but the total aggregation gives a difference of only 15% at most, so that an equally weighted average does not produce a major distortion in comparison with weighting according to production quantities.

4.10. Fluorescent whitening agents

Fluorescent whitening agents (FWAs) are colourless organic substances that absorb ultraviolet light and re-emit the energy absorbed mostly as blue fluorescent light (400 – 500 nm). They are added to laundry detergents and are adsorbed during the washing process by the textile fibres, where their fluorescence compensates for the natural yellow tone of the textiles (which increases with use) and produces more intense whiteness <Ullmann 1991>.

As an example, two important classes of FWAs are investigated here: triazinylaminostilbenes (DAS 1 for the detergent industry) which have been in use for some time, and the modern distyrylbiphenyls (DSBP). The latter have a more complicated synthesis, but because of their higher efficiency they can be applied in smaller quantities, and they also show almost complete photolytic degradability in surface waters <Kramer 1996>.

4.10.1. Flow diagrams

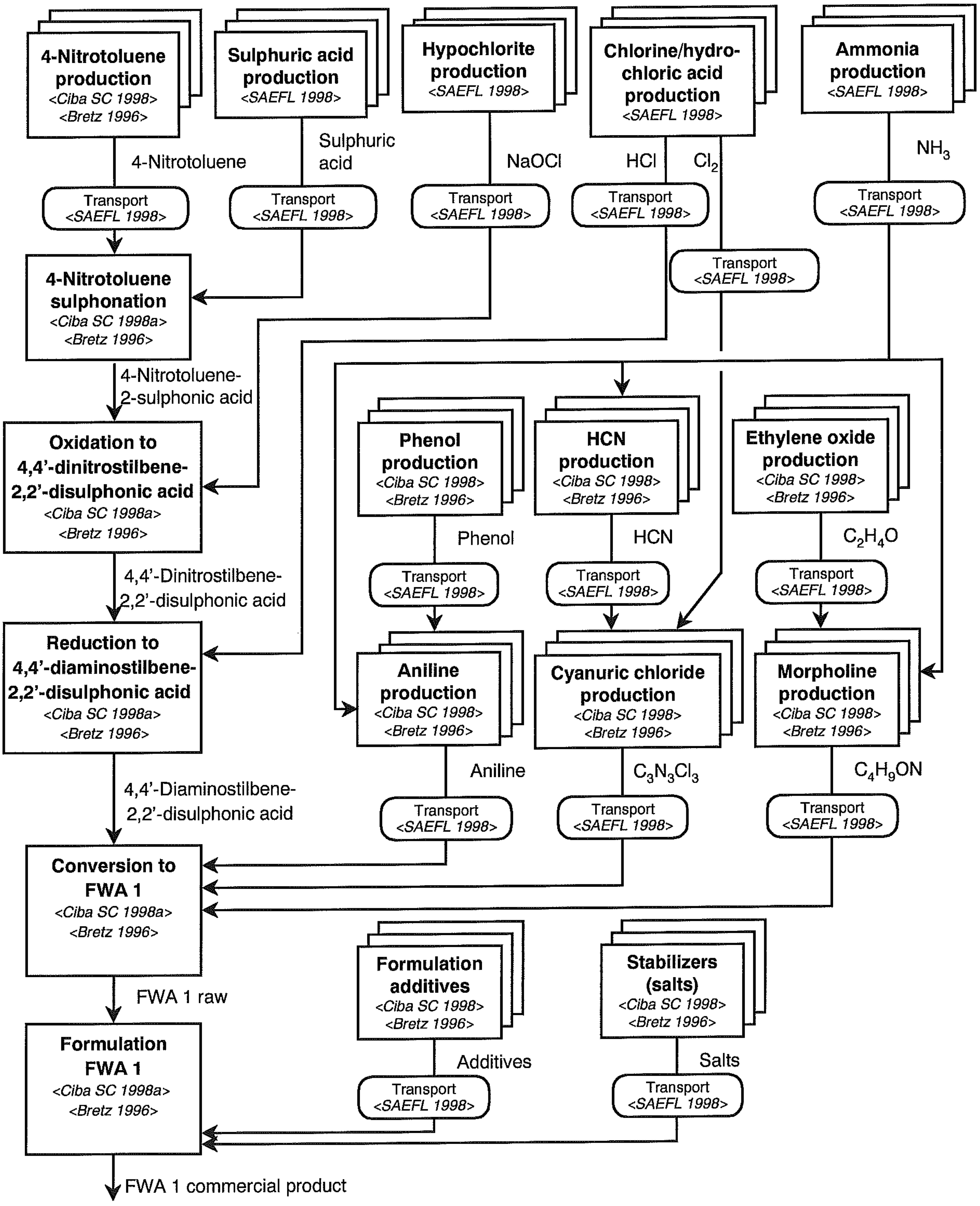


Fig. 4.15 Flow diagram of the manufacture of fluorescent whitening agents: DAS-1 triazinylaminostilbene type

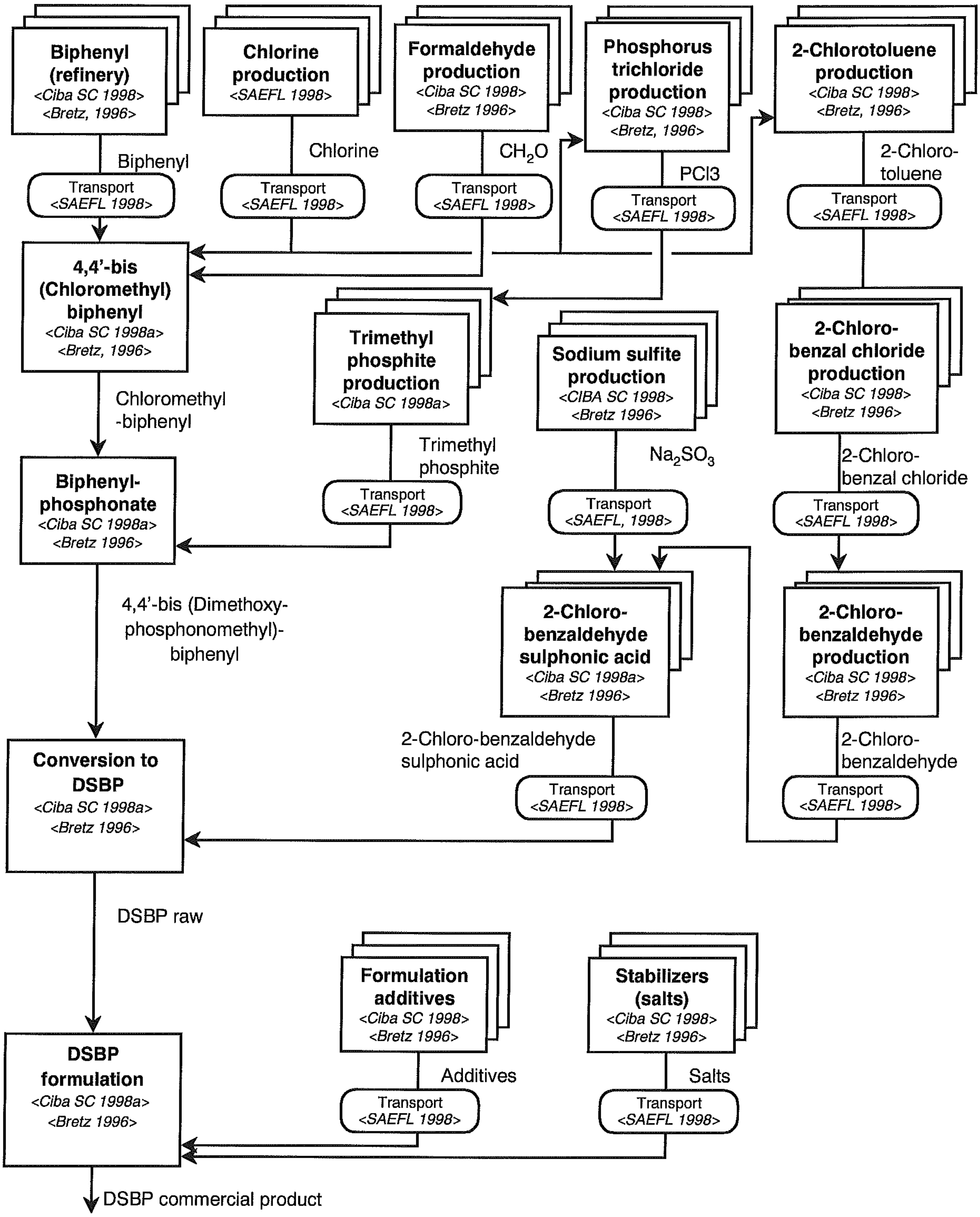
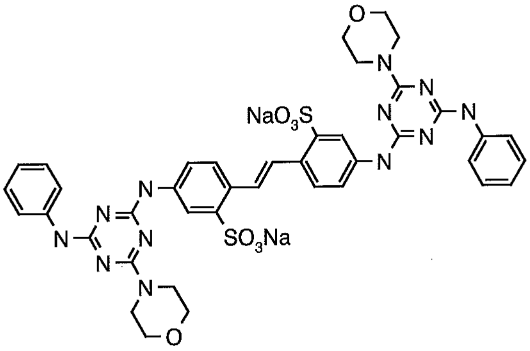


Fig. 4.16 Flow diagram of the manufacture of fluorescent whitening agents: DSBP distyrylbiphenyl type

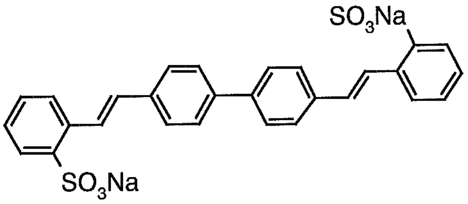
4.10.2. Summary of the production procedure

Triazinylaminostilbene example: DAS 1



The starting material for the triazinylaminostilbenes is 4,4'-Dinitrostilbene-2,2'-disulphonic acid, which is produced by the oxidation of 4-nitrotoluene-2-sulphonic acid with sodium hypochlorite. A subsequent Béchamps reduction with iron filings and HCl gives 4,4'-diaminostilbene-2,2'-disulphonic acid, which is reacted at both amino groups with cyanuric chloride. The two remaining Cl atoms in the cyanuric chloride rings then react one after another with two amines, in the case of DAS 1 with aniline and morpholine. Subsequent steps produce the desired β-crystal modification and deliver the finished commercial product, which contains 67% active substance.

Distyrylbiphenyl example: DSBP



The production of distyrylbiphenyl FWAs starts with biphenyl, which is produced along with other aromatic compounds during the refining of crude oil. Reacting it with chlorine and formaldehyde produces the intermediate 4,4'-bis(chloromethyl)biphenyl, which reacts with trimethylphosphite to give 4,4'-bis(dimethoxyphosphonomethyl)biphenyl. This symmetrical biphenylphosphonate is reacted with two molecules of an aromatic aldehyde. In the case of the DSBP under consideration, benzaldehyde-2-sulphonic acid is used, a compound which is produced from 2-chlor-benzaldehyde and sodium sulphite. The two sulphonic acid groups thus introduced give the final product DSBP the desired affinity to adsorb onto cellulose fibres. The commercial product contains 83% active substance.

4.10.3. Calculations performed and methodological variations

Original study used for the harmonisation:	• <Ciba 1994>
Studies carried out towards updating and harmonisation:	• New compilation of the inventories with current production data, and using the energy and basic data from <SAEFL 1998> • LCA for waste water treatment and energy production plants, in collaboration with the ETH Zurich, partial Critical Review of the synthesis processes <Halder 1997> • Introduction of further estimates for chemical starting products and transports

The LCAs of the two FWAs were compiled by the manufacturer <Ciba SC 1999>. The original study <Ciba 1994> was carried out as a contribution to the product line analysis of detergents by the Öko-Institut Freiburg <Griesshammer 1995> for the German Federal Office of the Environment. In the meantime, due to advances in technology the energy models and basic materials from <SAEFL 1991> had to be replaced by the appropriate modules from <SAEFL 1998>. LCAs have been compiled for substantial parts of the process infrastructure (especially plants for waste water treatment and energy supply), some in collaboration with the Laboratory for Technical Chemistry of the ETH Zurich <Halder 1997>. Also within the framework of this study, the synthesis description and process modelsfor triazinylaminostilbene FWAs were updated at the end of 1997 and critically reviewed. The data for the synthesis of distyrylbiphenyl were thoroughly reworked in 1999 after various modifications to the procedure.

Although the inventory data for the synthesis of FWAs come from a single manufacturer, they are reasonably representative (only one producer of distyrylbiphenyl FWAs in Europe and the USA; one of the four important suppliers of triazinylaminostilbene FWAs). It should however be noted that there are other methods of synthesising triazinylaminostilbene FWAs, to which the present data are *not applicable*.

As is generally the case in the speciality chemicals industry, the manufacturer does not start with the basic petrochemicals, but acquires high-quality starting materials from a chain of suppliers. These suppliers do not as a rule carry out LCAs for their products, or do not publish the results. Approximate LCAs for the products purchased have therefore been carried out using estimates based on the literature on chemical processes <Bretz 1996>. For all estimates it has been assumed that the production plants are connected to a waste water treatment plant. The data for one of the FWA manufacturer's waste water treatment plants, compiled by the ETH, have been used in the model <Halder 1997>.

Since the products purchased can usually be obtained from several sources, nothing is known about the transport data. A uniform transport distance of 300 km (200 km rail, 100 km 40 t lorry) has been assumed for each chemical substance obtained from another producer, even when it is suspected that many process chains with several synthesis steps are carried out by the same producer without intermediate transport.

The UCPTE mix has been used as an electricity model for all estimates <SAEFL 1998>. Since FWAs are manufactured partly in Germany and partly in Switzerland, the UCPTE mix was also used here for better comparability, where the electrical energy is not produced in a firm's own plant (with a known LCA).

Methodological variation from standard procedures:

The LCAs of the two FWAs were not calculated using the software of EMPA St Gallen, but using the manufacturer's ECOSYS system <Bretz 1994>, which itself relies on the process databases of the manufacturer <Ciba SC 1998a>. The system and the database for basic chemicals were subjected to Critical Review in 1998/99 by the GSF Munich in the course of a separate study <GSF 1999>.

Since there is still no generally accepted method to aggregate data quality indicators (DQIs) of single processes into a higher indicator for the whole system, the DQIs were not recorded in the ECOSYS database. The following assumptions are generally made for DQIs:

- Process steps carried out by the manufacturer: B (company), I (measured), m (average)
- Estimates for processes carried out by suppliers of precursors: inputs and product output: L (literature), I (measured), m (average)
- Estimates for processes carried out by suppliers of precursors: emissions and other outputs: L (literature), II (measured), x (other: stoichiometry and mass balances).

Not all the modules in the present version of the report were available at the time of the FWA LCA for use in ECOSYS, so that some older data <Boustead 1993a and later reports>; <ECOSOL 1995>, or the manufacturer's own estimates <Bretz 1996>, have been used. In these cases the original parameter lists were retained, which only partly agree with the list in 3.12.5.

The input materials (see 3.12.2), which could not be included in the inventory analysis for lack of information, were quantitatively insignificant (total < 0.5 g / kg of the commercial product, cumulated over the whole process tree). A detailed listing was thus not made and the flat rate energy of 50 MJ / kg not used.

In contrast to 3.12.4, downstream processes in production were generally considered. As long as they were carried out by the manufacturer, current data could be used. In the estimated processes it was assumed that non-aqueous organic wastes were incinerated. The emissions produced by the combustion of fuel oil EL <SAEFL 1991> serve as a model for the incineration of nitrogen-free wastes; estimates from Braunschweig 1993 were used for the disposal of nitrogen-containing special wastes. Further elements, halogens in particular, were considered separately, with the transfer coefficients from <SAEFL 1996>. For some recoverable wastes, notably in DSBP manufacture, the actual reuse (disposal or recycling) depends on the market situation at any given time. In doubtful cases we have assumed disposal (according to the precautionary principle), i.e. we have estimated environmental impacts for disposal and included them.

Because of the known allocation problems for the waste air treatment plants of multi-purpose chemical companies, individual atmospheric process emissions could not be allocated. The legal limits have been adhered to in all cases.

