CHALMERS

On the implementation of toxicological assessment at SCA Personal Care

Master of Science Thesis

KLARA NIKLASSON
Department of Energy and Environment
Division of Environmental System Analysis
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden, 2007
ESA Report No. 2007:7

REPORT NO. 2007:7

On the implementation of toxicological assessment at SCA Personal Care

KLARA NIKLASSON

Department of Energy and Environment
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden 2007

On the implementation of toxicological assessment at SCA Personal Care

KLARA NIKLASSON

ESA Report No 2007:7
ISSN 1404-8167
Environmental Systems Analysis
Chalmers University of Technology
SE-412 96 Göteborg
Sweden
Telephone + 46 (0) 31-772 10 00

Chalmers Reproservice
Göteborg, Sweden 2007

Abstract

In this master thesis the possibility and relevance of implementation of toxicological assessment are examined. At SCA Personal Care life cycle assessment (LCA) is used for environmental assessment of new design in the product development process. Now it will be investigated if it would be beneficial to implement toxicological assessment as an integrated part in the LCA practice. Different life cycle assessment methods for toxicological assessment are studied to find a method suitable for the purpose. Two different methods, EDIP and a risk phrase method based on the EDIP methodology, are applied to data sets from SCA's LCA data base. This toxicological assessment aims at showing how a toxicological assessment is carried out and highlighting procedural difficulties with it. According to the relevance of implementation, a lot of advantages are found. It is though evident that the toxicity assessment has to be carried out easily and cost-effectively to be beneficial for the company. The administration of the toxicity assessment has to be simple. Otherwise it will be too expensive to have it as an integrated part in the LCA practice. The method regarded most appropriate to use at SCA Personal Care is the EDIP method. It is a simple and well documented method which is easy to use.

Table of contents

1 Introduction

Environmental issues are indeed in focus today. A lot of different tools for environmental assessment have been developed: Environmental impact assessment, Ecological risk assessment, Material flow analysis and Life cycle assessment. All these environmental systems analysis tools have the purpose to reduce environmental impact of human activities.

In a life cycle assessment a product is followed from its "cradle" where raw materials are extracted from natural resources through production and use to its "grave", the disposal. Environmental impact from the product's life cycle is assessed and can be compared with the environmental impact from an equivalent product's life cycle. In life cycle assessment different impact categories are considered, e.g. global warming, acidification and toxicity. Toxicological assessment (TA) means assessment of different emissions' impact to the impact category of toxicity. Because of the significant differences among chemicals regarding the dose levels that are toxic, it is important to consider toxicity when comparing releases of different toxic chemicals.

At SCA, life cycle assessment has been used for environmental assessment of new design in the product development process of absorbent hygiene products during more than ten years. The LCAs at SCA Personal Care comprise information about use of resources and energy and potential impact on global warming, acidification, aquatic oxygen depletion and photochemical ozone creation. In this master thesis the possibility and relevance of implementation of TA are examined.

The task is to investigate if TA would be a good complement in the environmental work at SCA Personal Care. More specifically, investigate if the life cycle assessment work would benefit from implementation of toxicological assessment i.e. examine if the impact category toxicity is a good complement to the LCAs. The first question is if it is relevant to implement TA at SCA Personal Care. The second question is if it is possible to implement TA at SCA Personal Care. To find answers to these questions the following is done within the project.

- Inventory of potentially toxic substances in the products' lifecycles.
- Investigation of available models for toxicological assessment
- Application of suitable toxicological assessment methods to emission data in lifecycles of hygiene products.

The inventory serves to find what data is available and to find out what potentially toxic emitted substances appear in the lifecycles. It helps figure out if the data is satisfactory. It will help answer the question if, due to data gaps, a toxicological assessment based on available data would be misleading.

Knowledge of how the available models for toxicological assessment work and the differences between them is a necessity to answer the question if there is a suitable method for toxicological assessment at SCA. Knowledge of the models is also important to know what data is needed for toxicological assessment.

The investigation where suitable toxicological assessment methods are applied to datasets highlights the ability to use the LCA data in the TA methods and the problems associated with it. The investigation shows how TA works out in practice. The result of the TA shows which substances that contribute most to the impact category toxicity in the activities investigated.

Within the project answers to the questions associated with the general problems are found using a case study. The case study demonstrates how the toxicological assessment appears in a real LCA situation, a comparing LCA of two diapers.

2 Material and methods

The investigation is made through a case study on two diapers. In order to narrow the extent of the study some limitations have been done. The case study does not cover the whole life cycles of the diapers, it is limited to cover cradle to gate analysis of some materials included in the diapers. It is limited to comprise chemical pulp, super absorbents and elastic film since the biggest differences between the two diapers lie in their contents of these three materials.

To be able to answer the question if toxicological assessment should be included in the life cycle assessment an inventory of flows of potentially toxic substances in the lifecycles of the products manufactured by the company is made. The inventory comprises the three materials in the case study. The inventory includes:

- Study on the data in the LCA data base at the company.
- Investigation of data sources to the data in the LCA data base.
- Investigation of possibilities to get more accurate and complete data.
- Establishment of inventory reports of the emissions from the cradle to gate LCAs of elastic film, super absorbents and pulp respectively.

To know what data is needed for toxicological assessment it is necessary to know how it will be used. Therefore it is necessary to investigate models for toxicological assessment that could be used in the LCA practice at the company. Special attention was paid to the different models' data demand. The OMNIITOX models are investigated and the models that were investigated within the OMNIITOX project before the OMNIITOX models were constructed. The report "OMNIITOX –inventory and classification of LCA characterisation methods for toxic releases" (de Koning et al 2002) has been used as data source in the selection of models to be investigated and for description of these models. For some interesting models further information has been collected. The investigation of models was run parallel to the inventory.

A toxicological impact assessment is made, but in limited cover. This serves two purposes. Firstly, it shows how the toxicological impact assessment works in practice; it shows how the procedure works and uncovers weaknesses concerning data. Secondly, the toxicological assessment is used to highlight those substances that have the biggest environmental impact and therefore should be paid special attention.

3 Life cycle assessment

In this chapter the life cycle assessment concept is reviewed and the LCA practice at SCA Personal Care is examined.

3.1 The life cycle assessment concept

Life cycle assessment is a tool for evaluation of environmental impact, useful for environmental assessment of products. In a life cycle assessment a product is followed from its "cradle" where raw materials are extracted from natural resources through production and use to its "grave", the disposal, see figure 1. The general categories of environmental impacts needing consideration in an LCA include resource use, human health and ecological consequences. Risk is not dealt with in LCA. The results are related to the function of a product, which allows comparisons between alternatives. There is a series of international standards for LCA ISO 14040-14044, which was issued from 2006 onwards.

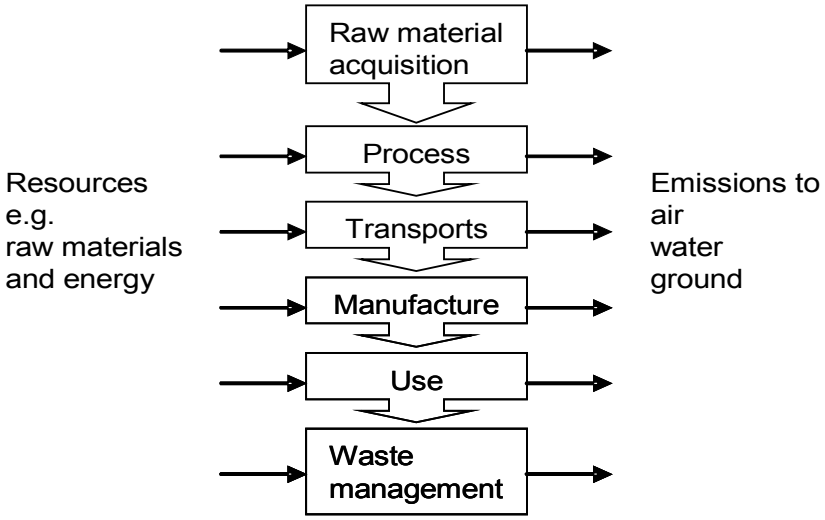

Figure 1. Life cycle

The LCA procedure includes several steps, see figure 2.

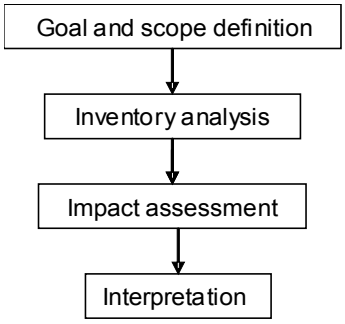

Figure 2. Life cycle assessment procedure

In the goal and scope definition the product to be studied and the purpose of the LCA are specified.

An inventory of inputs and outputs of the product system is compiled. The inventory analysis implies the construction of the life cycle model and calculation of the resources used and the emissions produced during the lifecycle. The model, usually represented as a flow chart, is a mass and energy balance over the system. The inventory of flows is an iterative process to find out which flows that are environmentally relevant.