4.11. Carboxymethyl Cellulose (CMC)

4.11.1. Flow diagram

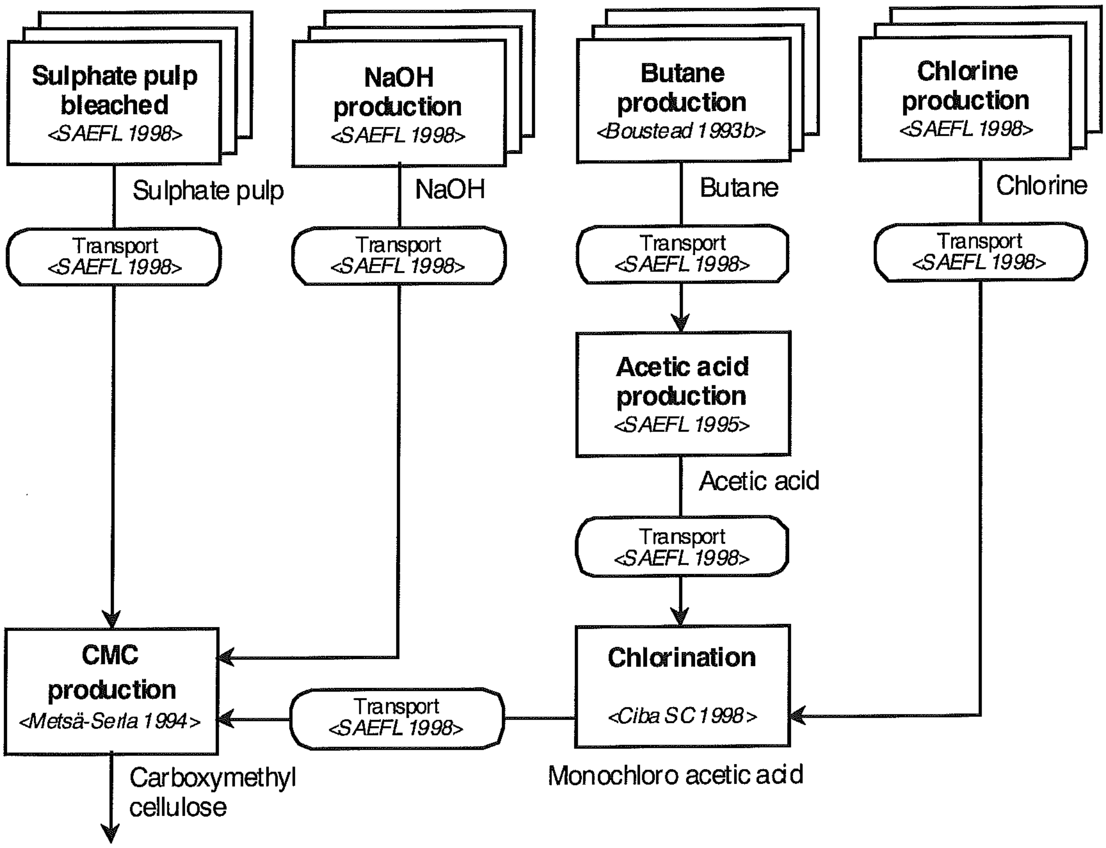


Fig. 4.17 Flow diagram of the production of carboxymethyl cellulose

4.11.2. Summary of the production procedure

Chemical structure of CMC: Cellulose-O-CH_2-COO^-Na^+

CMC is used in detergent as a soil carrier. It is also employed in other fields, for example as a thickener in salves, in the food industry as an emulgator and stabiliser, in the paint industry as a stabiliser or thickener, etc.

The starting product for its manufacture is cellulose sulphate or sulphite from pine wood. In a first step, the cellulose is activated using sodium salt. This may take place in the presence of absence of a solvent (e.g. isopropanol). Because of the production method the CMC produced contains sodium chloride and sodium glycolate. These salts are stepwise or continuously removed in a counter-current system. Residual alkali is neutralised with acid. Finally, the product is dried and ground. The end product is prepared as granulate or powder <Ullmann 1989c>.

4.11.3. Calculations performed and methodological variations

Original study used for the harmonisation:	• none
Studies carried out towards updating and harmonisation:	• Completely new calculation using energy and basic data from SAEFL SRU 250 <SAEFL 1998>

The inventory for CMC was newly calculated on the basis of details provided by one manufacturer. The data for butane production and acetic acid production stem from the study 'Comparative ecological evaluation of paint substances in the building industry " <SAEFL 1995>, which itself partly relies on the APME Report 4 <Boustead 1993b>.

The process "CMC production" was calculated using the UCPTE electricity model. Although it would have been possible to use a country-specific electricity model we did not do so, in order to make the data module more "European". There are various producers of CMC in Europe, and this method thus gives a better average than a country-specific one.

For the transport of sulphate cellulose from Sweden for CMC production an average transport distance of 500 km was assumed.

Methodological variation from standard procedures:

None

5. BASIC DATA AND LIFE CYCLE INVENTORIES

5.1. Raw materials, energy data and transports

The basic modules are the following LCAs: sand, salt, calcium carbonate, sodium hydroxide, sodium carbonate, chlorine, sulphuric acid, propylene, butane, acetic acid, benzene, aluminium oxide, aluminium hydroxide, sulphate pulp, transport data and energy data. The data for the basic modules are not printed in this study. A qualitative description of these data is provided by the fields in Chapter 3.7. Some fields are omitted in the following table.

Fields as in Chap. 3.7	**Sand extraction**	**Sodium chloride production**	**Calcium oxide production**	**Sodium hydroxide production**
Type	Non-terminated system	Non-terminated system	Non-terminated system	Non-terminated system
Time period	up to 1994	up to 1994	1989 - 1993	up to 1994
Energy values	Upper heating values	Upper heating values	Upper heating values	Upper heating values
Geographical validity	Western Europe	Western Europe	Western Europe	Western Europe
Technology	State-of-the-art	Mining of rock salt and extraction from salt water	State-of-the-art	State-of-the-art
Representativeness	n.i.	n.i.	1 company	14 companies
Original data generator	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology
First publication	<Fawer 1996>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>
Data sources	<Frischknecht et al. 1996>	APME Report 6 <Boustead 1994>	<Ullmann 1990> <Franklin 1989>	APME Report 6 <Boustead 1994>
German name	Sandextraktion	Salzabbau	Kalkabbau	NaOH Produktion
Infrastructure	Not considered	Not considered	Not considered	Not considered

Tab. 5.1. Qualitative description of the basic data

Fields as in Chap. 3.7	**Sodium carbonate production**	**Chlorine production**	**Sulphuric acid production**	**Propylene production**
Type	Non-terminated system	Non-terminated system	Non-terminated system	Non-terminated system
Time period	1995	up to 1994	up to 1995	up to 1993
Energy values	Upper heating values	Upper heating values	Upper heating values	Upper heating values
Geographical validity	Germany	Western Europe	Western Europe	Western Europe
Technology	State-of-the-art	State-of-the-art	Sulphur recovery in refineries, Contact process	State-of-the-art
Representativeness	1 company	14 companies	n.i.	19 crackers
Original data generator	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology
First publication	<Fawer 1997>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>
Data sources	Written communication by the producer	APME Report 6 <Boustead 1994>	<Lurgi 1995>	APME Report 2 <Boustead 1993a>
German name	Sodaproduktion	Chlorproduktion	Schwelfelsäureproduktion	Propylenproduktion
Infrastructure	Not considered	Not considered	Not considered	Not considered

Tab. 5.2. Qualitative description of the basic data (continued)

Fields as in Chap. 3.7	Butane production	Acetic acid production	Benzene production	Aluminium oxide production
Type	Non-terminated system	Non-terminated system	Non-terminated system	Non-terminated system
Time period	up to 1993	up to 1993	up to 1993	up to 1995
Energy values	Upper heating values	Upper heating values	Upper heating values	Upper heating values
Geographical validity	Western Europe	Western Europe	Western Europe	Western Europe
Technology	State-of-the-art	State-of-the-art	State-of-the-art	State-of-the-art
Representativeness	n.i.	n.i.	5 plants	n.i.
Original data generator	ökoscience AG, Zurich	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology
First publication	SRU 232 <SAEFL 1995>	None	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>
Data sources	APME Report 2 und 4 <Boustead 1993a,b>	SRU 232 <SAEFL 1995> <Franklin 1989>	APME Report 4 <Boustead 1993b>	<EAA 1995>
German name	Butanproduktion	Essigsäureproduktion	Benzolproduktion	Aluminiumoxid
Infrastructure	Not considered	Not considered	Not considered	Not considered

Tab. 5.3. Qualitative description of the basic data (continued)

Fields as in Chap. 3.7	Aluminium hydroxide production	Sulphate pulp production	Transport data	Energy data
Type	Non-terminated system	Non-terminated system	Terminated system	Terminated system
Time period	up to 1995	up to 1996	up to 1994	up to 1994
Energy values	Upper heating values	Upper heating values	Upper heating values	Upper heating values
Geographical validity	Western Europe	Sweden, Western Europe	Western Europe	Western Europe
Technology	State-of-the-art	State-of-the-art	State-of-the-art	State-of-the-art
Representativeness	n.i.	Swedish industrial average	Average values	Average values
Original data generator	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology	EMPA St Gallen, Section Ecology
First publication	<Fawer 1996>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>	SRU 250 <SAEFL 1996>
Data sources	<EAA 1995>	<STFI 1994>	<Frischknecht et al. 1996>	<Frischknecht et al. 1995,1996>
German name	Aluminium-hydroxidproduktion	Sulfatzellstoff Produktion	transportdaten	Energiedaten
Infrastructure	Not considered	Not considered	Not considered	Not considered

Tab. 5.4. Qualitative description of the basic data (end)

5.2. Detergent ingredients

Data description		LAS	AS	Soap	AE
Type		Non term. system	Non term. system	Non term. system	Non term. system
Version		1	1	1	1
Time period		1992	1992	1992	1992
Energy values		Gross calorific values	Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe	Western Europe
Technology		Sulphonation of LAB	Sulphonation of alcohols from palm kernel oil	Saponification of neutral oils (coconut oil, palm oil)	Ethoxylation of alcohols from petrochemical resources
Representativeness		Average data from several producers	Average data from several producers	Average data from several producers	Average data from several producers
Percent		>50%	>50%	>50%	>50%
Number of producers		n.i.	n.i.	n.i.	n.i.
Timestamp		14.12.98	14.12.98	14.12.98	14.12.98
Data entry by		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data generator		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data published in		this study	this study	this study	this study
Data sources		<Berna 1995>	<Hirsinger and Schick 1995>	<Postlethwaite 1995>	<Schul 1995>
		<Buwal 1998>	<Buwal 1998>	<Buwal 1998>	<Buwal 1998>
Functional unit					
CAS number		42615-29-2	-	68952-95-4	-
German name		Lin. Alkylbenzolsulfonate (LAS) aus petrochem. Rohstoffen	Fettalkoholsulfate (FAS) aus Palmkernöl	Seifenmischung aus kurzkettigen Fettsäuren aus Kokos-/Palmöl	Alkoholethoxylat (AE) mit 7 EO-Ketten aus petrochem. Rohstoffen
English name		Linear Alkylbenzene Sulphonate (LAS) from petrochemical feedstock	Alcohol sulfate (AS) from palm kernel oil	Soap; blend of short chain fatty acid from coconut / palm oil	Alcohol ethoxylate (AE) with 7 EO-chains from petroc. Feedstock
Amount	kg	1000	1000	1000	1000
Infrastructure		not included	not included	not included	not included

Tab. 5.5. Life cycle inventories of detergent ingredients

Data description		**Esterquat; coconut oil / palm kernel oil**	**Esterquat; tallow**	**Sodium silicate (hydrothermal liquor)**	**Sodium silicate (spray powder)**
Type		Non term. system	Non term. system	Non term. system	Non term. system
Version		1	1	2	2
Time period		1992-1998	1992-1998	1990-1995	1990-1995
Energy values		Gross calorific values	Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe	Western Europe
Technology		Fatty acid from coconut/palm kernel oil; Esterification of Triethanolamine; Quaternization with DMS	Fatty acid from cattle tallow; Esterification of Triethanolamine; Quaternization with DMS	Hydrothermal process	Hydrothermal process
Representativeness		Data from a single producer	Data from a single producer	Average data from several producers	Average data from several producers
Percent		n.i.	n.i.	93%	93%
Number of producers		1	1	13	13
Timestamp		16.3.99	16.3.99	26.8.98	26.8.98
Data entry by		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data generator		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	M.Fawer, EMPA St.Gallen	M.Fawer, EMPA St.Gallen
Data published in		this study	this study	<Fawer 1997>	<Fawer 1997>
Data sources		<Franklin 1999>	<Franklin 1999>	<Buwal 1998>	<Buwal 1998>
		<Buwal 1998>	<Buwal 1998>		
		<Buwal 1995>	<Buwal 1995>		
		<Kao 1998>	<Kao 1998>		
Functional unit					
CAS number		-	-	1344-09-8	1344-09-8
German name		Esterquat 85% in 2-Isopropanol	Esterquat 85% in 2-Isopropanol	Natriumsilikat Lösung 48%; SiO2 : Na2O = 2.0	Natriumsilikat, sprühgetr. Pulver 80%; SiO2 : Na2O = 2.0
English name		Esterquat 85% in 2-isopropyl alcohol	Esterquat 85% in 2-isopropyl alcohol	Sodium silicate; hydrothermal liquor 48%; SiO2 : Na2O = 2.0	Sodium silicate; spray powder 80%; SiO2 : Na2O = 2.0
Amount	kg	1000	1000	1000	1000
Infrastructure		not included	not included	not included	not included

Tab. 5.6. Life cycle inventories of detergent ingredients (continued)

Data description		**Sodium silicate (furnace lumps)**	**Sodium silicate (furnace liquor)**	**Sodium metasilicate (pentahydrate)**	**Layered sodium silicate (SKS-6)**
Type		Non term. system	Non term. system	Non term. system	Non term. system
Version		3	3	2	1
Time period		1990-1995	1990-1995	1990-1995	1990-1997
Energy values		Gross calorific values	Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe	Western Europe
Technology		Furnace process	Furnace process	Hydrothermal process	Hydrothermal process and tempering
Representativeness		Average data from several producers	Average data from several producers	Average data from several producers	Average and single producer data
Percent		93%	93%	93%	100%
Number of producers		13	13	13	1
Timestamp		26.8.98	26.8.98	26.8.98	19.8.98
Data entry by		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data generator		M.Fawer, EMPA St.Gallen	M.Fawer, EMPA St.Gallen	M.Fawer, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data published in		<Fawer 1997>	<Fawer 1997>	<Fawer 1997>	this study
Data sources		<Buwal 1998>	<Buwal 1998>	<Buwal 1998>	<Buwal 1998>
					<Fawer 1997>
					<Clariant 1998>
Functional unit					
CAS number		1344-09-8	1344-09-8	10213-79-3	
German name		Natriumsilikat Stückenglas 100%; SiO2 : Na2O = 3.3	Natriumsilikat Lösung 37%; SiO2 : Na2O = 3.3	Natriummetasilikat-5-hydrat 58%; SiO2 : Na2O = 1.0	Natriumschichtsilikat (SKS-6); gemahlen
English name		Sodium silicate; furnace lumps 100%; SiO2 : Na2O = 3.3	Sodium silicate; furnace liquor 37%; SiO2 : Na2O = 3.3	Sodium metasilicate pentahydrate 58%; SiO2 : Na2O = 1.0	Layered sodium silicate (SKS-6); ground
Amount	kg	1000	1000	1000	1000
Infrastructure		not included	not included	not included	not included

Tab. 5.7. Life cycle inventories of detergent ingredients (continued)

Data description		Sodiumtripoly-phosphat (STPP)	Zeolite A (powder)	Zeolite A (slurry)	Polycarboxylates
Type		Non term. system	Non term. system	Non term. system	Non term. system
Version		1	3	3	2
Time period		1986-1994	1990-1995	1990-1995	1989-1995
Energy values		Gross calorific values	Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe	Western Europe
Technology		Dihydrate system	Hydrogel route	Hydrogel route	Copolymerisation of maleic acid and acrylic acid
Representativeness		Betriebsspezifische Daten	Average data from several producers	Average data from several producers	Data from a single producer
Percent		n.i.	76%	76%	n.i.
Number of producers		1	5	5	1
Timestamp		20.11.98	26.8.98	26.8.98	12.2.99
Data entry by		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data generator		S.Dall'Acqua, EMPA St.Gallen	M.Fawer, EMPA St.Gallen	M.Fawer, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data published in		this study	<Fawer 1996>	<Fawer 1996>	this study
Data sources		<Buwal 1998>	<Buwal 1998>	<Buwal 1998>	<Fawer, Fecker 1993>
		<Landbank 1994>			<Buwal 1998>
					<Henkel 1992>
Functional unit					
CAS number		7758-29-4	1318-02-1	1318-02-1	-
German name		Natriumtripolyphosphat	Zeolith A Pulver	Zeolith A Aufschlämmung; 50% in Wasser	Polycarboxylate; 40% aktive Substanz
English name		Sodiumtripolyphosphate (STPP)	Zeolite A powder	Zeolite A slurry; 50% in water	Polycarboxylates; 40% active substance
Amount	kg	1000	1000	1000	1000
Infrastructure		not included	not included	not included	not included

Tab. 5.8. Life cycle inventories of detergent ingredients (continued)

Data description		Hydrogen peroxide	Perborate tetrahydrate	Perborate monohydrate	Percarbonate
Type		Non term. system	Non term. system	Non term. system	Non term. system
Version		2	2	2	2
Time period		1990-1995	1990-1995	1990-1995	1994
Energy values		Gross calorific values	Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe	Western Europe
Technology		Antraquinone system	Cristallisation from a solution of boron-containing minerals	Cristallisation from a solution of boroncontaining minerals, Dehydration	Cristallisation from an solution of Na-Carbonate and hydrogen peroxide
Representativeness		Average data from several producers	Average data from several producers	Average data from several producers	Average data from several producers
Percent		n.i.	85%	85%	n.i.
Number of producers		9	9	9	4
Timestamp		19.8.98	19.8.98	19.8.98	12.2.99
Data entry by		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data generator		S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen	S.Dall'Acqua, EMPA St.Gallen
Data published in		this study	this study	this study	this study
Data sources		<Bousted and Fawer 1998b>	<Bousted and Fawer 1998a>	<Bousted and Fawer 1998a>	<Buwal 1998>
		<Buwal 1998>	<Buwal 1998>	<Buwal 1998>	<Solvay 1994>
					<Aktivsauerstoff 1994>
					<Degussa 1993>
Functional unit					
CAS number		7722-84-1	007632-04-4	007632-04-4	15630-89-4
German name		Wasserstoffperoxid; in Lösung bezogen auf 100% Konzentration	Natriumperborat; tetrahydrat; 10 % aktives O2	Natriumperborat; monohydrat; 15% aktives O2	Natriumpercarbonat; min. O2 13.5%
English name		Hydrogen peroxide; solution; related to 100% concentration	Sodium perborate; tetrahydrate; 10% active O2	Sodium perborate; monohydrate; 15% active O2	Sodium percarbonate; min O2 13.5%
Amount	kg	1000	1000	1000	1000
Infrastructure		not included	not included	not included	not included

Tab. 5.9. Life cycle inventories of detergent ingredients (continued)

Data description		**CMC**	**Fluorescent Whitening Agents** **DAS-1 Triazinylaminostilbene-Type**	**Fluorescent Whitening Agents** **DSBP Distyrylbiphenyl-Type**
Type		Non term. system	Non term. system	
Version		2	3	3
Time period		1993	1997	1999
Energy values		Gross calorific values	Gross calorific values	Gross calorific values
Geography		Western Europe	Western Europe	Western Europe
Technology		Reaction of alkali cellulose with chloroacetic acid	Via 4,4'-Dinitrostilbene-2,2'-disulphonic acid (produced with Hypochlorite-Oxidation) and 4,4'-Di-aminostilbene-2,2'-di-sulphonic acid, produced with Béchamps reduction	Via 4,4'-bis (Chloromethyl)-bi-phenyl and Trimethylphosphite, via the 4,4'-bis (Dimethoxyphos-phonomethyl)-biphenyl, with Benzaldehyde-2-sulphonic acid
Representativeness		Data from a single producer	Data from a main producer	Data from the main producer
Percent		n.i.	< 50%	c. 98%
Number of producers		1	1	1
Timestamp		5.11.98	7.5.99	7.5.99
Data entry by		S.Dall'Acqua, EMPA St.Gallen	R. Bretz, CIBA SC, Basel	R. Bretz, CIBA SC, Basel
Data generator		S.Dall'Acqua, EMPA St.Gallen	R. Bretz, CIBA SC, Basel	R. Bretz, CIBA SC, Basel
Data published in		this study	<CIBA 1994>	<CIBA 1994>
Data sources		<Buwal 1998>	<CIBA SC 1999>	<CIBA SC 1999>
		<Buwal 1995>	Estimates for rawmaterial	Estimates for rawmaterial
		<Metsä-Serla 1994>	with <Bretz 1996>	with <Bretz 1996>
		<Ullmann 1989a,c>	<Buwal 1998>	<Buwal 1998>
Functional unit				
CAS number		009000-11-7	16090-02-1	27344-41-8
German name		Carboxymethyl-cellulose (NaCMC); 72% Trockensubstanz	DAS-1: Benzolsulfonsäure, 2,2'-(1,2- ethen-diyl)bis[5-[[4-(4-morpholinyl)-6-(phenylamino)-1,3,5-triazin-2-yl] amino]-, Dinatriumsalz; 67% Aktivsubstanz	DSBP: Benzolsulfonsäure, 2,2'-([1,1'-biphenyl]-4,4'-diyldi- 2,1-ethendiyl)bis-, Dinatriumsalz 83% Aktivsubstanz
English name		Carboxymethyl-cellulose (NaCMC); 72% solid	DAS-1: Benzenesulphonic acid, 2,2'-(1,2-ethene-diyl)bis[5- [[4-(4-morpholinyl)-6-(phenylamino)- 1,3,5-triazin-2-yl]amino]-, disodium salt; 67% Active ingredient	DSBP: Benzenesulphonic acid, 2,2'-([1,1'-biphenyl]-4,4'-diyldi- 2,1-ethenediyl)bis-, disodium salt; 83% Active ingredient
Amount	kg	1000	1000	1000
Infrastructure		not included	not included	not included

Tab. 5.10. Life cycle inventories of detergent ingredients (continued)

		LAS	AS	Soap	AE
Resources, commercial fuels					
Crude gas (natural gas)	Nm3	225	191	52.4	423
Crude oil from drilling well	kg	195	192	188	108
Raw brown coal	kg	73.6	65.1	25.1	88.1
Raw hard coal	kg	163	197	51.2	146
Uranium from ore	g	6.91	6.05	2.19	8.37
Biomass	kg		412	374	
Wood	kg	1.57	1.9	0.494	1.41
Pot. Energy water	MJ	458	401	145	556
Resources, feedstock					
Crude gas (as feedstock)	Nm3		7.55		546
Crude oil f. drilling well (as feedstock)	kg	841			613
Biomass (as feedstock)	kg		1750	1920	
Barytes	kg				
Bauxite	kg				
Boron	kg				
Diatomite (Kieselgur)	kg				
Dolomite	kg				
Fluorspar	kg				
Iron ore	kg				
Lead	kg				
Limestone	kg				
Magnesium	kg				
Nitrogen	kg				19
Oxygen	kg				504
Phosphate rock	kg				
Potassium	kg				
Rock salt	kg	99	111	98	
Sand, clay	kg				
SO2 secondary	kg				
Stibnite	kg				
Sulphur	kg	100	113		
Wood	kg				
Auxilliary material *	kg				
* Production not traced back to the resources (50 MJ/kg)					
Recoverable wastes (without downcycling)					
Aluminum residues	kg				
Filter residues	kg				
NaOH (ca. 15%-aq.)	kg				
Na-Silicate 47%	kg				
Disposal (Downstream processes not included)					
Industrial waste	kg	13.2	87.9	2.39	64.1
Inert chemicals	kg				
Mineral waste	kg				
Regulated & toxic chemicals	kg				
Slags & ashes	kg				

Tab. 5.11. Life cycle inventories of detergent ingredients (continued)

Resources, commercial fuels		**Esterquat; coconut oil / palm kernel oil**	**Esterquat; tallow**	**Sodium silicate (hydrothermal liquor)**	**Sodium silicate (spray powder)**
Crude gas (natural gas)	Nm3	177	225	38.1	230
Crude oil from drilling well	kg	147	466	22.1	40
Raw brown coal	kg	83	107	34.5	68.8
Raw hard coal	kg	152	137	54.9	123
Uranium from ore	g	8.62	13	2.82	6.19
Biomass	kg	602			
Wood	kg	1.41	1.26	0.0487	0.367
Pot. Energy water	MJ	745	686	155	314
Resources, feedstock					
Crude gas (as feedstock)	Nm3	252	269		
Crude oil f. drilling well (as feedstock)	kg	208	207		
Biomass (as feedstock)	kg	1950	1160		
Barytes	kg				
Bauxite	kg	0.995	0.994		
Boron	kg				
Diatomite (Kieselgur)	kg				
Dolomite	kg				
Fluorspar	kg				
Iron ore	kg	0.0511	0.0508	0.0942	0.167
Lead	kg				
Limestone	kg	0.0759	0.0757	2.19	3.8
Magnesium	kg				
Nitrogen	kg	4.38	4.38		
Oxygen	kg				
Phosphate rock	kg	8.63	43.5		
Potassium	kg	1.27	6.42		
Rock salt	kg	2.1	2.09	123	214
Sand, clay	kg	0.00522	0.00517	325	562
SO2 secondary	kg				
Stibnite	kg				
Sulphur	kg				
Wood	kg				
Auxilliary material *	kg			0.734	1.64
* Production not traced back to the resources (50 MJ/kg)					
Recoverable wastes (without downcycling)					
Aluminum residues	kg				
Filter residues	kg			0.653	
NaOH (ca. 15%-aq.)	kg				
Na-Silicate 47%	kg				
Disposal (Downstream processes not included)					
Industrial waste	kg	14.5	32.5	1.2	4.14
Inert chemicals	kg	0.000852	0.00429	1.69	3.03
Mineral waste	kg	2.21	2.2	20.2	28.9
Regulated & toxic chemicals	kg	0.00000259	0.000000271	0.004	0.00724
Slags & ashes	kg	10.8	0.923	2.25	3.98

Tab. 5.12. Life cycle inventories of detergent ingredients (continued)

		Sodium silicate (furnace lumps)	**Sodium silicate (furnace liquor)**	**Sodium metasilicate (pentahydrate)**	**Layered sodium silicate (SKS-6)**
Resources, commercial fuels					
Crude gas (natural gas)	Nm3	85.4	37	82.2	350
Crude oil from drilling well	kg	71.8	30.8	38.9	50.8
Raw brown coal	kg	15.6	6.55	68	141
Raw hard coal	kg	229	87.4	110	162
Uranium from ore	g	0.913	0.389	5.58	9.01
Biomass	kg				
Wood	kg	0.0754	0.0515	0.192	0.528
Pot. Energy water	MJ	44.5	18.9	300	439
Resources, feedstock					
Crude gas (as feedstock)	Nm3				
Crude oil f. drilling well (as feedstock)	kg				
Biomass (as feedstock)	kg				
Barytes	kg				
Bauxite	kg				
Boron	kg				
Diatomite (Kieselgur)	kg				
Dolomite	kg				
Fluorspar	kg				
Iron ore	kg			0.175	0.207
Lead	kg				
Limestone	kg	510	190	3.99	4.73
Magnesium	kg				
Nitrogen	kg				
Oxygen	kg				
Phosphate rock	kg				
Potassium	kg				
Rock salt	kg	638	237	224	266
Sand, clay	kg	772	287	293	702
SO2 secondary	kg				
Stibnite	kg				
Sulphur	kg				
Wood	kg				
Auxilliary material *	kg	0.0665	0.717	0.612	1.58
* Production not traced back to the resources (50 MJ/kg)					
Recoverable wastes (without downcycling)					
Aluminum residues	kg				
Filter residues	kg		1	0.812	1.41
NaOH (ca. 15%-aq.)	kg				
Na-Silicate 47%	kg				0.737
Waste treatment (Downstream processes not included)					
Industrial waste	kg		0.948	2.83	0.451
Inert chemicals	kg	0.65	0.268	3.71	3.16
Mineral waste	kg	127	47.2	27.6	24.8
Regulated & toxic chemicals	kg			0.00764	0.00902
Slags & ashes	kg			4.18	4.96

Tab. 5.13. Life cycle inventories of detergent ingredients (continued)

		Sodiumtripoly-phosphat (STPP)	**Zeolite A (powder)**	**Zeolite A (slurry)**	**Polycarboxylates**
Resources, commercial fuels					
Crude gas (natural gas)	Nm3	223	316	213	111
Crude oil from drilling well	kg	258	139	135	69.2
Raw brown coal	kg	41.3	95.6	88.7	35.4
Raw hard coal	kg	454	140	148	44.5
Uranium from ore	g	2.72	8.23	7.49	2.82
Biomass	kg				
Wood	kg	0.292	0.539	0.584	0.113
Pot. Energy water	MJ	319	455	418	191
Resources, feedstock					
Crude gas (as feedstock)	Nm3				140
Crude oil f. drilling well (as feedstock)	kg				149
Biomass (as feedstock)	kg				
Barytes	kg				0.0000234
Bauxite	kg		762	762	0.399
Boron	kg				
Diatomite (Kieselgur)	kg				
Dolomite	kg				0.0000234
Fluorspar	kg				0.00126
Iron ore	kg	0.00936			0.103
Lead	kg				0.0000234
Limestone	kg	1160	40	40	1.24
Magnesium	kg				
Nitrogen	kg				
Oxygen	kg				
Phosphate rock	kg	2340			
Potassium	kg				
Rock salt	kg	1220	222	222	69.5
Sand, clay	kg	0.00407	467	467	0.0516
SO2 secondary	kg	761			0.445
Stibnite	kg				
Sulphur	kg				0.18
Wood	kg				0.515
Auxilliary material *	kg	0.00339	1.88	1.88	
* Production not traced back to the resources (50 MJ/kg)					
Recoverable wastes (without downcycling)					
Aluminum residues	kg		3.12	3.12	
Filter residues	kg				
NaOH (ca. 15%-aq.)	kg		87.4	87.4	
Na-Silicate 47%	kg				
Disposal (Downstream processes not included)					
Industrial waste	kg	277			1.31
Inert chemicals	kg	0.142	10.4	10.4	0.952
Mineral waste	kg	351	252	252	8.8
Regulated & toxic chemicals	kg	0.000407	11	11	0.025
Slags & ashes	kg	0.224	5.14	5.14	1.52

Tab. 5.14. Life cycle inventories of detergent ingredients (continued)

		Hydrogen peroxide	Perborate tetrahydrate	Perborate monohydrate	Percarbonate
Resources, commercial fuels					
Crude gas (natural gas)	Nm3	348	221	537	203
Crude oil from drilling well	kg	63.8	60.7	137	68.7
Raw brown coal	kg	106	68.6	147	94.4
Raw hard coal	kg	98.2	63.5	135	468
Uranium from ore	g	10.4	6.69	14.2	6.61
Biomass	kg				
Wood	kg	0.961	0.621	1.33	0.795
Pot. Energy water	MJ	689	444	946	552
Resources, feedstock					
Crude gas (as feedstock)	Nm3	1.79	1.28	2.56	0.709
Crude oil f. drilling well (as feedstock)	kg	3.07	0.439		1.3
Biomass (as feedstock)	kg				
Barytes	kg	0.001	0.001	0.001	0.000395
Bauxite	kg	14	3	4.8	34.5
Boron	kg		70	110	
Diatomite (Kieselgur)	kg				
Dolomite	kg	0.001	0.002	0.004	0.000395
Fluorspar	kg	0.054	0.015	0.024	0.0213
Iron ore	kg	0.09	0.23	0.384	0.0368
Lead	kg	0.001	0.001	0.002	0.000395
Limestone	kg	0.38	2.7	4.4	891
Magnesium	kg		0.3	0.48	
Nitrogen	kg				
Oxygen	kg				
Phosphate rock	kg				
Potassium	kg				
Rock salt	kg	4.5	81	130	1240
Sand, clay	kg	1	0.44	0.84	5.79
SO2 secondary	kg	19	5.6	10	10.4
Stibnite	kg				
Sulphur	kg	7.7	2.4	3.8	3.66
Wood	kg	22	1.1	1.8	8.69
Auxilliary material *	kg				4.26
* Production not traced back to the resources (50 MJ/kg)					
Recoverable wastes (without downcycling)					
Aluminum residues	kg				
Filter residues	kg				0.0062
NaOH (ca. 15%-aq.)	kg				
Na-Silicate 47%	kg				
Disposal (Downstream processes not included)					
Industrial waste	kg	8.48	4.17	8.16	23.5
Inert chemicals	kg	6.3	29	46	4.67
Mineral waste	kg	49	15	24	251
Regulated & toxic chemicals	kg	0.968	0.473	0.946	0.387
Slags & ashes	kg	11	1.8	2.9	4.57

Tab. 5.15. Life cycle inventories of detergent ingredients (continued)