In the impact assessment phase, the emissions and the resources are related to various environmental problems. The potential environmental impact is evaluated by classification and characterisation of identified raw materials and emissions associated with the product life cycle. See figure 3.

Finally the different environmental impacts related to the life cycle may be put on the same scale through weighting. This part is though controversial and it is not part of the ISO standards for LCA.

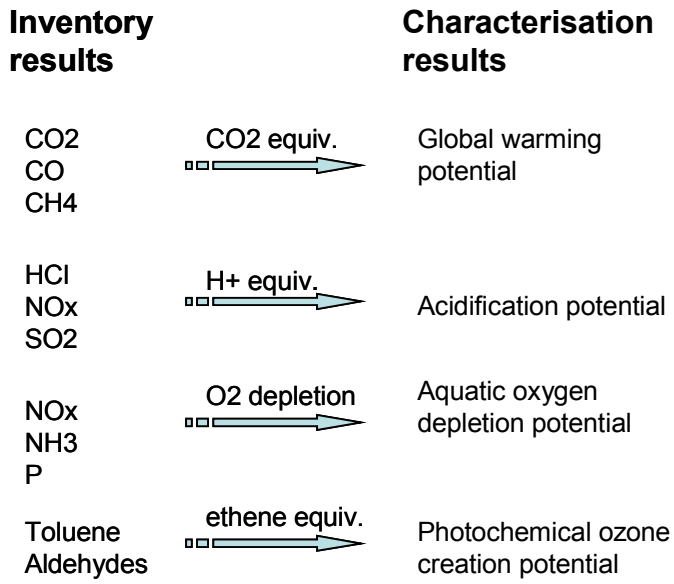

Figure 3. Characterisation

The life cycle impact assessment phase will be studied further below. Life cycle impact assessment (LCIA) aims at describing the environmental consequences of the environmental loads quantified in the inventory analysis. The impact assessment is achieved by translating the environmental loads from the inventory results into environmental impacts, such as acidification, eutrophication, global warming etc. As for the impact category toxicity, quantified emissions of for example benzene, cadmium and dioxins are converted into quantified contributions to ecotoxicity and human toxicity. There are several reasons for this translation: facilitate communication, making results more comparable and improve the readability by reducing the number of parameters. The set of impact categories in the LCA is a specification of environmental impacts considered relevant in the goal and scope definition. Several things should be considered when deciding on which impact categories to include:

- Completeness. The list of impact categories should cover all environmental problems of relevance.
- Practicality. You should not include too many categories.
- Independence. The categories should be mutually independent to avoid double-counting.
- Feasibility. It should be possible to link the life cycle inventory result parameters to chosen impact categories and characterisation methods.
- Environmental relevance. Indicators derived from characterisation methods should be environmentally relevant to the impact category and safeguard subjects.
- Scientific method. Characterisation methods should have scientific validity.

Classification simply means sorting the inventory parameters according to the type of environmental impact they contribute to. In the next step, characterisation, the relative contributions of the emissions and the resource consumption to each type of environmental impact are calculated. Characterisation is a quantitative step; the sizes of environmental impacts are calculated per category using equivalency factors. The definition of characterisation methods with suitable equivalency factors is in principle based on the physico-chemical mechanism of how different substances contribute to the different impact categories. Good characterisation methods exists for some of the impact categories (e.g. acidification) where the mechanisms are relatively simple and well known, but are less well developed for others e.g. ecotoxicity where the mechanisms are more complicated. There are a lot of toxic substances, having their effect through different mechanisms and having different types of impact. Moreover, different species react differently when exposed to a particular substance (Baumann & Tillman 2004).

3.2 Life cycle assessment vs Risk assessment

Life Cycle Assessment (LCA) is one approach to evaluate environmental impacts of chemical substances. Another approach is the Risk Assessment (RA). The most decisive difference between the two approaches is related to goal and scope. The results of an LCA is linked to the “functional unit” and the purpose is often to compare environmental impacts from “Product A” to the alternative “Product B”. The results are expressed as the marginal environmental impact from the manufacturing, use and disposal of the functional unit e.g. one product. The total number of the products produced is thus not considered. Risk Assessment

is often performed due to a requirement from the authorities. The RA is often site specific and the total amount of chemical substance involved is an important parameter by the assessment.

The data used to perform Life Cycle Impact Assessment (LCIA) and Risk Assessment is basically the same. However the way they are used and the need for specificity is different. Data used for LCIA are more often generic data that reflects the need for a best estimate of the environmental impacts. Data of this kind can also be used for a first rough estimate for a Risk Assessment, but the application of the data should reflect the need for a worst-case estimate. If the first estimate of the RA indicates a potential for adverse effects the Risk Assessment will usually pursue applying more site- and substance-specific data and models (Willum 2006, s. 19).

3.3 LCA practice at SCA Personal Care

At the hygiene product division at SCA the concept of life cycle assessment was introduced as early as in the beginning of 1990. By the mid 1990s, LCA studies became routine for some product groups (Baumann & Rex 2004). Today, LCA is a mandatory part in the product development process. The LCA practice has always been associated with a pragmatic approach. Thanks to this the company is able to use LCA as an important tool in the evaluation of their products' environmental impacts.[1] Most studies are made as part of the product development process, to assess the environmental consequences of new design (Baumann & Rex 2004).

Since 1996 SCA has participated in the successfully competence centre CPM, a competence centre for environmental assessment of product and material systems. CPM includes members from both industry and academia, it was established at Chalmers University of Technology in Gothenburg, Sweden in 1996.

The results of the LCAs are usually presented as a comparison of a reference product (old product) with its corresponding new designed product. In the LCA reports the results of the studies are presented in two different sections, see table 1. The first section, called resources and waste includes the parameters; Product weight, Land use forestry, Non-renewable material, Fossil resources, Total energy, Water consumption, Nuclear waste and Landfill waste. The second section, environmental effects, includes the environmental impact categories Global warming potential, Acidification potential, Aquatic oxygen depletion potential and Photochemical ozone creation potential.

Table 1. Parameters included in the LCAs at SCA Personal Care

Resources and waste		Environmental effects
Product weight	Total energy	Global warming potential
Land use forestry	Water consumption	Acidification potential
Non-renewable material	Nuclear waste	Aquatic oxygen depletion potential
Fossil resources	Landfill waste	Photochemical ozone creation potential

[1] Ellen Riise Environmental department SCA Personal Care 2006

The results of the comparison are shown as percentages showing the increase or decrease of a certain parameter in relation to the reference product, see table 2. The LCA report also includes an informing discussion of the results and a conclusion (Spak 2006).

Table 2. Results of a comparing LCA, as presented at SCA Personal Care (invented figures). (Spak 2006)

Impact category	Difference in % vs. current product	Judgement of environmental impact
Global warming potential	+7	Negative
Acidification potential	-5	Positive
Aquatic oxygen depletion potential	-14	Positive
Photochemical ozone creation potential	+4	Negative

The impact categories included in the LCA are not mutually different. For example NO_x emissions are accounted for in two impact categories; Acidification and Aquatic oxygen depletion. All substance emissions that have a significant impact according a specific impact category are included in the calculation of the potential environmental impact of that category. This is a worst case calculation for all impact categories, it is assumed that an emitted substance will have a 100% impact in all impact categories possibly affected.

Implementation of toxicological assessment at SCA Personal Care would mean a fifth impact category in the life cycle assessments. The concept of the flow chart models would still be the same but flows regarded as environmentally relevant may change, as toxic impact would be included in the assessment.

4 Background to toxicological assessment

In this chapter there is first a short introduction to toxicology. Thereafter follows a sub chapter concerning general structure of models for toxicological assessment. Then some key parameters in the TA models are dealt with; chemical partitioning and toxicity data.

4.1 Toxicology

Chemicals emitted as a consequence of human activities can contribute to ecotoxicity if they affect the function and structure of ecosystems by exerting toxic effects on the organisms which live in them. Emitted chemicals can also contribute to human toxicity via exposure though the environment. The most important exposure routes are inhalation and oral intake of water and food. If the concentrations of environmentally hazardous substances caused by the emission are high enough, the toxic effect can occur as soon as the substances are released. This form of toxic effect is called acute toxicity. It often results in the death of organisms exposed.

Toxic effects which are not acutely lethal and which first appear after repeated or long-term exposure to the substance are called chronic toxicity. Chronic toxicity is often caused by persistent substances, i.e. substances which have a low biodegradability in the environment and which can therefore remain for a long time after their emission. Some substances have a tendency to accumulate in living organisms, so that tissues and organs can be exposed to concentrations of the substance which are far higher than the concentrations in the surrounding environment. The chronic toxicity of a substance is thus determined by its toxicity, its biodegradability and its ability to accumulate in living organisms. The result of a chronic toxicity impact can for example be reduced reproductive capacity, which means that the species' chances of survival in the long term are reduced (Wenzel, Hauschild & Alting 1997, vol 1). Microbial degradation is crucial in the prediction of the longevity and thereby the long-term effects of a toxicant (Landis & Yu 1999).