		CMC	Fluorescent Whitening Agents DAS-1 Triazinylaminostilbene-Type	Fluorescent Whitening Agents DSBP Distyrylbiphenyl-Type
Resources, commercial fuels				
Crude gas (natural gas)	Nm3	458	882	2750
Crude oil from drilling well	kg	391	997	1340
Raw brown coal	kg	284	850	1310
Raw hard coal	kg	324	1230	2090
Uranium from ore	g	27.6	75.3	115
Biomass	kg	17.3		
Wood	kg	578	7.09	12.2
Pot. Energy water	MJ	2210	4620	32600
Resources, feedstock				
Crude gas (as feedstock)	Nm3	287	798	2110
Crude oil f. drilling well (as feedstock)	kg		546	1450
Biomass (as feedstock)	kg	415		
Barytes	kg			
Bauxite	kg	0.00711	5.08	6.46
Boron	kg			
Diatomite (Kieselgur)	kg	0		10.2
Dolomite	kg			
Fluorspar	kg			0.0194
Iron ore	kg	0.31	286	6.97
Lead	kg			
Limestone	kg	24.4	382	79.8
Magnesium	kg			0.00000886
Nitrogen	kg			
Oxygen	kg			
Phosphate rock	kg		6.12	1940
Potassium	kg		0.0923	0.000125
Rock salt	kg	500	2270	3350
Sand, clay	kg	0.114	2.16	54.9
SO2 secondary	kg	8.73		
Stibnite	kg			1.06
Sulphur	kg	2.82		
Wood	kg			
Auxilliary material *	kg	3.28		
* Production not traced back to the resources (50 MJ/kg)				
Recoverable wastes (without downcycling)				
Aluminum residues	kg			
Filter residues	kg			
NaOH (ca. 15%-aq.)	kg			
Na-Silicate 47%	kg			
Disposal (Downstream processes not included)				
Industrial waste	kg	41.4	54	523
Inert chemicals	kg	2.17		
Mineral waste	kg	37.4	178	233
Regulated & toxic chemicals	kg	0.0112	0.00000151	0.00000559
Slags & ashes	kg	3.41	69.5	44.1

Tab. 5.16. Life cycle inventories of detergent ingredients (continued)

Air pollutants		LAS	AS	Soap	AE
Ammonia (NH3)	g	0.796	0.741	0.258	12.9
Aromatic HC	g	8.7	8.32	5.8	8.16
Benzene (C6H6)	g	5.78	5.68	2.82	7.28
Cadmium (Cd)	g	0.222	0.221	0.225	0.112
Carbon dioxide fossil (CO2)	g	1670000	1380000	793000	2190000
Carbon dioxide non-fossil (CO2)	g		477000	447000	
Carbon monoxide (CO)	g	640	738	388	984
Chlorinated HC	g				
Chlorine (Cl2)	g	0.078	0.095	0.0611	
Dust/particulates	g	964	3140	2650	930
Fluor (F2)	g				
Halogenated HC	g	0.000181	0.000158	0.0000573	0.000219
Halon H1301	g	0.0465	0.046	0.0449	0.0259
Hydrochloric acid (HCl)	g	139	171	50.2	115
Hydrofluoric acid (HF)	g	8.57	9.39	3.41	8.01
Hydrogen (H2)	g				
Lead (Pb)	g	0.568	0.622	0.448	0.342
Manganese (Mn)	g	0.0591	0.0718	0.0184	0.0525
Mercaptans	g	0.00042	110	94	
Mercury (Hg)	g	0.347	0.366	0.338	0.0385
Metals	g				
Metals* (Energy modules SRU 250)	g	75.4	90.1	41.7	53.2
Methane (CH4)	g	3100	19800	15600	3800
Nickel (Ni)	g	4.83	4.82	4.7	2.6
Nitrogen oxides (NOx) as NO2	g	4290	3150	2050	4110
Nitrous oxide (N2O)	g	20.5	20.3	14.4	18.7
NMVOC non-methane HC	g	2710	3290	1890	17400
PAH policycl. arom. HC	g	0.0823	0.0704	0.0225	0.147
Radioactive substances	kBq	601000	526000	191000	728000
Sulphur oxides (SOx) as SO2	g	12000	11600	9730	7890
Zinc (Zn)	g	0.597	0.635	0.481	0.37
* do to assess (see 3.15.5)					

Tab. 5.17. Life cycle inventories of detergent ingredients (continued)

Air pollutants		Esterquat; coconut oil / palm kernel oil	Esterquat; tallow	Sodium silicate (hydrothermal liquor)	Sodium silicate (spray powder)
Ammonia (NH3)	g	4.37	54200	0.035	0.323
Aromatic HC	g	6.63	13.4	0.35	2.3
Benzene (C6H6)	g	3.48	7.97	0.27	2.59
Cadmium (Cd)	g	0.108	0.0638	0.000496	0.00153
Carbon dioxide fossil (CO2)	g	1330000	2450000	289000	892000
Carbon dioxide non-fossil (CO2)	g	365000	4100000		
Carbon monoxide (CO)	g	1250	7200	218	509
Chlorinated HC	g				
Chlorine (Cl2)	g				
Dust/particulates	g	2610	1220	667	1510
Fluor (F2)	g	0.122	0.614		
Halogenated HC	g	0.000134	0.000197	0.00000412	0.0000415
Halon H1301	g	0.0348	0.111	0.00145	0.00292
Hydrochloric acid (HCl)	g	84.1	79.5	34.5	73.5
Hydrofluoric acid (HF)	g	6.64	6.03	0.241	1.87
Hydrogen (H2)	g				
Lead (Pb)	g	0.285	0.247	0.00472	0.0198
Manganese (Mn)	g	0.0378	0.0362	0.00133	0.00837
Mercaptans	g				
Mercury (Hg)	g	0.0172	0.0202	0.00117	0.0141
Metals	g	10.6	10.5	0.418	0.723
Metals* (Energy modules SRU 250)	g	27.7	24.9	1.2	5.99
Methane (CH4)	g	13400	213000	128	1340
Nickel (Ni)	g	2.53	1.95	0.0215	0.0859
Nitrogen oxides (NOx) as NO2	g	6060	25500	1750	3490
Nitrous oxide (N2O)	g	53.2	70500	0.689	4.93
NMVOC non-methane HC	g	4130	10500	1450	2590
PAH policycl. arom. HC	g	0.0488	0.0668	0.0045	0.0611
Radioactive substances	kBq	445000	655000	13600	138000
Sulphur oxides (SOx) as SO2	g	7530	6960	2190	4180
Zinc (Zn)	g	0.402	1.53	0.0796	0.158
* do to assess (see 3.15.5)					

Tab. 5.18. Life cycle inventories of detergent ingredients (continued)

Air pollutants		Sodium silicate (furnace lumps)	Sodium silicate (furnace liquor)	Sodium metasilicate (pentahydrate)	Layered sodium silicate (SKS-6)
Ammonia (NH3)	g	237	88.3	0.184	0.524
Aromatic HC	g	1.84	0.824	0.939	4.15
Benzene (C6H6)	g	1.03	0.489	0.62	4.16
Cadmium (Cd)	g	0.00411	0.00413	0.000968	0.00279
Carbon dioxide fossil (CO2)	g	1070000	425000	570000	1290000
Carbon dioxide non-fossil (CO2)	g				
Carbon monoxide (CO)	g	3750	1410	404	2580
Chlorinated HC	g				
Chlorine (Cl2)	g				
Dust/particulates	g	3890	1450	1260	1670
Fluor (F2)	g				
Halogenated HC	g	0.0000152	0.00000692	0.0000194	0.0000855
Halon H1301	g	0.0172	0.00737	0.00232	0.00386
Hydrochloric acid (HCl)	g	62.1	25.9	67.1	105
Hydrofluoric acid (HF)	g	2.02	0.874	1.06	3.76
Hydrogen (H2)	g				
Lead (Pb)	g	0.0175	0.014	0.0102	0.0287
Manganese (Mn)	g	0.0023	0.00168	0.00444	0.0133
Mercaptans	g				
Mercury (Hg)	g	0.00472	0.00224	0.00366	0.0242
Metals	g			0.761	0.901
Metals* (Energy modules SRU 250)	g	2.41	2	3.02	11.1
Methane (CH4)	g	666	307	371	2100
Nickel (Ni)	g	0.165	0.119	0.0544	0.113
Nitrogen oxides (NOx) as NO2	g	3610	1420	3260	4320
Nitrous oxide (N2O)	g	1.54	0.844	1.61	8.1
NMVOC non-methane HC	g	1040	420	2640	3270
PAH policycl. arom. HC	g	0.00732	0.004	0.013	0.1
Radioactive substances	kBq	50200	22900	64400	285000
Sulphur oxides (SOx) as SO2	g	4700	1910	4080	5570
Zinc (Zn)	g	0.237	0.0972	0.0854	0.217
* not to assess (see 3.15.5)					

Tab. 5.19. Life cycle inventories of detergent ingredients (continued)

Air pollutants		Sodiumtripoly-phosphat (STPP)	Zeolite A (powder)	Zeolite A (slurry)	Polycarboxylates
Ammonia (NH3)	g	451	0.56	0.459	0.168
Aromatic HC	g	7.75	6.05	5.01	5.37
Benzene (C6H6)	g	5.15	4.79	3.48	0.872
Cadmium (Cd)	g	0.186	0.113	0.112	0.0043
Carbon dioxide fossil (CO2)	g	2720000	1420000	1210000	734000
Carbon dioxide non-fossil (CO2)	g				
Carbon monoxide (CO)	g	7720	730	664	280
Chlorinated HC	g				
Chlorine (Cl2)	g				0.0234
Dust/particulates	g	7540	4500	4470	633
Fluor (F2)	g				0.0234
Halogenated HC	g	0.0000475	0.000096	0.0000726	0.0000424
Halon H1301	g	0.0603	0.0265	0.0256	0.0161
Hydrochloric acid (HCl)	g	100	89.8	100	27.7
Hydrofluoric acid (HF)	g	4.86	3.8	3.66	1.08
Hydrogen (H2)	g				7.96
Lead (Pb)	g	0.454	0.228	0.242	0.0192
Manganese (Mn)	g	0.0472	0.0162	0.0187	0.00557
Mercaptans	g				0.0234
Mercury (Hg)	g	0.0159	0.0223	0.0156	0.00686
Metals	g	0.04	0.708	0.735	0.512
Metals* (Energy modules SRU 250)	g	34.5	22.4	26.7	2.41
Methane (CH4)	g	2220	2320	1740	855
Nickel (Ni)	g	4.69	2.47	2.41	0.197
Nitrogen oxides (NOx) as NO2	g	8750	4630	4450	2770
Nitrous oxide (N2O)	g	22.1	13.8	11.4	1.64
NMVOC non-methane HC	g	3550	3410	3410	3350
PAH policycl. arom. HC	g	0.0723	0.0955	0.0597	0.00579
Radioactive substances	kBq	158000	320000	241000	118000
Sulphur oxides (SOx) as SO2	g	19400	8790	8750	2410
Zinc (Zn)	g	0.492	0.373	0.377	0.0773
* do to assess (see 3.15.5)					

Tab. 5.20. Life cycle inventories of detergent ingredients (continued)

Air pollutants		Hydrogen peroxide	Perborate tetrahydrate	Perborate monohydrate	Percarbonate
Ammonia (NH3)	g	1.06	1.69	2.47	414
Aromatic HC	g	157	43.9	75.1	64.5
Benzene (C6H6)	g	5.25	3.54	8.49	3.09
Cadmium (Cd)	g	0.0519	0.0575	0.132	0.0239
Carbon dioxide fossil (CO2)	g	1200000	953000	2100000	1620000
Carbon dioxide non-fossil (CO2)	g				
Carbon monoxide (CO)	g	428	400	891	6430
Chlorinated HC	g		1	1	
Chlorine (Cl2)	g	1	1	1	0.395
Dust/particulates	g	652	1880	3530	7020
Fluor (F2)	g	1	1	1	0.395
Halogenated HC	g	0.000271	0.000175	0.000372	0.000155
Halon H1301	g	0.0152	0.0145	0.0327	0.015
Hydrochloric acid (HCl)	g	70.3	64.7	126	115
Hydrofluoric acid (HF)	g	7.81	5.51	10.7	7.93
Hydrogen (H2)	g	340	96	150	134
Lead (Pb)	g	0.157	0.143	0.321	0.0862
Manganese (Mn)	g	0.0347	0.0224	0.0478	0.0236
Mercaptans	g	1	1	1	0.395
Mercury (Hg)	g	0.0316	0.0203	0.0475	0.0189
Metals	g	1	1	1	0.487
Metals* (Energy modules SRU 250)	g	24.3	18.5	40.6	17.6
Methane (CH4)	g	2880	1910	4470	1770
Nickel (Ni)	g	1.4	1.4	3.16	0.701
Nitrogen oxides (NOx) as NO2	g	1950	2280	4510	4460
Nitrous oxide (N2O)	g	13.1	9.65	22.5	8.31
NMVOC non-methane HC	g	1220	1620	3020	1920
PAH policycl. arom. HC	g	0.121	0.0776	0.188	0.0619
Radioactive substances	kBq	901000	582000	1240000	516000
Sulphur oxides (SOx) as SO2	g	4280	4800	9940	8380
Zinc (Zn)	g	0.202	0.176	0.393	0.609
* do to assess (see 3.15.5)					

Tab. 5.21. Life cycle inventories of detergent ingredients (continued)

		CMC	Fluorescent Whitening Agents DAS-1 Triazinylaminostilbene-Type	Fluorescent Whitening Agents DSBP Distyrylbiphenyl-Type
Air pollutants				
Ammonia (NH3)	g	2.36	21300	93
Aromatic HC	g	18.6	50.6	157
Benzene (C6H6)	g	9	23.5	66.9
Cadmium (Cd)	g	0.35	0.763	0.879
Carbon dioxide fossil (CO2)	g	3060000	10100000	20700000
Carbon dioxide non-fossil (CO2)	g			
Carbon monoxide (CO)	g	1460	5210	10600
Chlorinated HC	g	330		
Chlorine (Cl2)	g	0.0666	0.000215	0.0006
Dust/particulates	g	4400	12500	17800
Fluor (F2)	g			
Halogenated HC	g	0.000634	0.00209	44.7
Halon H1301	g	0.0868	0.21	0.275
Hydrochloric acid (HCl)	g	226	1630	1700
Hydrofluoric acid (HF)	g	16	82.4	85.4
Hydrogen (H2)	g			2500
Lead (Pb)	g	0.768	3.22	4.29
Manganese (Mn)	g	0.0795	1.46	0.627
Mercaptans	g			0.000558
Mercury (Hg)	g	0.0489	0.16	0.343
Metals	g	1.21	4.31	7.59
Metals* (Energy modules SRU 250)	g	75.5	275	425
Methane (CH4)	g	5310	17100	35000
Nickel (Ni)	g	7.96	18.4	21.9
Nitrogen oxides (NOx) as NO2	g	11100	32600	58400
Nitrous oxide (N2O)	g	36.9	203	608
NMVOC non-methane HC	g	8060	19000	32900
PAH policycl. arom. HC	g	0.15	0.341	1.06
Radioactive substances	kBq	2050000	6490000	9870000
Sulphur oxides (SOx) as SO2	g	23400	71500	95200
Zinc (Zn)	g	0.933	4.67	12.7
* do to assess (see 3.15.5)				

Tab. 5.22. Life cycle inventories of detergent ingredients (continued)