4.2 General structure of models for toxicological assessment

The main aspects in toxicity-oriented problems are:

- Fate. The residence time of a chemical in a particular environmental compartment (air, water, ground). It depends on degradation mechanisms and transport processes, e. g. from air to soil by rain, from water to air by evaporation, from soil to water by run-off.

- Exposure/intake. The transfer of a substance from a given compartment to an exposure route leading to intake of the substance by an organism. The exposure depends on the food pattern, water intake and respiratory volume of the organism.

- Effect/damage. There is wide variation in the hazards posed by chemicals; some are more toxic than others.

Fate and exposure /intake are often modelled together. A number of compartments and sub-compartments are distinguished, e.g. air, soil, freshwater, marine waters and sediment. Environmental processes like rainfall, degradation, sedimentation and immobilisation (e.g. by burial in deeper sediments) are captured in model equations, which are then extended via exposure routes (air, water, crops, meat) to target organisms or to target ecosystems (terrestrial, freshwater, marine). The effect measure is often based on toxicologically-based yardsticks such as EC_{50}, defined as the concentration at which 50% of the target organisms show an effect. The higher the value, the less toxic is the substance. Extrapolation or safety factors may be applied to convert the results from the laboratory to the field, from rat to man, from single species to ecosystem etc., yielding for example ADIs (Acceptable Daily Intakes), TDIs (Tolerable Daily Intakes), PNECs (Predicted No Effect Concentrations) and MTCs (Maximum Tolerable Concentrations). The safety factors are also denoted assessment factors (de Koning 2002).

The framework for ecotoxicological models is generally based on three factors; an emission factor (summation of emissions of the particular chemical), a concentration to source (CSR) factor (where the chemical ends up and its ultimate concentration) and a toxicity effect factor (toxic effects to animals, plants at a given concentration). The CSR factor accounts for both fate and exposure. The product of the CSR factor and effect factor represent the ecological toxicity factor (the characterisation factor). Multiplication of all three factors gives the potential ecological toxicity impact (Gloria et al. 2006). See figure 4.

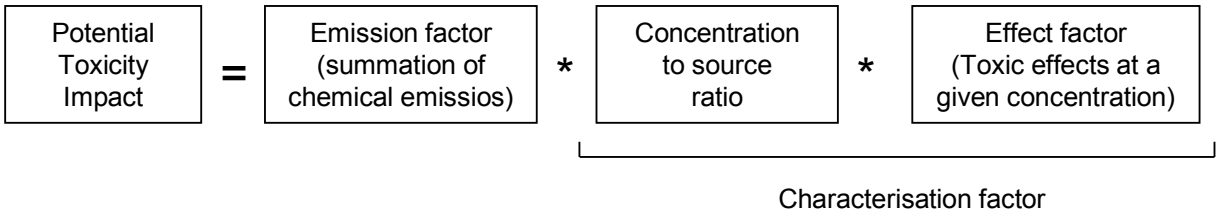

Figure 4. General framework for toxicological models (Gloria et. al 2006)

There is a trade off between accuracy and data requirements in the development of toxicity equivalents, also called characterisation factors. The more sophisticated fate analysis, the more data is needed for developing the characterisation factors of a substance. Since a large number of chemicals are used in our societies today we consequently need a large number of characterisation factors. The advantage of the simpler methods is that the equivalents are easier produced which means that equivalents can be calculated for a large number of chemicals, although at the expense of accuracy (Baumann & Tillman 2004, s. 152).

To assess human toxicity impact, the LCA-practitioner considers for each chemical involved the cumulative exposure associated with the mass released to a defined (indoor, urban, regional etc.) environment by multiplying the released amount by a measure of toxic impact to characterize the likelihood of health effects and their potential consequences.

At a workshop about human toxicity and LCIA, an adjunct activity of the 2004 SETAC World congress in Portland, Oregon, dose-response experts concluded that it is appropriate to include human toxicity in the LCIA process. The basis for this recommendation is that, in the absence of a toxicity metric, many LCIA practitioners will continue to rely on emissions magnitude as a measure of emissions impact. But, because of the significant differences among chemicals according the dose levels that are toxic, they consider that it is essential to

consider human toxicity when comparing releases of different toxic chemicals (McKone et al. 2006).

4.3 Chemical distribution among phases

Pure air is an example of a gas phase and pure water is an example of an aqueous phase. Solid phase include soil grains, solid particles suspended in water or air and pure solid chemicals. In addition, an immiscible liquid (i.e. a liquid that does not mix freely with water) can form its own non-aqueous phase liquid (NAPL). An oil film or a pool of grease solvent floating on a water surface is an example of a NAPL.

Chemical partitioning is a key step in toxicity modelling. Fate calculation includes estimation of the relative amounts of a chemical expected to end up in different phases that are in equilibrium with one another. Equilibrium concentrations are calculated. Aqueous solubility, a fundamental chemical-specific property, is defined as the concentration of a chemical dissolved in water when that water is both in contact and in equilibrium with the pure chemical. Vapour pressure, another chemical specific property, is defined as the partial pressure of a chemical in a gas phase that is in equilibrium with the pure liquid or solid chemical. Vapour pressure is temperature dependent; it can vary appreciably with a temperature change of 5 or 10˚C. A partition coefficient is the ratio of the concentrations of a chemical in two different phases, such as water and air, under equilibrium conditions, and it is a measure on how the chemical distributes itself. The Henry's law constant is a partition coefficient usually defined as the ratio of a chemical's concentration in air to its concentration in water at equilibrium. Henry's law constants generally increase with increased temperature, due to the significant temperature dependency of chemical vapour pressures.

Chemical partitioning also occurs between water and solid phases, in a process most generally termed sorption. There are to types of sorption; adsorption, in which a chemical sticks to the two-dimensional surface of a solid, and absorption, in which a chemical diffuses into a three-dimensional solid. Chemical sorption in the environment is much more difficult to predict than is chemical partitioning between air and water, partly because the types of sorptive solid phases (sorbents) vary enormously, and partly because there are many different mechanisms by which sorption can occur. The mechanisms by which sorption can occur include absorption into natural organic matter; adsorption to mineral surfaces via van der Waals, dipole-dipole, or other weak physical intermolecular forces; adsorption through electrostatic attractions to oppositely charged surface sites of the solids; and adsorption through covalent bonding to surface groups on the solids.

The symbol K_p is frequently used to represent a solid-water partition coefficient. K_d is a equivalent notation. The relation between dissolved and sorbed chemical concentration is often non-linear. Neutral organic chemicals with low water solubility tend to absorb into natural organic matter because they are non-polar. In general smaller molecules and more polar molecules dissolve more readily in water and have less tendency to sorb to solids. Larger molecules and less polar molecules are more likely to sorb to solids. The polarity of a chemical has a strong inverse correlation with the chemical's K_{ow}, the octanol-water partition coefficient. K_{ow} is the ratio of a chemical's concentration in octanol to its concentration in water at equilibrium. The relative concentration of a chemical in air, water or soil phases at equilibrium can be predicted from knowledge of the chemical's partition coefficients (i.e.

vapour pressure, Henry's law constant and distribution coefficient) (Hemond & Fechner-Levy 2000).

4.4 Toxicity data

Normally it is only possible to find *laboratory* data for a substance's toxicity. In the laboratory tests, selected organisms have been exposed to the substance under standardized conditions in a shorter or longer time.

In a short-term laboratory test (acute toxicity test), the concentration of the substance that kills e.g. 50% of the test organism (LC_{50}, Lethal Concentration 50%) is determined. For toxicity test of longer duration (chronic toxicity tests), the highest concentration of the substance which produces no observed effects on the test organisms (NOEC, No Observed Effect Concentration) or the lowest concentration which has resulted in observed effects on the test organisms (LOEC) is most often reported.

HRC, human reference concentration, is a measure of the concentration of the substance in air which is assessed as having no toxic effect on life-long inhalation. HRC is determined on the basis of the results of inhalation experiments with animals or observations on humans who has been exposed to a substance via the respiratory tract. HRD, the human reference dose, is a measure of the dose which is assessed not to have any toxic effect on life-long daily ingestion. The HRD is estimated in the same way as described for the HRC, with the difference that it must be based on results of ingestion experiments and thus dose values such as LD_{50}.

Different assessment factors will be applied according to the quality and the relevance of the available data. The PNEC value (Predicted No Effect Concentration) used to calculate substances' effect factors is estimated by dividing the lowest of the test results used (indicating highest toxicity) by the assessment factor (Wenzel, Hauschild & Alting 1997, vol 1).

4.5 QSAR

Quantitative structure-activity relationships (QSAR) is a method of estimating the toxic properties of a compound using the physical and structural makeup of the compound. The knowledge that similar compounds typically have similar modes of action makes QSAR a possibility. QSAR can be a useful tool in selecting compounds with desired properties but with low toxicity to the environment (Landis & Yu 1999).

5 Models for toxicological life cycle impact assessment

This chapter begins with a method chapter concerning the model study. Next follows a description of the OMNIITOX project and the OMNIITOX models. After that investigations of the following models are done:
EPS -Environmental Priority Strategies in product design
Ecopoints
Fh-IUCT
USES-LCA
GLOBOX
EDIP- Environmental Design of Industrial Products

In the end a deeper study is done on the EDIP method and an investigation of the risk-phrase method “Simple estimation of effect factors for toxicity used for screening LCA” is done. This method uses the EDIP methodology but uses risk-phrases as toxicity metric, instead of toxicity values.

5.1 Investigation of models – material and method

In this chapter the following models will be investigated:
OMNIITOX
EPS -Environmental Priority Strategies in product design
Ecopoints
Fh-IUCT
USES-LCA
GLOBOX
EDIP- Environmental Design of Industrial Products
Simple estimation of effect factors for toxicity used for screening LCA

OMNIITOX is a new and comprehensive project; many experts in the field have contributed in the development of the models. Within the OMNIITOX project an inventory of then current LCIA methods used for toxicological assessment was made. The inventory served as basis in the development of a new method. The results were compiled in the report “OMNIITOX – inventory and classification of LCA characterisation methods for toxic releases” (de Koning et al 2002). This report has formed basis in the choice of models to be investigated in this thesis. The report has been used as data source for description of the models. For some interesting models further information has been collected.

5.2 The OMNIITOX project

OMNIITOX (Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments) was an EU project within the "Competitive and Sustainable Growth"-Programme that ran 2001-2005. OMNIITOX aimed at facilitating decision-making regarding potentially hazardous compounds by improving methods and

developing information tools necessary for Life Cycle Assessment (LCA) and (Environmental) Risk Assessment (E)RA. The idea was that both decision-makers and practitioners will benefit from OMNIITOX results (IMI OMNIITOX project site 2005).

Given the limited availability of data for chemical properties, the OMNIITOX-project aimed at defining simplified operational models for characterisation of toxic impacts for a large number of substances. They should be implemented by a web-based information system facilitating data availability and model calculations, which also provides guidance on the use of LCIA and (E)RA (Molander 2002).

Information about the OMNIITOX project is available at the internet (OMNIITOX project website). The OMNIITOX Information System (IS), with the OMNIITOX models and the database is also available at the internet (OMNIITOX Information System).

The outcome of the project is two models for toxicological impact assessment; OMNIITOX base model and OMNIITOX simple base model. Since the base model is very data demanding a regression of this model were made to get a simplified model; OMNIITOX simple base model. An investigation of what properties that was the most important were made and an attempt to reduce the number of properties in the model to reduce data demand. Unfortunately the simple base model is just a little bit simplified, only a few properties were left out. An advantage of the OMNIITOX model is that it is transparent. A lot of work has been put in on doing a good documentation of how the model works.[2]

The OMNIITOX model is a fate, exposure and effect model. The calculated toxicological impact of an emitted chemical is a function of amount emitted, substance properties and environmental properties. The environmental properties are captured within the model. The user chooses if the calculation shall comprise Europe or the whole world. The model includes three emission compartments; air, freshwater and agricultural soil. Calculations of characterisation factors using the OMNIITOX base and simple base models in the OMNIITOX IS have resulted in 522 characterisation factors for 57 substances stored in the OMNIITOX database.

The OMNIITOX Information System provides characterisation factors for toxicity effects on human health (cancer and non-cancer) and fresh water aquatic ecosystems respectively (Rosenbaum 2005). The overall model frame work for human health impact characterisation is expressed as:

HDM = FM * XM * EM

HDM -Human damage factor matrix
FM -Fate factor matrix
XM -exposure factor matrix
EM -Effect factor matrix

[2] Johan Tivander, IMI Industriell miljöinformatik, Chalmers University of Technology 2006-10-06

The human damage factor [cases / kg emitted substance] can be interpreted as the increase in number of cancer or non-cancer diseases, as a consequence of an emission in the initial compartment.

The overall model frame work for ecotoxicological characterisation is expressed as:

EIM = FM * EEM

EIM Ecotoxicological impact factor matrix
FM Fate factor matrix
EEM Ecotoxicological effect matrix

The ecotoxicological impact factor [PAF * m^3 * year/ kg] can be interpreted as the increase in the fraction of species which are affected by adverse effects in a specific volume of the final compartment and during a specific time, due to an emission into a specific compartment.
PAF = potentially affected fraction. (Rosenbaum 2005)

Concerning data demand see appendix 1, Minimum requirement list of substance properties.

OMNIITOX – inventory and classification of LCA characterisation methods
In the OMNIITOX project an inventory of then current LCIA characterisation methods were made. This investigation formed a basis for the challenging work of creating a new method for toxicological assessment.
The report "OMNIITOX – inventory and classification of LCA characterisation factors for assessing toxic releases." (de Koning et al. 2002) describes the inventory, classification and first evaluation of LCIA characterisation methods. It consists of an inventory of current LCIA characterisation methods for toxic substances and a set of criteria combined with a scoring system for evaluation of the characterisation methods.

First a complete inventory of characterisation methods where made. The resulting long list of methodologies where reduced by applying some rules including:

- The characterisation model is operational and used to calculate characterisation factors.
- The characterisation method is the original and most recent version.
- The characterisation method is well documented in the English language.
- The characterisation method has been submitted for analysis by one of the OMNIITOX participants.
- If two methods described by different authors are similar, they will be considered as a group and one representative method will be analysed further.

Ten methodologies remained for further investigation and description: Fh-IUCT, Ecopoints, EDIP-characterisation, USES-LCA, CalTOX, Impact 2002, EPS default method version 2000, GLOBOX, Eco-indicator and Ecosense. These methods are examined and described in the report. From these ten the OMNIITOX participants then selected some methods to be investigated further. The descriptions of the methods given in the report have been reviewed by the method owners (de Koning et al. 2002).

Models that are ranked the highest level of sophistication, level 5, is excluded from this investigation since it is obvious that they are too advanced for the purpose; tox assessment in the LCA practice at SCA Personal Care. The level 5 models have been developed for damage assessment. Models on this level can take into account exposed populations, exposure pathways and backgrounds. Models classified as level 5 are: Ecoindicator 99, IMPACT 2002, Ecosense and EPS. A short explanation of the EPS model is made because it uses a very diverging methodology and to make clear that it is not a model for separate toxicological assessment. CalTOX is excluded since it not comprises ecotoxicological assessment.

5.3 EPS - Environmental Priority Strategies in product design

The EPS method includes characterisation and weighting. The weighting is based on "Willingness to pay", a notion from environmental economics. Five "safeguard subjects" or areas of protection are considered; abiotic stock resources, human health, ecosystem production capacity, biodiversity and cultural and recreational values. The impact categories are summed up into the endpoint category human health. The characterisation factors reflect all environmental impact that lead to negative consequences for human health. This means that there is no separate characterisation factor for toxicology (de Koning et al. 2002).

5.4 Ecopoints

The ecopoints are given by the ratio between the actual anthropogenic emission of a substance and the critical emission of that substance. For determination of the critical flow the method uses politically defined targets and scientifically supported goals as a basis for evaluation. Ecofactors are time and space dependent. The ecofactors vary according to in which year and in which country the flows are measured, due to differences in politically goals that in turn are dependent of technological and economic situations, environmental situations, scientific discussion and social goals. This method do not account for fate and exposure, it assumes that fate and exposure for all toxic substances are equal (de Koning et al. 2002).

5.5 Fh-IUCT

This characterisation method for both human toxicity and ecotoxicity was developed by the Fraunhofer-institut für Umweltechemie und Ökotoxikologie (Fh-IUCT). The method comprises the emission compartments air and water.

The human toxicological assessment method is a semi-quantitative screening method. The characterisation is made by assigning substances to five different Hazard Potential Classes (HPC), representing increasing toxicity. Allocating substances to the different classes is done in a two step procedure. In the first step the substances are classified on basis of toxicological characteristics only, using exposure limits or risk phrases. The second step modifies the classification made in the first step based upon exposure criteria like persistence,

accumulation and indoor versus outdoor emissions. If a substance is very persistent or emitted indoors it is allocated one class higher. After the classification, summation of the emissions within each class is performed on the basis of mass units. No further aggregation occurs.

The method for ecotoxicity has a two tiered approach. The first step in tier 1 organises the chemical stressors into different classes representing an increasing ecotoxicity. The chemical stressors are ranked by a combination of three environmental key parameters: (1) persistence as defined by the OECD-TG, (2) accumulation as given by logPow>3 or a BCF>100, (3) ecotoxicity as defined by LC_{50} or EC_{50}. Based upon these three environmental key properties emissions are classified into five ecotoxicological impact classes all having a different ecotoxicological potential factor (ETP). See table 3.