		LAS	AS	Soap	AE
Water pollutants					
Waste water quantity	m3				
Aluminium (Al)	g	263	316	82.1	235
Ammonium (NH4+)	g	29.2	10.9	9.91	11.1
Antimony (Sb)	g				
AOX as Cl-	g	0.0338	0.0334	0.0326	0.0188
Aromatic HC	g	8.67	8.51	8.07	5.36
Arsenic (As)	g	0.53	0.638	0.171	0.473
Barium (Ba)	g	45.2	49.2	30.1	32.2
BOD	g	470	320	3370	1440
Boron (B)	g				
Cadmium (Cd)	g	0.0242	0.0267	0.0144	0.0183
Chlorate (ClO3-)	g				
Chloride (Cl-)	g	7950	6820	5450	4400
Chlorinated CH	g	0.0118	0.0112	0.00888	0.0111
Chromium (Cr)	g	7.11	5.84	1.1	9.72
COD	g	1330	2880	9310	2730
Copper (Cu)	g	1.32	1.59	0.425	1.17
Cyanide (CN-)	g	0.0416	0.0411	0.0374	0.0256
DOC	g	3.16	2.65	0.631	6.15
Fats/oils	g	302	307	316	171
Fluoride (F-)	g	3.71			0.949
H2O2	g				
Inorg. salts and acids	g	7830	11700	16000	4250
Iron (Fe)	g	201	201	676	214
Lead (Pb)	g	1.44	1.7	0.473	1.32
Mercury (Hg)	g	0.0309	0.0278	0.0385	0.00158
Metals	g	86.7	91.5	67.2	57.6
Nickel (Ni)	g	3.54	1.64	0.473	1.23
Nitrate (NO3-)	g	8.77	8.4	6.79	6.56
Nitrogen org. bound	g	0.977	0.967	0.934	0.553
Nitrogen total	g	9.69	79.6	689	5.44
PAH policycl. arom. HC	g	0.127	0.126	0.123	0.0707
Phenols	g	2.06	1.42	1.36	0.907
Phosphate (PO4 3-)	g	17.8	18.9	4.98	17.5
Radioactive substances	kBq	5540	4850	1760	6710
Silicates	g				
Sulphate (SO4 2-)	g	3290	3370	732	2340
Sulphide (S 2-)	g	110	2.3	2.99	29.2
Suspended solids	g	1070	1580	2470	844
TOC	g	291	254	116	459
Toluene (C7H8)	g	1.19	1.17	1.12	0.709
Zinc (Zn)	g	3.51	3.38	1.08	4.6
Water consumption					
Cooling water	m3	n.i.	n.i.	n.i.	n.i.
Process water	m3	n.i.	n.i.	n.i.	n.i.
Washing water	m3	n.i.	n.i.	n.i.	n.i.
Delivered energy (additional information)					
Electricity	MJ	1770	1510	450	2220
Biomass	MJ		1630	1480	
Diesel	MJ				
Natural gas	MJ	7330	6130	1410	14600
Heating oil EL	MJ				
Heating oil S	MJ				
Oil fuels	MJ	6590	6580	6850	3190
Coal	MJ	1790	2570	545	1220
Energy not specified	MJ				
Total delivered (final) energy	MJ	17500	18400	10700	21200
Energy production & delivery	MJ	7570	6950	3710	8210
Auxiliary material (50 MJ/kg)	MJ				
Feedstock	MJ	38300	31000	34800	49200
Recovered energy	MJ				
Total primary energy	MJ	63400	56300	49300	78700

Tab. 5.23. Life cycle inventories of detergent ingredients (continued)

		Esterquat; coconut oil / palm kernel oil	Esterquat; tallow	Sodium silicate (hydrothermal liquor)	Sodium silicate (spray powder)
Water pollutants					
Waste water quantity	m3			0.105	0.469
Aluminium (Al)	g	187	164	7.95	59.4
Ammonium (NH4+)	g	277	395	0.6	1.36
Antimony (Sb)	g				
AOX as Cl-	g	0.0262	0.0881	0.00104	0.0021
Aromatic HC	g	6.42	20.1	0.281	0.851
Arsenic (As)	g	0.391	0.4	0.0162	0.12
Barium (Ba)	g	33.1	71.1	1.39	6.25
BOD	g	2230	1710	0.652	1.15
Boron (B)	g				
Cadmium (Cd)	g	0.0462	0.177	0.000891	0.00377
Chlorate (ClO3-)	g				
Chloride (Cl-)	g	5050	13400	6320	11200
Chlorinated CH	g	0.00636	0.0208	0.000452	0.00333
Chromium (Cr)	g	2.1	2.67	0.0829	0.614
COD	g	3000	1580	9.8	6.34
Copper (Cu)	g	1.02	1.24	0.0401	0.296
Cyanide (CN-)	g	0.0392	0.0996	0.00152	0.00716
DOC	g	3500	3500	0.182	2.72
Fats/oils	g	264	834	8.55	23.4
Fluoride (F-)	g				
H2O2	g				
Inorg. salts and acids	g	6350	9990	1030	2070
Iron (Fe)	g	825	176	5.1	37.1
Lead (Pb)	g	1.43	1.59	0.0441	0.323
Mercury (Hg)	g	0.00232	0.00924	0.0000498	0.000673
Metals	g	129	223	17.3	35.2
Nickel (Ni)	g	1	1.15	0.0408	0.3
Nitrate (NO3-)	g	8.26	17.9	0.446	1.55
Nitrogen org. bound	g	1.32	7.72	0.0938	0.165
Nitrogen total	g	744	193	0.553	1.02
PAH policycl. arom. HC	g	0.0952	0.303	0.00397	0.00802
Phenols	g	1.36	3.44	0.042	0.112
Phosphate (PO4 3-)	g	258	1460	0.482	3.54
Radioactive substances	kBq	4100	6030	125	1270
Silicates	g			1640	23600
Sulphate (SO4 2-)	g	1470	1860	871	1840
Sulphide (S 2-)	g	0.845	1.33	0.00885	0.0218
Suspended solids	g	1820	3100	892	4200
TOC	g	3690	3870	14.9	189
Toluene (C7H8)	g	0.883	2.78	0.038	0.102
Zinc (Zn)	g	1.98	2.03	0.0821	0.6
Water consumption					
Cooling water	m3			0.0126	0.0734
Process water	m3	71.6	72.7	1.72	5.46
Washing water	m3			0.302	0.372
Delivered energy (additional information)					
Electricity	MJ	1540	1650	970	2200
Biomass	MJ	4800			
Diesel	MJ	1730	15600	124	182
Natural gas	MJ	3560	4790	1160	7410
Heating oil EL	MJ	71.2	1390	407	705
Heating oil S	MJ	1990	297	6.31	8.79
Oil fuels	MJ	18.7			
Coal	MJ	519	559	267	467
Energy not specified	MJ	6530	7350	41.7	1010
Total delivered (final) energy	MJ	20800	31600	3010	12100
Energy production & delivery	MJ	5960	8600	2360	5930
Auxiliary material (50 MJ/kg)	MJ			36.7	82.1
Feedstock	MJ	50800	34700		
Recovered energy	MJ				
Total primary energy	MJ	77500	74900	5370	18000

Tab. 5.24. Life cycle inventories of detergent ingredients (continued)

Water pollutants		Sodium silicate (furnace lumps)	Sodium silicate (furnace liquor)	Sodium metasilicate (pentahydrate)	Layered sodium silicate (SKS-6)
Waste water quantity	m3	0.301	0.122	0.0743	0.393
Aluminium (Al)	g	12.5	8.56	31.1	87.2
Ammonium (NH4+)	g	122	45.4	1.04	1.98
Antimony (Sb)	g				
AOX as Cl-	g	0.0123	0.00531	0.00174	0.00279
Aromatic HC	g	3.18	1.37	0.476	1.22
Arsenic (As)	g	0.0277	0.0183	0.0629	0.175
Barium (Ba)	g	9.99	4.55	3.69	8.92
BOD	g	0.347	0.142	1.18	1.44
Boron (B)	g				
Cadmium (Cd)	g	0.00448	0.00209	0.00237	0.00589
Chlorate (ClO3-)	g				
Chloride (Cl-)	g	375000	139000	11500	14200
Chlorinated CH	g	0.00418	0.00181	0.000953	0.00517
Chromium (Cr)	g	0.161	0.101	0.317	0.902
COD	g	3.91	1.64	14.1	21.8
Copper (Cu)	g	0.0682	0.0452	0.156	0.434
Cyanide (CN-)	g	0.0138	0.00595	0.00386	0.00513
DOC	g	1	0.446	0.518	4.33
Fats/oils	g	97.7	42	14.3	32.9
Fluoride (F-)	g				
H2O2	g				
Inorg. salts and acids	g	230000	85400	4540	2850
Iron (Fe)	g	15.8	8.28	22.8	139
Lead (Pb)	g	0.0757	0.0488	0.17	0.493
Mercury (Hg)	g	0.00027	0.00012	0.000158	0.00107
Metals	g	26.5	11.5	32.8	45.6
Nickel (Ni)	g	0.0724	0.0472	0.158	0.439
Nitrate (NO3-)	g	2.52	1.1	1.16	2.73
Nitrogen org. bound	g	0.456	0.19	0.144	0.227
Nitrogen total	g	3.94	1.67	0.871	1.39
PAH policycl. arom. HC	g	0.0469	0.0201	0.00635	0.0106
Phenols	g	0.52	0.224	0.0706	0.156
Phosphate (PO4 3-)	g	0.775	0.524	1.86	5.2
Radioactive substances	kBq	463	212	593	2620
Silicates	g			580	16900
Sulphate (SO4 2-)	g	169	89.1	1710	2620
Sulphide (S 2-)	g	0.108	0.0466	0.0161	0.0249
Suspended solids	g	28800	10700	605	2200
TOC	g	96.1	42.3	39.2	299
Toluene (C7H8)	g	0.437	0.188	0.0631	0.143
Zinc (Zn)	g	0.156	0.0989	0.316	0.88
Water consumption					
Cooling water	m3	1.12	0.392	0.0317	0.285
Process water	m3	6.16	3.19	3.05	3.4
Washing water	m3		0.03	0.806	0.651
Delivered energy (additional information)					
Electricity	MJ	144	63.7	1990	2860
Biomass	MJ				
Diesel	MJ	135	49	225	268
Natural gas	MJ	2990	1290	2420	11100
Heating oil EL	MJ	252	93.8	644	879
Heating oil S	MJ	2310	1010	4.47	13.6
Oil fuels	MJ				
Coal	MJ	4090	1550	443	577
Energy not specified	MJ	3.19	25.5	5.71	78.4
Total delivered (final) energy	MJ	9930	4120	5760	15700
Energy production & delivery	MJ	1730	742	4810	8250
Auxiliary material (50 MJ/kg)	MJ	3.33	35.9	30.6	79.1
Feedstock	MJ				
Recovered energy	MJ	-710	-240		
Total primary energy	MJ	11000	4620	10600	24100

Tab. 5.25. Life cycle inventories of detergent ingredients (continued)

Water pollutants		Sodiumtripoly-phosphat (STPP)	Zeolite A (powder)	Zeolite A (slurry)	Polycarboxylates
Waste water quantity	m3	45.5	3.02	2.84	
Aluminium (Al)	g	48.5	2510	2500	26.3
Ammonium (NH4+)	g	239	6.79	6.42	2.11
Antimony (Sb)	g				
AOX as Cl-	g	0.0448	0.0193	0.0186	0.0132
Aromatic HC	g	11.1	5.2	4.84	3.1
Arsenic (As)	g	0.107	0.182	0.199	0.0539
Barium (Ba)	g	35.5	20.9	21.1	10.4
BOD	g	0.739	1.37	1.39	301
Boron (B)	g				
Cadmium (Cd)	g	4.06	0.0138	0.0129	0.00519
Chlorate (ClO3-)	g				
Chloride (Cl-)	g	715000	13900	14200	3770
Chlorinated CH	g	0.0138	0.00891	0.00714	0.00443
Chromium (Cr)	g	0.606	1.16	1.16	0.292
COD	g	15.8	85.6	62.3	1120
Copper (Cu)	g	0.263	0.556	0.557	0.132
Cyanide (CN-)	g	0.0497	0.0254	0.0232	0.0141
DOC	g	2.69	3.93	2.38	4.92
Fats/oils	g	341	157	148	36.4
Fluoride (F-)	g	71600			
H2O2	g				
Inorg. salts and acids	g	441000	29600	28100	893
Iron (Fe)	g	52	90.8	78.9	34.9
Lead (Pb)	g	0.287	0.528	0.546	0.158
Mercury (Hg)	g	0.000756	0.00104	0.000671	0.000401
Metals	g	89.8	68.3	68.6	77.8
Nickel (Ni)	g	0.278	0.468	0.504	0.136
Nitrate (NO3-)	g	8.86	905	904	9.85
Nitrogen org. bound	g	1.87	0.682	0.653	1.19
Nitrogen total	g	15.1	6.03	5.8	3.19
PAH policycl. arom. HC	g	0.165	0.0725	0.0698	0.043
Phenols	g	1.82	0.834	0.789	0.374
Phosphate (PO4 3-)	g	3.01	35.6	26.3	2.33
Radioactive substances	kBq	1460	2940	2220	1090
Silicates	g				
Sulphate (SO4 2-)	g	685	2260	2240	786
Sulphide (S 2-)	g	0.39	0.173	0.165	0.948
Suspended solids	g	2890000	8350	8250	592
TOC	g	283	310	203	126
Toluene (C7H8)	g	1.52	0.701	0.66	0.419
Zinc (Zn)	g	51.1	1.04	1.08	0.286
Water consumption					
Cooling water	m3		14.1	14.1	
Process water	m3	16.9	2.22	2.22	1.21
Washing water	m3		2.71	2.71	
Delivered energy (additional information)					
Electricity	MJ	1340	2630	2400	977
Biomass	MJ				
Diesel	MJ	1890	552	514	148
Natural gas	MJ	7570	10500	6900	3990
Heating oil EL	MJ	29.3	668	686	166
Heating oil S	MJ	5210	3380	3350	31.6
Oil fuels	MJ				2260
Coal	MJ	8000	414	731	138
Energy not specified	MJ				
Total delivered (final) energy	MJ	24000	18200	14700	7710
Energy production & delivery	MJ	7020	8250	7720	2420
Auxiliary material (50 MJ/kg)	MJ	0.17	94	94	
Feedstock	MJ				12200
Recovered energy	MJ				
Total primary energy	MJ	31100	26500	22400	22400

Tab. 5.26. Life cycle inventories of detergent ingredients (continued)

		Hydrogen peroxide	**Perborate tetrahydrate**	**Perborate monohydrate**	**Percarbonate**
Water pollutants					
Waste water quantity	m3				0.0124
Aluminium (Al)	g	189	111	232	143
Ammonium (NH4+)	g	5.94	5.18	10.3	210
Antimony (Sb)	g				
AOX as Cl-	g	0.0111	0.0105	0.0238	0.0107
Aromatic HC	g	3.33	2.97	6.78	2.98
Arsenic (As)	g	0.321	0.208	0.444	0.266
Barium (Ba)	g	20.5	15.7	34.4	18.3
BOD	g	230	67.2	100	91.2
Boron (B)	g		2200	3600	
Cadmium (Cd)	g	0.0123	0.00902	0.0196	0.0104
Chlorate (ClO3-)	g				
Chloride (Cl-)	g	6730	7580	14100	718000
Chlorinated CH	g	0.00802	0.00596	0.014	0.00534
Chromium (Cr)	g	1.64	1.06	2.28	1.35
COD	g	2800	873	1410	1740
Copper (Cu)	g	0.791	0.513	1.1	0.656
Cyanide (CN-)	g	0.0175	0.0151	0.0336	0.0146
DOC	g	5.07	3.2	7.8	2.51
Fats/oils	g	98.8	89.8	203	90.3
Fluoride (F-)	g				
H2O2	g				3000
Inorg. salts and acids	g	3340	2800	5650	424000
Iron (Fe)	g	218	142	303	166
Lead (Pb)	g	0.966	0.625	1.33	0.756
Mercury (Hg)	g	0.00136	0.000874	0.00208	0.00076
Metals	g	105	70.5	141	66.8
Nickel (Ni)	g	0.803	0.522	1.11	0.666
Nitrate (NO3-)	g	386	114	180	155
Nitrogen org. bound	g	0.328	0.309	0.696	0.643
Nitrogen total	g	4.21	4.04	7.86	4.79
PAH policycl. arom. HC	g	0.0416	0.0396	0.0894	0.041
Phenols	g	1.51	1.47	2.07	0.854
Phosphate (PO4 3-)	g	42.9	24.8	42.5	314
Radioactive substances	kBq	8300	5360	11400	4750
Silicates	g				15.6
Sulphate (SO4 2-)	g	1890	1750	3440	8370
Sulphide (S 2-)	g	0.103	0.0963	0.217	0.0932
Suspended solids	g	2150	1120	2050	50700
TOC	g	375	244	588	198
Toluene (C7H8)	g	0.433	0.395	0.896	0.4
Zinc (Zn)	g	1.62	1.05	2.25	1.34
Water consumption					
Cooling water	m3	150	61.1	120	
Process water	m3	6.6	17	30	14.5
Washing water	m3				
Delivered energy (additional information)					
Electricity	MJ	2940	1880	3960	1990
Biomass	MJ				
Diesel	MJ				535
Natural gas	MJ	11800	7470	18300	6930
Heating oil EL	MJ				767
Heating oil S	MJ				719
Oil fuels	MJ	1350	1610	3710	
Coal	MJ				7140
Energy not specified	MJ				180
Total delivered (final) energy	MJ	16100	11000	26000	18300
Energy production & delivery	MJ	8600	5750	12600	6330
Auxiliary material (50 MJ/kg)	MJ				213
Feedstock	MJ	220	70	100	86.9
Recovered energy	MJ	-740	-1070	-1670	
Total primary energy	MJ	24200	15700	37000	24900

Tab. 5.27. Life cycle inventories of detergent ingredients (continued)