Table 3. The ecotoxicological impact classes with associated ecotoxicological potential factors (de Koning et al. 2002)

Impact class 0 with property combination:	Impact class A with property combination:	Impact class B with property combination:	Impact class C with property combination:	Impact class D with property combination:
$LC_{50} > 10$ mg.l^{-1} degradable non-accumulating ($\log P_{ow} < 3$)	$LC_{50} > 100$ mg.l^{-1} persistent and/or accumulating ---------- or ---------- $LC_{50} < 10$ mg.l^{-1} degradable non-accumulating	$LC_{50} = 10 - 100$ mg.l^{-1} persistent and/or accumulating	$LC_{50} = 1 - 10$ mg.l^{-1} persistent and/or accumulating	$LC_{50} < 1$ mg.l^{-1} persistent and/or accumulating
⇩	⇩	⇩	⇩	⇩
0	1	10	100	1000

For metals and metal compounds the environmental key properties persistence and bio-accumulation are not well defined, metals are allocated to ecological impact classes on the basis of expert judgement. A general discussion of the allocation of metals to classes is lacking. Since environmental impact is a function of both chemical properties and loading, in the next step, the derived ecological potential factor, for a substance, are multiplied with the amount of emitted substance to give a potential ecotoxicological loading for the given substance. The sum of all ecotoxicological loadings of a product system is the potential ecotoxicological loading of the product which can be used in comparative assessments. Then calculation of normalised data can be made.

In the methodology of Fh-IUCT the first tier is a selection method and the second tier is comparable to a full characterisation step using more sophisticated methodologies. The second tier is though not well documented and the OMNIITOX participants conclude that it is not operational (de Koning et al. 2002).

BCF, Bioconcentration factor represents the equilibrium ratio of the concentration of a specific chemical in a fish relative to that dissolved in the surrounding water, provided that the diffusion mechanism represents the only source of the substance for the fish. BCF values vary not only from chemical to chemical but also, to a certain extent, from one type of fish to another, particularly because of variations in the abilities of different fish to metabolize a given substance (Baird & Cann 2005, s. 319).

The partition coefficient, K_{ow}, is defined as $K_{ow} = [S]_{oktanol} / [S]_{water}$. 1-oklanol is used since it has been found experimentally that it is a suitable surrogate for the fatty portion of fish. Chemicals with high K_{ow} tend to bioaccumulate (Baird & Cann 2005, s. 319). The partition coefficient K_{ow} is sometimes assigned P_{ow} (Willum 2006, appendix 2).

5.6 USES-LCA - Uniform system of valuation of substances

This model is a sophisticated fate, exposure and effect characterisation method which modelling environmental mechanisms. It is a global fate model that combines the regional, continental and global scales with arctic, temperate and tropical zones. Together with physico-chemical property factors of substances, the model can theoretically describe how a substance is dispersed between soils, air and waters. The model is used to calculate the predicted environmental concentration (PEC) of a substance in air, water and soil. The PEC is related to the predicted no-effect level (PNEC) of that substance to form a measure of the degree of impact. This value is then related to that of a reference substance, 1,4-dichlorobenzene, a known pesticide. Easy to say the USES-LCA toxicological assessment model assesses the degree to which the no-effect level is disturbed.

Fate analysis of substances is performed with the SimpleBox 3.0 which is part of the USES 2.0 model. SimpleBox 3.0 has been adapted to meet LCA-specific demands.

The USES-LCA model was updated 2005, after the comparison of toxicological assessment models were done within the OMNIITOX project. SimpleBox 3.0 is used in the model instead of SimpleBox 2.0 and significant changes has been done in the structure of the air and soil compartments in the new version of USES-LCA; distinction between rural and urban air (air emissions to areas of low respective high population density), inclusion of rain-no rain conditions and inclusion of soil depth dependent intermedia transport. The new fate and exposure module of USES-LCA has been applied to calculate human population intake fractions and fate factors of freshwater, marine and terrestrial environment for 3393 substances, emitted to 7 different emission compartments (Huijbregts et al. 2005).

Apart from the fate and exposure update, a new method to derive cancer and non-cancer human damage and effect factors of toxic pollutants has been developed, starting from a lognormal dose-response function. Human damage factors are expressed as Disability Adjusted Life Years (DALY). Human effect factors contain a disease-specific and a substance-specific component. The disease-specific component depends on the probability of disease occurrence and the distribution of sensitivities in the human population. The substance-specific component, equal to the inverse of the ED50, represents the toxic potency of a substance. The new method has been applied to calculate combined human damage and effect factors for 1192 substances (Huijbregts 2006).

Emission compartments included in the model are:
Urban air, rural air, freshwater, seawater, agricultural soil, industrial soil, natural soil

Environmental receptors are:
Terrestrial environment, freshwater environment, marine environment

Human exposure routes are:

Inhalation and ingestion via root crops, leaf crops, meat products, dairy products, eggs, freshwater fish, marine fish, and drinking water (Huijbregts et al. 2005).

The authors of "The Hitch Hiker's Guide to LCA" (Baumann & Tillman 2004) conclude that despite its level of sophistication, there are many uncertainties in the USES-LCA model, especially in its assessment of metals.

5.7 GLOBOX

GLOBOX is a global multimedia fate, exposure, and effect model, largely based on the European Union model EUSES (version 1.00). It has primarily been constructed for the calculation of spatially differentiated LCA characterisation factors on a global scale. GLOBOX is spatially differentiated with respect to fate and human intake on the level of separate, interconnected countries, seas, and oceans. Alternatively, the user can choose to differentiate on a number of lower levels, or to turn off spatial differentiation altogether. GLOBOX has been harmonised with the ecoinvent Life Cycle Inventory database, which implies that all regional divisions distinguished in this database are also included as levels of differentiation in GLOBOX. The choice for the level of differentiation can be made separately for every individual emission, depending on the spatial information available on each specific (industrial) process. The chosen level of spatial differentiation will influence the accuracy of the resulting characterisation factors. The idea behind GLOBOX is that it should be possible to construct location specific characterisation factors for any emission at any location in the world, taking into account the summed impacts of such emission in all countries and at all seas and oceans among which it is dispersed during its lifetime.

It is written at the homepage of the Leiden University that the model is not yet fully operational, and it is due to be released in 2006. More information will be made available through the website (Wegener Sleeswijk 2005).

5.8 EDIP - Environmental Design of Industrial Products

Hauschild & Wenzel (1998) developed characterisation factors based on environmental key properties to model fate, exposure and effect for human toxicity and ecotoxicity releases. The aim was to develop a method which is transparent to the user and allows an easy calculation of missing characterisation factors without losing the environmental relevance of the results. The EDIP method was designed for product development purposes (Baumann & Tillman 2004).

The EDIP method is well documented in the two books Environmental Assessment of Products volume 1 and 2 (Wenzel, Hauschild & Alting 1997).

Human toxicity
The characterisation factor Human toxicity potential (HTP) for a substance *i* emitted to an emission compartment *ecomp*, leading to exposure via route *r*, is calculated as follows:

$$HTP_{i,ecomp,r} = \sum_{fcomp} f_{i,ecomp,fcomp} * BIO_i * T_{i,fcomp,r} * I_r * E_{i,r}$$

$HTP_{i,ecomp,r}$	the Human Toxicity Potential
$f_{i,ecomp,fcomp}$	the intermedia transport factor, the fraction of substance *i* emitted to emission compartment *ecomp* that reaches final compartment *fcomp*
BIO_i	the biodegradability factor
$T_{i,fcomp,r}$	the transfer factor, the fraction of substance *i* transferred from *fcomp* to exposure route *r*
I_r	the intake factor, intake of medium (kg medium/kg body weight/day)
$E_{i,r}$	the effect factor

Depending of exposure route concerned, the effect factor, $E_{i,r}$ is either the inverse of the Human Reference Dose, HRD (comparable to Acceptible Daily Intake, ADI) or the Human Reference Concentration, HRC. The HRD and HRC are based on animal test data, and derived by extrapolation methods using safety factors and in some cases policy targets.

The method of Hauschild & Wenzel (1998) yields three separate indicator results for human toxicity, one for each of the three exposure routes air; water (fish); soil (plants, animals, milk or direct ingestion).

$$\text{Human toxicity}_r = \sum_{i} \sum_{ecomp} m_{i,ecomp} * HTP_{i,ecomp,r}$$

$m_{i,ecomp}$	the emission of substance *i* to compartment *ecomp*

These three indicator results are measured in different units, as dilution volumes of the respective compartment, hence no aggregation to a single indicator results (de Koning et al. 2002).

HTPs are available for approx. 170 different chemicals emitted to air, water or soil (The Danish EPA).

Data needed:
Emitted amount of the substance
The emitted substance's partition ratio between water and land
If the substance's half-life in air is more than one day
If the substance is "ready biodegradable" or "inherent biodegradable" according to OECD guidelines or similar biodegradability tests
The transfer factor e.g. water fish: BCF or K_{ow}
Intake factor
Human reference dose or concentration (comparable to acceptable daily intake)

Ecotoxicity
There are characterisation factors for aquatic, terrestrial and sewage treatment plant ecotoxicity. The aquatic ecotoxicity characterisation factor is subdivided in acute and chronic, according the type of impact considered.

The four characterisation factors are calculated:

$$AETP_{i,ecomp,acute} = f_{i,ecomp,fcomp} * E_{i,\ aquatic,acute}$$
$$AETP_{i,ecomp,chronic} = f_{i,ecomp,fcomp} * BIO_i * E_{i,\ aquatic,chronic}$$
$$TETP_{i,ecomp,chronic} = f_{i,ecomp,fcomp} * BIO_i * E_{i,terrestrial}$$
$$STPETP_{i,stp,acute} = E_{i,sewagetreatmentplant}$$

The distribution factors, $f_{i,ecomp,fcomp}$ describe the final distribution of the substance.

The effect factors are calculated as the inverse of a Predicted No Effect Concentration, PNEC. The PNEC is based on single species ecotoxicological data, and derived by using extrapolation methods. For acute toxicity to wastewater treatment plants, the effect factor is based on the Lowest Observed Effect Concentration (LOEC) for aerobic heterotrophic bacteria.

The four different ecotoxicity indicators are calculated:

$$\text{Ecotoxicity} = \sum_i \sum_{ecomp} m_{i,ecomp} * \text{characterisation factor}$$

For explanation of the expressions see human toxicity above.

The various indicator results are not aggregated further to a single indicator result as part of the characterisation step (de Koning et al. 2002). Ecotoxicological characterisation factors are available for approx. 190 different chemicals emitted to air, water or soil (The Danish EPA).

The toxicity equivalents are expressed in m^3 of air, water or soil into which the emission should be diluted for its concentration to be so low that no toxicological effects could be expected (Baumann & Tillman 2004).

The characterisation factors for ecotoxicity depend exclusively on the characteristics of the substance. These will be the same independently of the context in which the emission occurs. Therefore the characterisation factors have to be calculated only once for each substance. The factors calculated can be reused every time the substance appears in an inventory to be assessed (Wenzel, Hauschild & Alting 1997, vol.1).

Data needed:
Emitted amount of the substance
The emitted substance's partition ratio between water and land
If the substance's half-life in air is more than one day
If the substance is "ready biodegradable" or "inherent biodegradable" according to OECD guidelines or similar biodegradability tests
PNEC

5.9 Extension of the investigation

As EDIP seemed to be a suitable model for toxicological assessment at SCA Personal Care a deeper investigation of the model was done. Moreover, a variant of the EDIP method, "Simple estimation of effect factors for toxicity used for screening LCA", was investigated. This model uses the EDIP methodology, but the substances' toxicity data is based on risk

phrases, representing toxicity intervals, instead of toxicity values. The risk phrase method was published 2006, after the OMNIITOX project.

5.10 EDIP – deeper study

The EDIP project started in 1991 with the goal of developing methods for including environmental aspects in the product development phase. The project was carried out in close collaboration between the Danish EPA, the Technical University of Denmark (Institute for Product Development and Department of Technology and Social Sciences), Confederation of Danish Industries and five leading companies: Bang & Olufsen A/S, Danfoss A/S, Gram A/S, Grundfos A/S and KEW A/S (The Danish EPA).

The EDIP method is well documented in the books Environmental Assessment of Products volume 1 and 2 (Wenzel, Hauschild & Alting 1997). Volume 1 includes a manual on how to calculate missing characterisation factors. There is LCA software, GaBi, including the EDIP methodology and EDIP database. Information about this software can be found at LCA-center at the internet (LCA-center). EDIP characterisation factors for human and ecotoxicity can be downloaded at LCA-center (LCA-center).

In the calculation of characterisation factors for human toxicity three emission compartments are considered; air, water and soil. For soil, four routes are considered; direct ingestion of soil, ingestion of plants, ingestion of meat and ingestion of milk. The product of the intake factor and transfer factor are calculated for the four sub-compartments. The route leading to the highest exposure (greatest value) is selected to represent the soil compartment. For the exposure routes direct inhalation of air, direct consumption of ground water and direct consumption of soil the transfer factors is one. The transfer factor for water via consumption of fish is equal to the substance's bio concentration factor, BCF. For consumption of plants, meat and milk the transfer factors are calculated by means of the substance's stem concentration factor (SCF) and coefficient of adsorption in soil (K_d); SCF, K_d and beef transfer factor (B_b); BCF, K_d and milk transfer factor (B_m) respectively. For some substances these factors are available in Hauschild et al Environmental Assessment of Products. For others, instructions on how to calculate them from the substance's P_{ow} are available.

The distribution factors, $f_{i,ecomp,fcomp}$ describe the final distribution of the substance. A substance deposited from air is assumed not to re-evaporate from the water or soil compartment, even if it is volatile. For calculation of the distribution factor knowledge is needed of whether the Henry's law constant for the substance is greater than 10^{-3} atm m^3/ mol and if its atmospheric half-life is more than 1 day (Wenzel, Hauschild & Alting 1997, vol 1).

The effect factors are calculated as the inverse of a Predicted No Effect Concentration, PNEC. The PNEC is based on single species ecotoxicological data, and derived by using extrapolation methods. If the calculation of the effect factor is based on a $PNEC_{water,\ chronic}$ that was estimated on the basis of data for acute ecotoxicity and the substance's P_{ow} is greater than 1000, the PNEC value may be adjusted due to the substance's capacity for bioaccumulation. Wenzel, Hauschild and Alting (1997, vol 1) discusses when and how this should be done.

Within the EDIP methodology a qualitative assessment of ecotoxicity and human toxicity has been developed. It was developed for use as a screening method in order to focus work in a quantitative assessment. When the quantitative assessment is that simple that it is just to multiply the emissions with ready to use characterisation factors no qualitative assessment is required. The method can be used as an aid in the decision on with substances from an inventory should be regarded as contributors to the toxicity impact categories. It can also be used in a simple ranking of alternative products on the basis of the toxicity of the substances emitted during the products life cycle.

The qualitative assessment is a simple scoring system made up of an exposure factor and a toxicity factor. The exposure factor is based on risk-phrases indicating long-term adverse effects in the environment, the criteria for these phrases are associated with the substance's biodegradability and potential for bioaccumulation. The toxicity factors are based on the risk-phrases assigned. The qualitative assessment of a chemical is expressed in an impact score, which is the product of the exposure score and the human toxicity score or ecotoxicity score. A manual for how the qualitative assessment is carried out is available in the documentation of the EDIP methodology, in the book Environmental Assessment of products, vol. 1 (Wenzel, Hauschild & Alting 1997).

5.11 Simple estimation of effect factors for toxicity used for screening LCA

The approach of this method is based on the assumption that relevant toxicity data can be extracted from the risk-phrases that have been assigned to the chemical substances and published on official and advisory lists, and that this information can be transformed into one figure representing the level of toxicity.

It is often difficult and time consuming to get access to relevant data for chemical substances and it often takes the knowledge of a specialist to interpret these data and to calculate effect factors as it is done in the EDIP Method. Due to this, the effects of the emission of chemical substances are likely to be omitted from many LCAs. The overall purpose of developing this method was to facilitate the integration of the assessment of chemical substances in Life Cycle Assessment. Michael Hauschild, The Department of Manufacturing Engineering and Management at the Technical University of Denmark, says that the situation today is that it takes a skilled person one man-day to collect data and calculate a set of effect factors for one chemical substance in accordance with the EDIP Methodology. At the Department of Manufacturing Engineering and Management (IPL) at the Technical University of Denmark so far effect factors have been calculated for approx. 200 substances. There is a substantial need to facilitate the calculation of effect factors for chemical substances.

Within the project a database with data on human toxicity and ecotoxicity for chemical substances derived from risk-phrases and software that can calculate effect factors according to the EDIP methodology have been established. The results of this project are:

- "Simple estimation of effect factors for toxicity used for screening LCA" (Project publication and appendices) (Willum 2006).

- Effect Factor Calculator - the calculation tool in MS Access format containing the entire functionality and all applied data (Effect factor calculator, Access).

- Effect Factor Calculator - the calculation tool in MS Excel format" with reduced functionality designed to calculate effect factors from individual data. The file must be applied with macros activated.

- Effect Factors calculated for 23.029 substances based on toxicity data derived from risk-phrases in MS Excel format (Effect factor calculator, Excel).

All these documents are available at the internet. Toxicity data have been taken from lists where substances have been assigned risk-phrases according to the EU legislation. The total outcome from these lists sum up to 27.322 substances with unique CAS numbers. The values behind this list have been estimated by means of computer models, so-called QSAR models (Quantitative Structure-Activity Relationships). In the database that has been established within this project the origin of each dataset can be identified.

It is also necessary to uncover the fate of the substance when it is emitted to the environment. To do this a set of physical/chemical data have been extracted from the EPIWIN software. Some values are genuine experimental data while others are estimated based on the chemical structure of the respective substance or by a property/property estimation technique. These parameters are stored in the software and the origin of the data is also specified. Values for all relevant parameters have been extracted for 28.033 substances with unique CAS numbers.