Water pollutants		CMC	Fluorescent Whitening Agents DAS-1 Triazinylaminostilbene-Type	Fluorescent Whitening Agents DSBP Distyrylbiphenyl-Type
Waste water quantity	m3	40		
Aluminium (Al)	g	383	1850	3870
Ammonium (NH4+)	g	24.1	2080	3900
Antimony (Sb)	g		0.0205	69.2
AOX as Cl-	g	216	6480	0.2
Aromatic HC	g	16.2	39.2	54.5
Arsenic (As)	g	0.776	3.73	6.25
Barium (Ba)	g	75.5	256	391
BOD	g	4910	20.5	32.8
Boron (B)	g			
Cadmium (Cd)	g	0.0408	0.152	0.227
Chlorate (ClO3-)	g	855		
Chloride (Cl-)	g	31800	922000	480000
Chlorinated CH	g	0.022	0.0538	0.0964
Chromium (Cr)	g	4.04	19.1	31.7
COD	g	18600	122	180
Copper (Cu)	g	1.92	9.67	22.6
Cyanide (CN-)	g	0.0814	1.92	1.2
DOC	g	14.2	97600	14300
Fats/oils	g	511	1250	1740
Fluoride (F-)	g		20.4	15.8
H2O2	g			
Inorg. salts and acids	g	10900	1320000	50600
Iron (Fe)	g	481	1850	5850
Lead (Pb)	g	2.33	10.8	17.6
Mercury (Hg)	g	0.00195	0.0053	0.0128
Metals	g	184	565	823
Nickel (Ni)	g	1.95	10.4	15.2
Nitrate (NO3-)	g	20.3	3390	10800
Nitrogen org. bound	g	2.14	5.89	8.48
Nitrogen total	g	168	15000	799
PAH policycl. arom. HC	g	0.237	0.576	0.771
Phenols	g	2.66	9.22	9.87
Phosphate (PO4 3-)	g	101	2180	2320
Radioactive substances	kBq	18900	59400	90400
Silicates	g			
Sulphate (SO4 2-)	g	6690	152000	224000
Sulphide (S 2-)	g	0.568	3	2110
Suspended solids	g	3030	18900	11400
TOC	g	3250	98900	20600
Toluene (C7H8)	g	2.22	5.38	7.34
Zinc (Zn)	g	3.97	20.6	171
Water consumption				
Cooling water	m3			
Process water	m3	1.88	467	1340
Washing water	m3		467	1340
Delivered energy (additional information)				
Electricity	MJ	8490	26100	39800
Biomass	MJ	11800		
Diesel	MJ	638		
Natural gas	MJ	14400	28500	92900
Heating oil EL	MJ	547		
Heating oil S	MJ	10500		
Oil fuels	MJ	235	34500	45700
Coal	MJ	712	15900	28200
Energy not specified	MJ	1120		
Total delivered (final) energy	MJ	48300	105000	207000
Energy production & delivery	MJ	24100	39100	78400
Auxiliary material (50 MJ/kg)	MJ	164		
Feedstock	MJ	19500	49800	132000
Recovered energy	MJ			
Total primary energy	MJ	92000	194000	417000

Tab. 5.28. Life cycle inventories of detergent ingredients (end)

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APPENDIX A: CRITICAL REVIEW REPORT ON "LIFE CYCLE INVENTORIES FOR THE PRODUCTION OF DETERGENT INGREDIENTS"

Reviewer:

Rolf Bretz
Life Cycle Assessment
Consumer Care Division
Ciba Specialty Chemicals
P.O. Box
CH-4002 Basel / Switzerland

Summary

This Critical Review Report reflects the assessment of the reviewer on the study "Ökoinventare für die Produktion von Waschmittel-Inhaltsstoffen" by EMPA St.Gall (S. Dall'Acqua, Dr. M. Fawer, R. Fritschi and C. Allenspach).

The present study gives a very positive impression; the scientific and technical methods applied are sound, and the authors adhere carefully to the requirements set by the ISO standards. The data used in this study come from very reliable, state-of-the-art sources; they were checked or collected with great care, and transformed according to the goals of the study by well-documented methods.

The publication of the study is strongly recommended.

The following improvement options were identified, which could further improve the value of the study:

- One process estimation (cationic tensides) should be based on more reliable data for its input materials. The authors agree with this measure and the work is in progress.
- The inclusion or exclusion of waste treatment processes in the system boundaries should be clarified and applied consistently (point accepted by the authors).
- Double counts in the water emissions (the TOC / DOC / COD problem) need to be avoided on the inventory level, since this correction is no longer possible in the subsequent impact assessment step (which is not part of this study).
- The sum emission parameter "metals to air" comprises both harmless elements (Na, K, Ca, Mg) and actually toxic heavy metals. It leads to distortions in some impact assessment methods (such as Eco-Indicator 95 <Goedkoop 1995>). The authors agreed to reconsider the definition and use of this parameter. **Important:** This problem is not limited to the present investigation, but afflicts all life cycle inventories based on emission data in the BUWAL study SRU 250 <BUWAL 1998>.
- Boron emissions to water should not be concealed in the sum parameter "salts and acids", since they are used in impact assessment methods, e.g. in Eco-Indicator 95. Boron effluents are particularly important in the washing process.
- The transparent representation of data in the original, published studies (separate lists for process and energy-related data, data for individual process steps) is not maintained in the present investigation. This transparency (which was endorsed by the data suppliers) should not unnecessarily be given up for the sake of uniformity. The draft international standard ISO 14043 <ISO 1998a> strongly recommends such structured LCI inputs and outputs in Annex A, as a tool for anomaly detection and for dominance and influence analysis.

1. Introduction

The study "Ökoinventare für die Produktion von Waschmittel-Inhaltsstoffen" was commissioned to EMPA St. Gall (S. Dall'Acqua, Dr. M. Fawer, R. Fritschi and C.Allenspach) in spring 1997 as a sub-project of the more comprehensive investigation "Gewerbliche Wasch- und Reinigungsmittel" by the German Umweltbundesamt (UBA).

The reviewing process started with a whole-day introductory meeting with S. Dall'Acqua and Dr. M. Fawer on Sept. 29, 1998. Shorter meetings on Nov. 26, Dec. 4 and 7, 1998, and Jan. 27, 1999 with either author served to define the scope of this review and the details of cooperation. After the appropriate secrecy agreements had been signed, draft reports and data were exchanged. A series of telephone conferences between February and April 1999, supported by exchange of intermediate results via e-mail, served to clarify individual questions.

This Critical Review is based on the 3rd draft (January 1999) and the 4th draft (4. March 1999). Since the latter contains a substantial number of enhancements and improvements, the subsequent comments refer mostly to the 4th draft. The review covers all sections of the draft report, except section 4.10 on optical brighteners (and the corresponding data about brighteners in section 5.2), since the reviewer actively participated in the preparation of this section.

The review follows the guidance for performing a peer review in the SETAC 'Code of Practice' <SETAC 1993>, as well as the more recent requirements of ISO standards 14040 <ISO 1997> and 14041 <ISO 1998>.

2. General Comments

The present study gives a very positive impression; the scientific and technical methods applied are sound, and the authors adhere carefully to the requirements set by the ISO standards. The data used in this study come from three sources:

- published studies of internationally accepted quality, by reputable third-party authors, mostly peer-reviewed
- previous studies by EMPA (mostly by the authors of this investigation, generally peer-reviewed) that were reassessed and updated
- new or reassessed studies by material suppliers, mostly in cooperation with EMPA and under critical survey of the authors.

The reviewer is convinced that these data reflect the state of the art and meet present-day quality criteria as closely as possible, thus being appropriate for the purpose of the study.

Many of the original data sources are accessible, and all operations performed to collect and harmonize the data are transparently stated in the final report. Wherever limitations occur (mostly in data availability and/or transparency), these are explicitly described, and in most cases, an estimate of the consequences of such limitations for the overall quality is given.

In accordance with the original goal, the study is not a full LCA, but is deliberately limited to a life cycle inventory which will supply data on input materials to the overall "industrial washing" investigation of UBA. Therefore, a critical review of the impact assessment and improvement assessment was not applicable, and there are no interpretations and conclusions to be compared with the goal of the study and to be judged in view of the data quality.

3. Goal and Scope of the Study

3.1. *Goal*

The primary goal of the investigation, harmonization of the considerable number of existing studies on detergent ingredients, adaptation to the present requirements of ISO 14040 and 14041, and consistent use of up-to-date energy, transport, and basic material modules <BUWAL 1998>, is clearly stated and adhered to throughout the study.

The second goal, filling of data gaps by new studies (on SKS-6, polycarboxylate, percabonate, cationic tensides, CMC) is harder to achieve. In most cases, authentic industry data of good quality could be collected, though normally only from one supplier. To the reviewer's judgement, the data quality reached in the cationic tensides study is not comparable to the other data sets, since for many of the immediate precursors, only very rough estimates were available. Improvements were announced by the authors.

Generally, the goals of the study are appropriate for its intended application (inclusion in the overall project "Gewerbliche Wasch- und Reinigungsmittel"), and the data are of high interest for the target audiences (authorities, industries, and NGOs interested in the laundry washing process). However, the study cannot be directly used for benchmarking purposes by the involved manufacturers.

3.2. *System Definition and Boundaries*

The functional unit (1000 kg of marketable ingredient) is appropriate for the inclusion into the overall project. However, comparisons between ingredient alternatives cannot be made on a weight basis, but must consider the individual efficiencies of various substances for a given purpose.

The exclusion of the infrastructure (production equipment etc.) is justified in most of the production processes, due to the long useful life of such installations and their relatively small contribution to the overall environmental burdens of the processes.

It could be argued that this is not true for some sectors of energy supply, especially hydroelectric and nuclear power generation, where the ecological impacts of construction and end-of-life dismantling may dominate. However, the omission of capital goods follows a current practice established in many other LCA studies, and may facilitate the comparability of the results.

The exclusion of production waste treatment (section 3.5) is not quite in accordance with the goal of a "cradle-to-factory gate" analysis; besides, it is not consistently applied throughout the study: At least in the flow diagram 4.5.1 (sodium tripolyphosphate), there is an explicit module "waste treatment" inside the boundaries; in other instances, this may be the case implicitly (e.g. the burning of fibers and shells in the ECOSOL studies <ECOSOL 1995>). This uncertainty may impede the comparability with other studies. A more detailed accounting of the various waste types and treatments was announced by the authors.

3.3. *Data Availability and Quality, Assumptions*

To a great extent, the study had to rely on the data as presented in the original studies. Unfortunately, their quality is not in all cases fully documented and appears heterogeneous. Very useful attempts were made by the authors to check and improve the plausibility of the existing data, and to fill data gaps by additional research.

As in any complex LCI study, many assumptions and estimations had to be made, especially to fill the remaining data gaps and keep the time and effort for the investigation manageable. These assumptions are clearly stated in all cases, and often supported by sensitivity considerations.

Especially well-documented are the assumptions necessary to harmonize the surfactant data (4.2.3) and the sodium tripolyphosphate data (4.5.3) with the primary goal of this study. These choices are vital for the meaning of the results and could raise lots of discussion; they are documented and rationalized in an impressive way.

Other assumptions, such as the arbitrary allocation of 50 MJ of primary energy per kg of non-examined auxiliary material, without any emissions or raw material consumptions, are neither very consistent nor helpful. An improvement could be made by a rough classification (basic inorganics / basic organics / manufactured products etc.) and substitution by typical representatives of each class (e.g. soda / acetic acid / etc.). However, the consequences for the overall results will presumably be marginal.

3.4. Choice of Parameters

A severe problem in the harmonization of the underlying studies is the inconsistency of their parameter lists, ranging from the very brief lists in the early APME studies on chemical intermediates <Boustead 1993> to the multitude of emissions recorded for energy systems by ETH-ESU <Frischknecht 1994>. The authors fit all data to the emission list of SRU 250 <BUWAL 1998>, following the rules stated therein. This generally appears to be a reasonable compromise, however, there are three serious problems with this approach:

3.4.1. Double Counts in Water Emissions

In section 3.12.5, there is a warning that due to the presently popular sum parameters, some water emissions may be counted twice (e.g. organic carbon in BOD and TOC). This should be considered during impact assessment.

This shift in responsibility is unacceptable, since the end user of the data, unlike the data generator, has no means to eliminate this double count. Therefore, the problem has to be solved on the inventory level.

In the reviewer's own practice, a set of assumptions and rules is used to solve the TOC/DOC/COD/BOD problem and harmonize inventories with reasonable scientific judgement <Bretz 1999>. This could possibly serve as a help to deal with the heterogeneous data found in the various sources. The authors recognized the problem and will seek for solutions.

3.4.2. Unspecific Metals

In SRU 250 <BUWAL 1998>, table 16.2, a number of metal emissions to air is summarized under "metals". These emissions, of non-specified molecular nature (probably not the pure elements) include some harmless nutrient constituents (Na, K, Mg, Ca), as well as potentially hazardous metals such as Cr (Cr^{VI} is considered a carcinogen), Co (toxic via inhalation), Cu (salts are irritants, fungicides), Sb (SbH_3 is highly toxic), Th (radioactive), Tl, Be, etc.

When the Eco-indicator 95 (EI 95) impact assessment method <Goedkoop 1995> is applied to the module "UCPTE electricity" of <BUWAL 1998>, and "metals to air" are weighted with the factor for "air heavy metals" (same as lead!), this single unspecific parameter accounts for 70% of the total EI 95 points. The influence of the "heavy metals" class as a whole is absolutely dominant (80% ot the total). If the unspecific "metals to air" are excluded from the assessment, on the other hand, the remaining influence of this class is reduced to a more realistic value of 34%.

The reviewer compared these values to a similar module "UCPTE electricity" based on ETH data <Frischknecht 1994>, taken from the standard database in SimaPro™ <Halder 1997>. As expected, most emissions are some 20-30% higher in the ETH module, due to the inclusion of capital goods. The individual heavy metals that correspond to the sum parameter "metals to air" amount to 33 mg/kWh (compared to 22 mg/kWh in <BUWAL 1998>). 44% thereof are the nutrient metals (Na, K, Mg, Ca), another 55% represent other low-toxicity metals (Al, V, Ti, Cu, Sr) plus Boron (which does not appear in the BUWAL conversion list, but is nevertheless missing in the <BUWAL 1998> data). Only 1% (weight) comes from toxic elements (Ba, Cr, Co, Th, U, As, Sb). An impact assessment with EI 95 shows a "heavy metals" contribution of 37%.

Obviously, the simplified sum parameter "metals to air", as defined in <BUWAL 1998> and used in this study, substantially distorts the results of at least one widely-used impact assessment method, and should therefore be avoided. The authors acknowledge this and will take appropriate action.

The observation made in the comparison between original and harmonized ECOSOL data <ECOSOL 1995> in section 4.2.3 about the higher heavy metal impact in the new data probably needs revision - the higher "heavy metals" are presumably due to the erroneous sum parameter.

It should be noted that these remarks are equally applicable to any study using <BUWAL 1998> energy modules or other data from this source.

3.4.3. Inorganic Salts and Acids

A similar effect (with opposite sign) is caused by the water emission sum parameter "inorganic salts and acids" (<BUWAL 1998>, table 16.3). That parameter is not normally considered in impact assessment methods, but contains the boron emissions to water, which would have an EI 95 weighting factor in their own right. Especially in a washing process study, boron should not be hidden in any sum parameter, since boron emissions to waste water are one of the important (and controversial) issues in the laundering process.

Again, the remarks made above are equally applicable to any study using data from <BUWAL 1998>.

4. Inventory

4.1. Methodology, Process Descriptions

The LCI methodology follows the established EMPA standards that have shown their usefulness and validity in many other investigations, such as <BUWAL 1998>. A considerable weakness lies in the simplified parameter list discussed in section 3.4 of this review.

The processes are adequately described with rather detailed flow charts. Some improvements in the representation of chemical reaction equations were already adopted by the authors.

4.2. Data Collection, Literature Sources, Validation, Transformations

To the best of the reviewer's knowledge, the literature data used in this study are taken from the most recent, representative publications in the field. The data collection forms used to fill data gaps are well-designed and were tested in previous studies. The actual accuracy of such collected data and their validation could not be assessed in this review, but remains in the responsibility of the authors and the data suppliers (manufacturers).

The transformations performed with the data are adequately described in the respective sections "Durchgeführte Arbeiten und methodische Abweichungen"; they are consistent with the state of the art and the goal of the study.

4.3. Allocation Procedures

Weight allocation was used throughout the study. Though theoretically often disputed, this technique is still the one most frequently found in LCA studies. In most cases, weight allocation had already been introduced by the original studies and had to be maintained. There are no obvious cases where any other allocation method would have been more reasonable.

4.4. *Data Aggregation and Presentation*

The original ECOSOL data <ECOSOL 1995> were presented in a very transparent way, with energy and waste profiles for the individual production steps and separate result columns for fuel-related and process emissions. The original publications by EMPA itself <EMPA 1996>,<EMPA 1997> go even further and show individual emissions for process steps, or at least a distinction between process / thermal energy / electrical energy / transport.

The draft international standard ISO 14043 <ISO 1998a> strongly recommends such structured LCI inputs and outputs in Annex A, as a tool for anomaly detection and for dominance and influence analysis.

A distinction between foreground processes (under the control of the manufacturer) and background processes (such as energy supplies, communal waste water treatment, etc.) would be beneficial, since it would allow individual manufacturers to use the study for benchmarking, which is impossible now due to the aggregation.

The reviewer acknowledges that some of these transparency requests may be in conflict with the legitimate interests of the manufacturers to protect their fabrication secrets. However, the transparency found in the original publications, in accordance with the data suppliers, should not unnecessarily be given up for the sake of uniformity. Different degrees of detail in various sections of the study appears to be the lesser evil than the deliberate loss of publicly available information.

5. Concluding Remarks

It is an inherent feature of all critical reviews that they dwell more on occasional weaknesses than on the general high quality of a study. The reviewer is convinced that the present investigation adheres to very demanding professional standards and provides an important, useful set of data for the LCA community.

In this sense, any criticism shall serve to point out improvement options. The reviewer experienced a very open and constructive cooperation with the authors, and hopes that the remarks made above will help to further enhance the clarity and applicability of this study.

A publication of the results as a generally available EMPA report is highly recommended.

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APPENDIX B: STATEMENT ON THE CRITICAL REVIEW REPORT

The Critical Review Report was made using the 4th draft of this report. In response to the Critical Review, some points were removed or improved in this final version, others must remain open to criticism.

3.1 Data quality of cationic tensides:
We were able to use process data for the production of coconut oil, palm kernel oil and beef tallow from the study "Resources and Environmental Profile Analysis of Petrochemical and Oleochemical Surfactants Produced in Europe" <Franklin 1999>. The data quality of these precursor products is now comparable with that of other raw materials.

3.2 Non-inclusion of production wastes:

Here we have been more precise: processes involved in the disposal of production wastes, e.g. incineration or landfill dumping, are considered in this study only when detailed routes of disposal and waste composition are known, or if useful assumptions can be made. Where this is not possible, the waste quantities are categorised according to Chapter 3.13.4 and shown in the inventory tables. An estimate of the environmental impacts of these wastes, based on an average composition, is not made as this would introduce errors.

3.3 Energy supplement of non-traceable materials without emission burdens:

This criticism was left standing. It was however noted that an additional addition of emissions would raise the total profile only negligibly.

3.4.1 Multiple entries of TOC/DOC and COD/BOD parameters:

Multiple entries (recording the same emission under different parameters) have largely been avoided. Exceptions: in the energy modules based on the LCAs of energy systems <Frischknecht et al. 1996> the emissions of organic substances into water in refining, regional distribution and the transport of crude oil and oil products, have been recorded partly as a single substance and also as COD. However, in the cases identified so far, according to <öbu 1998>, they have had negligible if any influence on the results of the impact assessment.

3.4.2 Nonspecific metal emissions:

Nonspecific metal emissions of an unknown composition, taken from the modules for energy production, are shown separately from the other metal emissions, and labelled as "Metals (Energy modules SRU 250)". <öbu 1998> recommends that an assessment of these parameters should not be made, since they are quantitatively primarily non-heavy metals. The conclusions on heavy metal made in Figure 4.5 are correct.

3.4.3 Boron emissions under inorganic salts and acids:

The sum parameter "Inorganic salts and acids" contains boron emissions from the modules for energy production. According to Eco-indicator 95 however, these are small enough to be ignored in making an impact assessment (1 kWh electricity UCPTE: 0.2% of the Eco-indicator points in the category heavy metals). The production-dependent boron emissions, perborates, are by contrast shown separately and not summed under inorganic salts and acids. Production-dependent boron emissions were not recorded for any other detergent raw materials.

4.4 Difference between foreground and background processes:

This criticism has been left.

APPENDIX C: THE TOC/DOC AND COD/BOD PARAMETERS

Author:

Rolf Bretz
Life Cycle Assessment
Consumer Care Division
Ciba Specialty Chemicals
P.O. Box
CH-4002 Basel / Switzerland

Organic pollutants of waste water have traditionally been determined by oxidative titration with chromate, which probes COD (chemical oxygen demand).

This must not be confused with BOD (biological oxygen demand, also referred to as BOD5, biological oxygen demand in a 5-day test). The former is a chemical oxidation under strict conditions which gives the total oxidisable substances; the latter, in a (more or less accurate) simulation of a waste water treatment plant gives a value (oxygen demand) for the quantity of *biologically degradable* organic compounds that can be converted into CO_2 in five days in the presence of activated sludge, using oxygen from the air. COD is therefore a measure of the total pollution (including non-degradable organic compounds), while BOD gives a reference for the pollution of a waste water treatment plant: the oxygen demand must be supplied by aeration, and this costs electricity and also limits the capacity of the plant.

There is no direct relationship between the BOD and COD values, except for a trivial one: BOD $\leq$ COD. The BOD / COD relationship gives no information on degradability, while the difference gives the refractive carbon content.

Neither value is carbon-specific (COD more so than BOD); the presence of inorganic reductants (e.g. pyrosulphites and thiosulphates, which are commonly used in the textile industry) raises the COD of a probe, while any oxidants (such as the whitening agents chlorite and peroxide) lead to lower values.

The determination of total organic carbon (TOC) is more recent and requires more effort in terms of apparatus. It is however not influenced by inorganic disrupting environmental factors. However, it cannot be assumed that COD and TOC are measured at the same time in the same process waste water – the choice of measurement depends not only on the laboratory equipment but also on local traditions and the authorities' regulations.

Measurement can take place using either the unchanged probe, where it gives the *total* organic carbon (TOC); alternatively the probe may first be ultrafiltered, which gives the *dissolved* organic carbon (DOC).

There is no clear relationship between TOC and COD. As an extreme example, formic acid needs

16 g O for 12 g C, i.e. COD / TOC = 1.33,

according to the formula

$HCOOH + \frac{1}{2} O_2 \rightarrow CO_2 + H_2O$

while methane requires

64 g O for 12 g C, i.e. COD / TOC = 5.33,

according to the formula

$CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$.

Average values can be found for ethanol, for example. According to the formula

$C_2H_6O + 3 O_2 \rightarrow 2 CO_2 + 3 H_2O$

96 g O are needed for 24 g C, i.e. COD / TOC = 4,

or for sugar, where according to the formula

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$ 192 g O are required for 72 g C, i.e. COD / TOC = 2.66.

Non-oxidisable (or completely oxidised) foreign atoms (such as halogens or sulphur in SO_3 groups) in place of hydrogen reduce the COD / TOC relationship, while oxidisable groups ($-NH_2$, -S-) raise it. SAEFL 133 and 297 assume an empirical relationship COD / TOC ≈ 3; our own measurements give 2.6 - 2.8.

There is no strict connection between DOC and TOC, except for the trivial: DOC ≤ TOC. The difference TOC - DOC is a measurement for the particularly bound carbon, which is also given by the parameter "Total undissolved substances".

Evaluation of the parameters varies: Eco-indicator 95 and SAEFL 133 and 297 all view COD as the primary parameter. Eco-indicator 95 gives no reason why, and with what weighting, COD is evaluated in the impact class "Eutrophication" – but it does give a factor. SAEFL 297 argues oxygen depletion below the inflow point, which however – at least with substances which are difficult to degrade – is associated not with COD but with BOD. SAEFL 133 and 297 initially give only the conversion factor DOC ≈ 3 * COD; Volume 297 also suggests converting TOC (as "worst case" estimate) with the same factor, if the other two parameters are missing.

Why the refractive (non-degradable) dissolved carbon in DOC, but not the particularly bound carbon in TOC, should have a eutrophicating effect makes no sense to me. Waste water treatment professionals assume that the carbon fraction in "Total undissolved substances" may be of biological origin (from activated sludge), and thus could certainly be degradable under conditions of oxygen depletion.

Ciba's conclusions:

1. if only COD or only DOC (i.e. not TOC) appears in an imported inventory, the respective parameter in both processes is evaluated. The value 18 UBP/g from SAEFL is used. For Eco-indicator 95 no extension for DOC has been introduced, but a factor of 0.066 has been introduced for TOC, i.e. three times greater than the COD value of 0.022. According to the equation DOC ≤ TOC the minimum assumption TOC = DOC is obtained and added to the inventory.
2. if COD and DOC (but not TOC) appear in a system, we assume that these values have been measured by different laboratories for different processes, and thus they are treated additively (according to the precautionary principle), i.e. enter both of them and evaluate them. Adding TOC = DOC in the inventory is carried out as in point 1.
3. if both parameters appear in one step which is clearly identifiable as a single process (which has not been the case so far), the factor COD / TOC (≈ 3?) is tested for its plausibility, and under the precautionary principle the higher value is entered. The conversion TOC = DOC in the inventory is carried out as in point 1.
4. if instead of DOC the total organic carbon (TOC) appears, the inventory is supplemented with DOC = TOC, again according to the precautionary principle. TOC is evaluated in Eco-indicator 95 but not in SAEFL 297 (in contrast to the original source), since the simultaneous use of the value 18 UBP/g for both DOC and TOC would lead to multiple entries. Instead, the assessment is carried out by supplementing the inventory with DOC. Simultaneously appearing COD is evaluated in parallel as in point 2 (or for single processes, left out, as in point 3).
5. if DOC and TOC appear together, the plausibility of DOC ≤ TOC is tested. If this is acceptable, both values are entered unchanged into the database. SAEFL 297 then evaluates DOC (for reasons of authenticity, but contradicting the precautionary principle), Eco-indicator 95 evaluates TOC (with the additionally introduced factor 0.066, as in point 1). If, on the other hand, DOC > TOC, which unfortunately sometimes occurs, we enter TOC = DOC in the inventory again and ignore the smaller value.

APPENDIX D: DIFFERENT TERMS USED FOR PARAMETERS

Table D.1 below compares terms used for parameters. The terms used in this study and in SRU 250 <SAEFL 1998> are to be found in the column "EMPA (German)" and "EMPA (English)". The Ökoinstitut Freiburg i.Br. uses the appropriate column. The column "SPOLD" contains the English terms as recommended by the Society for Promotion Of Life-cycle assessment Development <SPOLD 1997>. Note that the terms do not always completely agree.

Resources, commercial fuels				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
129521-66-0	Rohbraunkohle	Braunkohle (RiL)	Raw brown coal	Coal (brown, in ground)
008006-14-2	Rohgas (Erdgas)	Erdgas (RiL)	Crude gas (natural gas)	Natural gas (in ground)
-	Rohöl ab Bohrloch	Erdöl (RiL)	Crude oil from drilling well	Oil (in ground)
-	Rohsteinkohle	Steinkohle (RiL)	Raw hard coal	Coal (hard, unspecified, in ground)
-	Uran ab Erz	Uran (RiL)	Uranium from ore	Uranium (U, in ground)
-	Biomasse	Biomasse, unspez. (RiL)	Biomass	-
-	Holz	Holz (RiL)	Wood	wood
-	Pot. Energie Wasser	Wasserkraft	Pot. energy water	Potential energy (stock, in barrage water)

Resources, feedstock				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
008006-14-2	Rohgas (Erdgas) (als Feedstock)	Erdgas (RiL)	Crude gas (as feedstock)	Natural gas (in ground)
-	Rohöl ab Bohrloch (als Feedstock)	Erdöl (RiL)	Crude oil (as feedstock)	Oil (in ground)
-	Biomasse (als Feedstock)	Biomasse, unspez. (RiL)	Biomass (as feedstock)	-
-	Baryt	Baryt (RiL)	Barytes	-
001318-16-7	Bauxit	Bauxit (RiL)	Bauxite	Bauxite (Al2O3.2H2O, in ground)
-	Blei	-	Lead	Lead (Pb, in ground)
-	Bor	-	Boron	-
016389-88-1	Dolomit	-	Dolomite	Dolomite (CaMg(CO3)2, in ground)
-	Eisenerz	Eisen (RiL)	Iron ore	Iron (Fe, in ground)
-	Fluorit	-	Fluorspar	-
-	Holz	Holz (RiL)	Wood	Wood (unspezified, standing)
-	Kalkstein	Kalkstein (RiL)	Limestone	-
-	Magnesium	-	Magnesium	Magnesium (Mg, in ground)
-	Phosphatgestein	Rohphosphat (RiL)	Phosphate rock	Phosphate rock (in ground)
-	Sand, Ton, Lehm	-	Sand, clay	-
-	Sauerstoff	-	Oxigen	-
-	Schwefel	Schwefel (RiL)	Sulphur	Sulfur (S, in ground)
-	SO2 sekundär	-	SO2 secondary	-
-	Steinsalz	Steinsalz (RiL)	Rock salt	Sodium chloride (NaCl, unspezified natural origin)
-	Stickstoff	-	Nitrogen	-
-	Additive	-	Additives	-

Recoverable wastes				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
-	Aluminiumrückstände	-	Alu-residues	-
-	Filterrückstände	-	Filter residues	-
-	NaOH (ca. 15%-aq.)	-	NaOH (ca. 15%-aq.)	-
-	Wasserglas 47%	-	Sodium silicate 47%	-

Disposal				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
-	Industrieabfälle	-	Industrial waste	Municipal waste and similar commercial, industrial and institutional waste (unspecified)
-	Inerte Chemieabfälle	Abfälle, inert (AzB)	Inert chemicals	Stabilized/soldified waste (unspecified)
-	Mineralische Abfälle	Abraum (AzB)	Mineral waste	Waste from mineral excavation (unspezified)
-	Schlacke	Aschen u. Schlacken (AzB)	Slag & ashes	Waste from incineration of municipal and similar waste (bottom ash and slag)
-	Sonderabfall	Sondermüll (AzB)	Regulated & toxic chemicals	-

Air pollutants

CAS No.	EMPA (German)	Ökoinstitut Freiburg i.Br. (German)	EMPA (English)	SPOLD (Englisch)
007664-41-7	Ammoniak (NH3)	Ammoniak (L)	Ammonia (NH3)	Ammonia (NH3)
-	Aromatische KW	-	Aromatic HC	Volatile organic compounds (hydrocarbons, aromatic)
000071-43-2	Benzol (C6H6)	Benzol (L)	Benzene (C6H6)	Benzene (C6H6)
007439-92-1	Blei (Pb)	Blei (L)	Lead (Pb)	Lead (Pb)
000744-04-9	Cadmium (Cd)	Cadmium (L)	Cadmium (Cd)	Cadmium (Cd)
007782-50-5	Chlor (Cl2)	Chlor (L)	Chlorine (Cl2)	Chlorine (Cl2)
-	Chlorierte KW	NMVOC, chlor. (L)	Chlorinated HC	-
007782-41-4	Fluor (F2)	Fluor (L)	Fluorine (F2)	Fluorine (F2)
007664-39-3	Flussäure (HF)	Fluorwasserstoff (L)	Hydrofluoric acid (HF)	Hydrofluoric acid (HF)
-	Halogenierte KW	NMVOC, halog. (L)	Halogenated HC	Halogenated hydrocarbons (unspecified)
0075-63-8	Halon H1301	Halon 1301 (L)	Halon H1301	-
000124-38-9	Kohlendioxid fossil (CO2)	Kohlendioxid, fossil (L)	Carbon dioxide fossil (CO2)	Carbon dioxide (CO2, fossil)
	Kohlendioxid biogen (CO2)	Kohlendioxid, regenerativ (L)	Carbon dioxide non fossile (CO2)	Carbon dioxide (CO2, biomass)
000630-08-0	Kohlenmonoxid (CO)	Kohlenmonoxid (L)	Carbon monoxide (CO)	Carbon monoxide (CO)
010024-97-2	Lachgas (N2O)	Distickstoffmonoxid (L)	Nitrous oxide (N2O)	Nitrogen oxide (N2O)
007439-96-5	Mangan (Mn)	Mangan (L)	Manganese (Mn)	Manganese (Mn)
-	Mercaptane	Mercaptane (L)	Mercaptans	Mercaptans (unspezified)
-	Metalle	Metalle, unspez. (L)	Metals	Metals (unspecified)
000074-82-8	Methan (CH4)	Methan (L)	Methane (CH4)	Methane (CH4)
007440-02-0	Nickel (Ni)	Nickel (L)	Nickel (Ni)	Nickel (Ni)
-	NMVOC Nicht-Methan KW	NMVOC, unspez. (L)	NMVOC non-methane HC	Volatile Organic Compounds (non-methane, unspecified origin)
-	PAH Polyzykl. arom. KW	PAK, unspez. (L)	PAH polycycl. arom. HC	Polycyclic aromatic hydrocarbons (PAH)
007439-97-6	Quecksilber (Hg)	Quecksilber (L)	Mercury (Hg)	Mercury (Hg)
-	Rad. Substanzen	-	Radioactive substances	-
007647-01-0	Salzsäure (HCl)	Chlorwasserstoff (L)	Hydrochloric acid (HCl)	Hydrochloric acid (HCl)
007446-09-5	Schwefeloxide (SOx) als SO2	Schwefeldioxid (L)	Sulfur oxides (SOx) as SO2	Sulfur dioxide (SO2)
-	Staub/Partikel	Staub (L)	Dust/particulates	Particulates (unspecified)
011104-93-1	Stickoxide (NOx) als NO2	NOx (L)	Nitrogen oxides (NOx) as NO2	Nitrogen oxides (NOx)
001333-74-0	Wasserstoff (H2)	Wasserstoff (L)	Hydrogen (H2)	Hydrogen (H2)
007440-66-6	Zink (Zn)	Zink (L)	Zinc (Zn)	Zinc (Zn)