Software in the shape of a Microsoft Access file has been developed and effect factors for 23.029 substances have been calculated. Effect factors calculated by the conventional method for 120 substances were compared to effect factors calculated by the risk-phrase method. This comparison (though insufficient) provides an indication of how good an estimate the risk-phrase method can generate. Though this comparison is based on a limited number of substances it indicates that effect factors calculated by the risk-phrase method represent a fairly good estimate. The effect factors calculated from toxicity values derived from the risk-phrases will inevitably be connected with some uncertainty. The uncertainty will differ depending on the risk-phrase applied, and the origin of the underlying data. To each set of effect factors calculated is attached some “Comments on data quality”, that serves to characterize the quality of the underlying toxicity data. For list of all notes used to characterize quality of the toxicity data see appendix 2.

Behind each risk-phrase is a set of criteria specifying when a substance should be assigned the respective risk-phrase, see table 4. If e.g. a substance is assigned the risk-phrase R25 (Toxic if swallowed) it means that it has an LD50 between 25 – and 250 mg/kg body weight. The next step is to transform this interval into one figure. For risk-phrases that have criteria set up in terms of an interval the midpoint value is chosen for a good estimate. For substances having the risk-phrase R25 the representative level of toxicity can be set to the midpoint value (LD50 = 112.5 mg/kg body weight).For risk-phrases where the criteria is defined by a toxicity value lower than a specific threshold value the representative toxicity level is set to 10% of the threshold value. This estimation was done after a data set of 357 substances with known L(E)C50 values below 1.000 mg/ m3 water were analysed. The logarithmic mean value for these substances turned out to be 10% of the threshold value. Therefore it is assumed that 10% (100 mg/ m3 water) of the threshold value is a good estimation of the toxicity level of this category.

The risk-phrases used are all based on LC_{50} values since this toxicity information is applicable to the EDIP methodology.

Table 4. Risk-phrases used for calculation of the effect factors (Willum 2006)

Risk phrase number	Phrase in English	Toxicity information specified in the criteria [3]	Representative toxicity level employed for calculation of effect factors	Unit	Comments
R20	Harmful by inhalation.	LC_{50} is between 2.000 and 20.000 mg/m^3/4 hr	11.000	mg/m^3 air/4 hr	The values for gas are used, as the values for aerosol seems unlikely to apply in this context. Midpoint value used.
R22	Harmful if swallowed.	LD_{50} is between 200 and 2.000 mg/kg	1.100	mg/kg body	Midpoint value used.
R23	Toxic by inhalation.	LC_{50} is between 500 and 2.000 mg/m^3/4 hr	1.250	mg/m^3 air/4 hr	Midpoint value used.
R25	Toxic if swallowed.	LD_{50} is between 25 and 200 mg/kg	112,5	mg/kg body	Midpoint value used.
R26	Very toxic by inhalation.	LC_{50} is lower than 500 mg/m^3/4 hr	50	mg/m^3 air/4 hr	A representative value of 10% of the "limit value" have chosen.
R28	Very toxic if swallowed.	LD_{50} is lower than 25 mg/kg	2,5	mg/kg body	A representative value of 10% of the "limit value" have chosen.
R50	Very toxic to aquatic organisms.	At least one of the values for 96 hr LC50 (for fish) or 48 hr EC50 (for daphnia) or 72 hr IC50 (for algae) is lower than 1.000 mg/m^3	100	mg/m^3/water	A representative value of 10% of the "limit value" have chosen.
R51	Toxic to aquatic organisms.	At least one of the values for 96 hr LC50 (for fish) or 48 hr EC50 (for daphnia) or 72 hr IC50 (for algae) is between 1.000 and 10.000 mg/m^3. And no ones are lower.	5.500	mg/m^3/water	Midpoint value used.
R52	Harmful to aquatic organisms.	At least one of the values for 96 hr LC50 (for fish) or 48 hr EC50 (for daphnia) or 72 hr IC50 (for algae) is between 10.000 and 100.000 mg/m^3. And no ones are lower.	55.000	mg/m^3/water	Midpoint value used.

By the calculation of effect factors for human toxicity the *"Human Reference Dose"* (HRD) has to be derived from the available toxicity data. The HRD is the dose (in mg/kg bodyweight) which is assessed as not causing any effects on the exposed individual on life long exposure.
You can usually not find HRD values in the literature and this value is thus determined by the equation:

HRD=Lowest relevant and reliable toxicity data found / Assessment Factor

By the calculation of effect factors for ecotoxicity the *"Predicted No Effect Concentration"* (PNEC) is the value that needs to be derived. PNEC is the concentration of a substance in the environment expected not to cause ecotoxicological effects. The PNEC is determined from the equation:

PNEC=Lowest available toxicity data found / Assessment Factor
Assessment factors are applied in the EDIP Methodology in order to compensate for the quality and the relevance of the toxicity data available. For human toxicity the values derived are based on LD50 or LC50 and for such data the EDIP methodology sets a high assessment factor of 100.000. For ecotoxicity the EDIP Methodology operates with one assessment factor for chronic ecotoxicity and another for acute ecotoxicity:

• For chronic ecotoxicity the assessment factor is set to 100 as the values extracted from the risk-phrases fall in the category "Data for acute ecotoxicity (EC50) available for at least one species from each of the classes fish, crustacea and algae".

• For acute ecotoxicity the assessment factor is set to 10 as the values extracted from the risk-phrases fall in the category "Data for acute ecotoxicity (EC50) available for at least one species from each of the classes fish, crustacea and algae". It is thus the same data that is

applied to calculate effect factors for acute and chronic ecotoxicity. The only difference is the assessment factor.

As the criteria for the risk-phrases relevant to ecotoxicity are based on ecotoxicity data of higher quality and relevance than those for human toxicity, the applied assessment factors are considerably lower than for human toxicity. This indicates that the calculated assessment factors for ecotoxicity are less uncertain than those for human toxicity.

Ole Willum concludes that the highest degree of uncertainty by the calculation of effect factors is related to the toxicity data. The uncertainty is higher for human toxicity than for ecotoxicity. This conclusion is considered to be true for both the risk-phrase method and the method based on individual data.
The notes "Comments on data quality" should be studied carefully and taken into consideration when assessing the results of the LCA in question and the importance of an uncertainty should be uncovered by the sensitivity analysis. If you need to narrow the interval of uncertainty it is recommended to search for specific toxicity data for the particular substances and recalculate the effect factor by using "Calculation of effect factors based on individual data" model 2. In this case the calculator will apply physical/chemical data for the specified substance from the database with 28.033 substances and your individual toxicity data.

To calculate human toxicity indicators from the factors the following formula is used:

$$\text{Human toxicity}_r = \sum_i \sum_{ecomp} m_{i,ecomp} * HTP_{i,ecomp,r}$$

$m_{i,ecomp}$ the emission of substance *i* to compartment *ecomp*

The ecotoxicity indicators are calculated:

$$\text{Ecotoxicity} = \sum_i \sum_{ecomp} m_{i,ecomp} * \text{characterisation factor}$$

The characterisation factors in the database are given in the unit m^3/g (Willum 2006).

5.12 Model defaults - Toxicological assessment of metals

There are problems with the toxicological assessment models. An investigation, comparing five different methods available to perform ecotoxicological impact assessment for metals, highlights this. Two different cradle-to-gate case studies were selected and examined by applying different freshwater ecological toxicity impact models (Uses-LCA, Ecoindicator 99, IMPACT 2002, EDIP 97 and CalTOX-ETP). The result of the investigation showed that there were several procedural difficulties and that the results were inconsistent, there was a big variation of results between the different methods applied. The authors concluded that the investigation illustrates the need to proceed with caution when applying LCIA ecotox methodologies to life cycle studies that include metals. Until further improvements are made the deficiencies should be clearly communicated as part of the LCIA reporting. Business and policy decisions should not without further discussion be based solely on the results of the currently available methods for assessing ecotoxicity in LCIA.

The result, that there are deficiencies in the LCIA ecotox methods are further supported by the participants at the Apeldoorn Workshop (April 15th, 2004, Apeldoorn, NL) where specialists in LCA and Risk Assessment discussed current practices and complications of the LCIA ecological toxicity methodologies for metals. The consensus of the workshop was that LCIA ecotox methods currently available do not appropriately characterize potential impacts of metals due to lack of fundamental metals chemistry in the models (Gloria et al. 2006).

Toxicological assessment of metals – ion and elementary metal

CAS, Chemical Abstracts Service, registers unique chemical substances. CAS registers a. o. specific alloys, ions, isotopes and elementary particles, so it is clear that elements and ions have different CAS numbers (CAS 2006). This is verified by a search on Chromium in the Swedish database "Ämnesregistret" (register of substances), a database from "Kemikalieinspektionen", a Swedish authority informing about chemicals. Chromium metal has CAS number 7440-47-3 and Chromium (VI) ion has CAS number 18540-29-9.

Chromium (VI) ion 18540-29-9 does not exist in the database Chemical substances, used at the Environment and Product safety department at SCA Personal Care. In this database, no ions are included. In the toxicological information of Chromium 7440-47-3 it is said that the Chromium (VI) salts can cause cancer and allergy. In the toxicological information of Copper 7440-50-8 it is written in parenthesis that the ecotox values for algae are valid for free copper ions. It seems that there is one common toxicity value for both the elemental and the ion form of a substance. Probably this is due to a substance's shifting between these to forms.