Water pollutants

CAS No.	EMPA (German)	Ökoinstitut Freiburg i.Br. (German)	EMPA (English)	SPOLD (Englisch)
-	Abwassermenge	Abwasser, unspez.	Waste water quantity	Wastewater (unspecified)
007429-90-5	Aluminium (Al)	Aluminium (W)	Aluminium (Al)	Aluminium (Al)
014798-03-9	Ammonium (NH4+)	Ammonium (W)	Ammonium (NH4+)	Ammonium ion (NH4+)
-	Anorg. Salze und Säuren	Anorgan. Salze u. Säuren (W)	Inorg. salts and acids	-
-	AOX als Cl-	AOX (W)	AOX as Cl-	AOX (Adsorbable Organic Halogen)
-	Aromatische KW	Aromaten, unspez. (W)	Aromatic HC	Volatile organic compounds (hydrocarbons, aromatic)
007440-38-2	Arsen (As)	Arsen (W)	Arsenic (As)	Arsenic (As)
007440-39-3	Barium (Ba)	Barium (W)	Barium (Ba)	-
007439-92-1	Blei (Pb)	Blei (W)	Lead (Pb)	Lead (Pb)
-	BOD	BSB-5 (W)	BOD	BOD5 (Biochemical Oxygen Demand)
007440-42-8	Bor (B)	-	Boron (B)	Boron (B)
000744-04-9	Cadmium (Cd)	Cadmium (W)	Cadmium (Cd)	Cadmium (Cd)
014866-68-3	Chlorat (ClO3-)	-	Chlorate (ClO3-)	Chlorate (ClO3-)
016887-00-6	Chlorid (Cl-)	Chlorid (W)	Chloride (Cl-)	Chloride (Cl-)
-	Chlorierte KW	Stoffe, org., chlor,unspez.(W)	Chlorinated HC	-
007440-47-3	Chrom (Cr)	Chrom (W)	Chromium (Cr)	Chromium (Cr)
-	COD	CSB (W)	COD	COD (Chemical Oxygen Demand)
-	Cyanid (CN-)	Cyanid (W)	Cyanide (CN-)	Cyanides (CN)
-	DOC	DOC (W)	DOC	DOC (Dissolved Organic Carbon)
007439-89-6	Eisen (Fe)	Eisen (W)	Iron (Fe)	Iron (Fe)
-	Fette/Öle	Fette und Öle (W)	Fats/oils	Oils (unspecified)
007722-84-1	Wasserstoffperoxid (H2O2)	-	Hydrogen peroxide (H2O2)	Hydrogen peroxide (H2O2)
016984-48-8	Fluorid (F-)	Fluorid (W)	Fluoride (F-)	Fluoride (F-)
007440-50-8	Kupfer (Cu)	Kupfer (W)	Copper (Cu)	Copper (Cu)
-	Metalle	Metalle, unspez. (W)	Metals	Metals (unspecified)
007440-02-0	Nickel (Ni)	Nickel (W)	Nickel (Ni)	Nickel (Ni)
014797-55-8	Nitrat (NO3-)	Nitrat (W)	Nitrate (NO3-)	Nitrate (NO3)
-	PAH Polyzykl. arom. KW	PAK, unspez. (W)	PAH policycl. arom. HC	Polycyclic aromatic hydrocarbons (PAH)
000108-95-2	Phenole	Phenole (W)	Phenols	Phenol (C6H6O)

014265-44-2	Phosphat (PO4 3-)	Phosphat (W) Phosphate (als P2O5) (W)	Phosphate (PO4 3-)	Phosphate (PO4 3-)
007439-97-6	Quecksilber (Hg)	Quecksilber (W)	Mercury (Hg)	Mercury (Hg)
-	Rad. Substanzen	-	Radioactive substances	-
015593-90-5	Silikate (SiO3--)	-	Silicate (SiO3--)	Silicate (SiO3--)
-	Stickstoff gesamt	Stickstoffverbind. als N (W)	Nitrogen total	Nitrogen (total)
-	Stickstoff org. gebunden	Org. geb. Stickst. a. N. (W)	Nitrogen org. bound	-
014808-79-8	Sulfat (SO4 2-)	Sulfat (W)	Sulfate (SO4 2-)	Sulfate (SO4 --)
018496-25-8	Sulfid (S 2-)	Sulfide (W)	Sulfide (S2-)	Sulphide (S --)
-	Suspendierte Stoffe	Feststoffe, suspensiert (W)	Suspended solids	Suspended solids (unspecified)
-	TOC	TOC (W)	TOC	TOC (Total Organic Carbon)
000108-88-3	Toluol (C7H8)	Toluol (W)	Toluene (C7H8)	Toluene (C6H5CH3)
007440-66-6	Zink (Zn)	Zink (W)	Zinc (Zn)	Zinc (Zn)

Water consumption				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
-	Kühlwasser	Kühlwasser	Cooling water	-
-	Prozesswasser	Rohwasser	Process water	-
-	Waschwasser	-	Washing water	-

Final energy requirement				
CAS No.	**EMPA (German)**	**Ökoinstitut Freiburg i.Br. (German)**	**EMPA (English)**	**SPOLD (Englisch)**
-	Elektrizität	Energie, elektrisch	Electricity	-
-	Biomasse	-	Biomass	-
-	Diesel	Diesel	Diesel	-
-	Erdgas	Erdgas	Natural gas	-
-	Heizöl EL	Heizöl, leicht	Heating oil EL	-
-	Heizöl S	Heizöl, schwer	Heating oil H	-
-	Erdöl-Produkte	-	Oil fuels	-
-	Kohle	Kohle	Coal	-
-	Energie unspezifiziert	-	Energy unspecified	-
-	Total Endenergie	-	Total delivered (final) energy	-
-	Energiebereitstellung total	-	Energy production & delivery	-
-	Energie für Hilfsmaterial (50 MJ/kg)	-	Energy for auxiliary material (50 MJ/kg)	-
-	Feedstock	Feedstock	Feedstock	-
-	Rückgewonnene Energie	-	Recovered energy	-
-	Total (Primärenergie)	Kumulierter Energieaufwand	Total primary energy	-

Tab. D.1 Comparison of the different terms used for parameters

APPENDIX E: GLOSSARY OF TERMS

Allocation	In LCAs, allocation refers to the assignment of environmental impacts (depletion of raw materials, emissions) to main and co-products.
Cradle-to-factory-gate	LCA of a product system that does not include the whole life cycle, but only considers the manufacture up to the producers factory gate.
Eco-inventory	Synonym for the ISO 14040 term **Life cycle inventory**
Efficiency	In general, the relationship between usable energy and energy used.
Emission factor	Specific emissions into air, water and/or soil per activity (per energy, per mass or per transport unit over a particular time period).
Environmental burden	Environmental burdens are environmental impacts assessed in terms of their danger to the environment.
Environmental parameter	All quantities which are determined in the input-output analysis and are associated with the removal from or release of substances and energy into the environment (e.g. emissions into the atmosphere and water, energy consumption etc.). They are acquired in the data collection for the inventory analysis and are the basis for determining environmental interventions.
Feedstock energy	Energy introduced into a system by energy resources not used to provide energy. The feedstock energy is bound up in the input material. It is determined as the upper heating value of the input material, since the feedstock is often used as fuel.
Feedstock	This is generally a synonym for all material inputs into a system <Boustead 1992b>. In our case feedstock is regarded as material inputs which could be but are not used to provide energy (energy resources). Feedstock is also used as an abbreviation for feedstock energy.
Final energy source	The form in which the energy is stored by the consumer (e.g. diesel fuel, electricity).
Final energy	The energy available to the consumer.
Functional unit	Quantified performance of a product system for use as a reference unit in a life cycle assessment study (ISO 14040).
Life cycle assessment (LCA)	Compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle.
Life cycle impact assessment	Phase of life cycle assessment aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts of a product system.
Life cycle interpretation	Phase of life cycle assessment in which the findings of either the inventory analysis or the impact assessment, or both, are combined consistent with the goal and scope in order to reach conclusions and recommendations.

Life cycle inventory analysis	Phase of life cycle assessment involving the compilation and quantification of inputs and outputs, for a given product system throughout its life cycle.
Life cycle	The life cycle of a product contains all process steps from the acquisition of primary and secondary raw materials up to waste treatment and recovery.
Parameter	See **Environmental parameter**
Primary energy source	The energy source from which the energy is delivered (hard coal, brown coal, wood etc.).
Product system	Collection of the modules linked by material and energy flows, that fulfil one or more established functions.
Recoverable wastes	Recoverable wastes occur in a production process in addition to the main and co-products and are materially recovered, or in exceptional cases used energetically. These are not considered in the allocation.
Recovery	Recovery of raw and other materials from wastes.
Substance	A substance is a chemical element or compound (molecule), eg iron, carbon, nitrogen dioxide.
Supply energy	The energy used to supply the final energy from an energy source to the energy consumer.
System boundaries	Boundaries between a product and its environment or other product systems.
Terminated system	Product system for which there are no more flows from or to the technosphere.
Waste disposal	The disposal of wastes comprises their physical, chemical or biological change including subsequent deposition on a landfill, as well as the preliminary stages of collection, transport, intermediate storage and treatment (LPE modification of 10. June1997).
Wastes	According to the LPE (modification of 10. June1997), wastes are moveable entities which are disposed of by the owner or whose disposal is in the public interest.

APPENDIX F: STANDARD QUESTIONNAIRE FOR COLLECTING DATA

Standard questionnaire for single processes (modules) for calculating a life cycle assessment

Code OEKOBIL\DAEINGB

PROCESS NAME (as in flow diagram):				
Date:				**Data quality indicator (DQI):**
Company:				I: measured
Contact person		Tel.:		II: calculated
Factory location:				III: average value
Country:				IV: estimate
Process output:	*Main product:*			**Origin of the data: (e.g. III F)**
Reference unit:	*(Functional unit):*			L: Literature data
Reference year:		*Start:*	*End:*	F: Factory-specific data
Transports:	No:	Yes, see separate transport data form:		X: Other

Notes, more detailed explanation of the process (e.g. specific conditions, hazards or industrial accidents)::

ENERGY INPUTS	**Quantity**	**Unit**	**DQI**
Electricity			
Grid			
Internally produced			
Energy sources			
Hard coal			
Brown coal			
Coke			
Wood			
Natural gas			
Hydrogen			
Heating oil H/M			
Heating oil L			
Diesel			
Petrol			
Other (specify)			
Power-heat coupling			

MATERIAL INPUTS	**Quantity**	**Unit**	**DQI**
Raw materials			

*) Give whether 1) open or 2) closed cycle and give temperature

MATERIAL OUTPUTS	**Quantity**	**Unit**	**DQI**
Main product			
Co-Products			
Steam as appropriate			
Energy surplus as approriate			
(specify.)			

Water consumption	**Quantity**	**Unit**	**DQI**
Process water			
Cooling water*)			
Washing water			

Additional materials			
Air pressure [bar]			
Steam [bar]			

Process-dependent air pollutants			
	Quantity	Unit	DQI
Aldehydes (R-CHO)			
Ammonia			
Hydrogen chloride			
Fluorine			
Hydrofluoric acid			
CO2: renewable			
CO2: fossil			
Carbon monoxide			
Nitrous oxide (N2O)			
Mercaptans			
Sulphur oxides			
Hydrogen sulphide			
Dust, particulates			
Nitrogen oxides (NOx)			
Heavy metals			
Lead			
Mercury			
Other			
Hydrocarbons (VOC)			
Methane			
Chlorinated HC			
(specify)			
CFC			
(specify)			
Polycyclic HC			
(specify)			
Miscellaneous organis substances			
(specify)			
Other emissions			
(specify)			

- = No emissions can be detected

Process-dependent water pollutants			
Measurement location **(before or after internal water purification plant):**			
	Quantity	Unit	DQI
Waste water quantity:			
BOD			
COD			
Dissolved inorganic substances			
Boron (borates)			
Cadmium			
Chloride			
CN-			
Fats / oils			
Fe ions			
Hydrofluoric acid			
NH4+ ions			
Nitrates			
Pb ions			
Phenols			
Phosphates			
Mercury			
Hydrochloric acid			
Acids as H+ ions			
Suspended solids			
(specify)			
Other metals			
(specify)			
Hydrocarbons			
Chlorinated HC (AOX)			
(specify)			
Dissolved organic carbon (DOC)			
Total organic carbon (TOC)			
Other emissions			
(specify)			

n.i. = Such emissions exist, but we have no information

Wastes	**Quantity**	**Unit**	**DQI**	Type of landfill or type of recycling

Tab. F.1 Standard form for data collection

Listing of the official «EMPA Reports», arranged according to the report numbers

1 *Roš M.:* Die zukünftigen schweizerischen Normen für Bindemittel auf Grundlage von Untersuchungsergebnissen der EMPA in den Jahren 1922 bis 1924 (1925).

1a *Roš M.:* Bericht Nr. 1, zweite Auflage, deutsch und französisch (1925).

2* *Roš M.:* Der hochwertige Baustahl, St. 58 (1925).

3* *Roš M.:* Das kommende schweizerische Regulativ über die Prüfung der Behälter für den Transport verflüssigter, verdichteter und unter Druck gelöster Gase (1925).

4 *Zschokke B.:* Die Widerstandsfähigkeit des Betons gegen chemische Einflüsse der Böden und Grundwässer (1925).

5 *Roš M.:* SIA Normen für Holzbauten. Der Bau von Gerüsten und Hochbauten aus Holz in der Schweiz (1925).

Brunner J.: Der Bau von Brücken aus Holz in der Schweiz (1925).

The «EMPA Report» (or copies of the out-of-print numbers) are available through: EMPA Dübendorf, Bibliothek, Überlandstrasse 129, CH-8600 Dübendorf. Prices given upon inquiry.

6 *Sonderegger A.:* Theorie und Praxis der elektrischen Lichtbogenschweissung (1925).

7* *Roš M.:* Die Festigkeit des Mörtels und des Betons/La résistance des mortiers et bétons (1925).

8 *Roš M:* Die Druckelastizität des Mörtels und des Betons – Das elastische Verhalten von ausgeführten Beton- und Eisenbeton-Bauwerken (1925).

9 *Roš M.:* Der neue F-Stahl. Ergebnisse der Festigkeits-Untersuchungen (1926).

10 *Roš M.:* Die zukünftigen schweizerischen Normen für Bindemittel auf Grundlage von Untersuchungsergebnissen der EMPA: Die Prüfung der Zemente mit plastischem Mörtel (1926).

11 *Keel C. F.:* Theorie und Praxis der autogenen Schweissung (1926).

12 *Höhn E./Sonderegger A.:* Über elektrisch und autogen geschweisste Konstruktionen (1926).

13* *Roš M./Brunner J.:* Die Knicksicherheit von an beiden Enden gelenkig gelagerten Stäben aus Konstruktionsstahl (1926).

14* *Roš M./Eichinger A.:* Versuche zur Klärung der Frage der Bruchgefahr (1927).

15 *Roš M.:* Das neue schweizerische Regulativ über die Prüfung der Behälter für den Transport verdichteter, verflüssigter und unter Druck gelöster Gase (1930).

16 *Feret R.:* L'essai des liants hydrauliques en prismes de mortier plastique (1926).

17 *Portevin A.:* Les essais mécaniques des fontes (1926).

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ISSN 0258-9745
ISBN 3-905594-09-9