A further indication that ions and elements are not treated separately in toxicological assessment is the different nomenclature used in different data bases. Sometimes the transfer of a dataset between different data bases imply a change in nomenclature, this translation sometimes include changes of ions to elements.

5.13 Discussion of suitable methods for toxicological assessment at SCA Personal Care

The EDIP method is fundamentally diverging from OMNIITOX and USES-LCA since the inputs to the model is not encountered at a cardinal scale, a continual numerical scale with indefinite accuracy. In the EDIP method the data is classified into groups representing a numerical interval. Each group is given a score, a value on a non-continual scale with fixed values e g 0.2, 0.5, 1. The EDIP method has been criticized for this methodology, with the argument that the method is not consistent with the reality. In the reality processes are of cardinal nature. The OMNIITOX and USES-LCA models have input data on cardinal scales. These models are trying to assess toxicological impacts values as correct as possible by using methods that are similar to the reality. The typical substance for these models is a non-polar organic substance, average sized. These models were ultimately developed to handle emissions of substances similar to the typical substance. The USES-LCA method has been criticized for its assessment of metals. Metals are fundamentally different from the organic typical substance, for example metals are un-degradable per definition. Metals do not follow the pattern the method developers had in mind when they were evolving the method. As they

do not fit in the model the assessment of metals has been misleading. Another group of substances that diverge from the typical substance is amphiphilic substances. Within the OMNIITOX project ideas were formulated on how to handle these two substance groups. Metals are handled in a different way from organic substances, and processes that take away active metals are included in the model for assessment of metals. Unfortunately time was not enough which had the consequence that all ideas were not implemented in the model. EDIP uses a simple toxicity estimation and therefore the toxicological assessment of metals is not a big problem in this model.

There is agreement that chemical ranking and scoring should be used only for a screening level assessment, to identify substances that require more detailed evaluation in an LCA study (Hertwich et al. 2002. s. 106).

A site specific characterisation of toxic emissions in LCA requires knowledge of the release site or region and its characteristics. Most LCAs today lack information on the release site, at least for some of the processes in the life cycle. Even if it is possible to characterise all the release sites, it may be too expensive and the variations associated with releases at different regions may negate each other's effect, to yield predictions similar to those of the generic models. To justify the additional effort of a site-specific approach, significant variation in exposure and /or effect must exist and information on these variations must be available. If the differences from site to site are small or difficult to characterise, the gains of information from considering the release site will be too small to justify the effort (Hertwich et al. 2002. s. 117).

5.14 Results of the investigation of models for toxicological assessment

The OMNIITOX models are data demanding and too advanced for the purpose; toxicological assessment at SCA Personal Care. Ecopoints has a big disadvantage in that it is based on political targets that vary over time and space. Using that method would cause a lot of extra work since the products' lifecycles mean emission all over the world. Concerning the FhIUCT method the first tire has problem with its assessment of metals and the second tire is not operational. The first tire is a screening method, it is too simplified to be a good TA method.

USES-LCA is unnecessary advanced, it would be demanding to work with such a high detail level. A simpler model is to be preferred. Regarding GLOBOX, there is no need for spatially differentiated characterisation factors. Site- specific characterisation would imply a lot of more work and a great data demand.

EDIP is a simple and well documented fate, exposure and effect model. It uses a simple methodology that is easy to understand and practice. It is a quite old method, used a lot and acknowledged as a TA method. The risk-phrase method Simple estimation is using a simple methodology and it is well documented, but it is connected with a big uncertainty, especially for substances that lack risk-phrases relevant for human- or ecotoxicology. The advantage is that it is easy to calculate characterisation factors according this method, there are already a lot of characterisation factors calculated. It is though a screening method and it should not be used solely as a TA method because the result would be accomplished with a big uncertainty and would not be reliable.

6 Case study

The case study shows how the toxicological assessment appears in a real LCA situation, a comparing LCA of two diapers. In order to narrow the extent of the case study some limitations have been done. The case study does not cover the whole life cycles of the diapers, it is limited to comprise cradle to gate analysis of some materials included in the diapers; elastic film, super absorbants and pulp. These three materials were chosen since the biggest differences between the two diapers lie in their contents of these materials.

The case study does not comprise a whole life cycle scenario since that would be too time consuming for this project. Manufacture of products is not included. The manufacture of hygiene products in the converter factory does not imply any other toxic emissions than emissions associated with usage of electricity. The use phase of the hygiene products does not have any environmental impact. Emissions from consumer waste are not included in the case study since the model used at SCA Personal Care to calculate these emissions is under reconstruction.

"The most effective way to improve the environmental performance for converters is to minimize or substitute input raw material and/or make their retailers aware of there role" (IFEU 2004).

6.1 Inventory: potentially toxic substances

To be able to answer the question if toxicological assessment should be included in the life cycle assessment at SCA Personal Care an inventory of flows of potentially toxic substances in the lifecycles of the products manufactured by SCA is made. The inventory comprises the three materials in the case study. The inventory includes:

- Study on the data in the LCA data base at the company.
- Investigation of data sources to the data in the LCA data base.
- Investigation of possibilities to get more accurate and complete data.
- Establishment of inventory reports of the emissions from the crade to gate LCAs of elastic film, super absorbents and pulp respectively.

Inventory reports of emitted substances from the cradle to gate LCAs of elastic film, super absorbants and pulp respectively are established. Emissions of radioactive substances reported as kBq was excluded from the inventory. The toxicological assessment methods do not handle this sort of emissions.

6.1.1 Elastic film

Data is taken from the LCA database Ecolab at SCA Personal Care environmental department. Data sources for the emission data are Plastics Europe and the data sources presented below for electricity and transport. The Plastics Europe data for elastic film in Ecolab was a rounded version where substance flows smaller than 1 mg per kg elastic film produced were not specified. As toxicological assessment often deals with small emission flows, many substance flows relevant to toxicity is not included in that version. Therefore the Plastics Europe data was exchanged for un-rounded Plastics Europe data sets (Plastics Europe, Ecoprofiles). An inventory report on production of elastic film was thereafter made in Ecolab.

6.1.2 Super absorbents

EDANA, the European Disposables and Nonwovens Association, has done life cycle assessment of materials used in diapers, among others super absorbents (SAP). The result of the LCA on SAP is available in the report *Life cycle data for incontinence products* (IFEU 2004). The results are presented in two versions, a shorter one including key parameters and a comprehensive non aggregated one including more flows. In Ecolab the shorter one is used, since it include relevant data for doing company standards life cycle assessments. Emissions relevant to the impact category toxicity are presented in the comprehensive version, therefore that one is used in the inventory.

6.1.3 Chemical pulp

The chemical pulp that is bought and used in the SCA Personal Care factories is fluff pulp made in Kraft pulp mills.

In the Kraft process the fibres are liberated in the cooking plant by dissolving the lignin and part of the hemicellulose in the cooking chemical solution (white liquor), which contains sodium hydroxide and sodium sulphide as active chemicals. (IPPC 2001. s. 17) The pulp industry is indeed using a lot of chemicals. For example it is stated in the Skutskär mill environmental report 2005 that the total amount chemicals used is 369 kg /ton pulp produced, fuels included (Stora Enso 2005).

Polychlorinated dibenzo-p-dioxins (PCDDs) and polychlorinated dibenzo-p-furans (PCDFs) have been identified in emissions from the pulp industry. They have been detected in stack gases from the burning of condensed black liquor. PCDDs and PCDFs are also produced during pulp bleaching with elemental chlorine (Murray 1992). Because of the problems of producing dioxins and furans most pulp and paper mills have changed bleaching agent from elemental chlorine to chlorine dioxide from which the dioxin and furan output is much smaller, even undetectable in many cases (Baird & Cann 2005, s. 377).

Data concerning production of chemical pulp is data from pulp supplier questionnaires.

LCA data of the chemicals used in the pulp production is taken from different LCA data bases and LCAs performed by different organisations, for example Plastics Europe and EDANA (see 7.2). Data concerning electricity and transports is taken from other sources (see 7.2).

There may be more data available than are asked for in the supplier questionnaires of SCA Personal Care. Some suppliers have given data not asked for in the questionnaires. The comparison between data from the different paper mills shows a big difference in production chemicals but also in the emissions stated. Lack of data can be due to that some emissions are not measured or that the data is not supplied because it is not inquired by SCA. If TA will be implemented the supplier questionnaires should also ask for data on emissions of chelators EDTA/DTPA, chlorate, VOC and PAH.

6.2 Inventory: data sources

To perform LCAs, a lot of data is needed. SCA Personal Care uses site specific data from their own production and from their suppliers. The supplier data is collected through supplier environmental questionnaires. To get data from the whole life cycles of the products produced other data sources are also needed. LCA data bases and LCAs made by different organisations are used.

6.2.1 Electricity data

Electricity data is an intrinsic chapter. First, the amount of electricity used is needed. Second, data according emissions from different types of electricity production are needed. Third, data concerning different electricity mixes being used in different parts of the world are needed.

Emissions from electricity production
Figures are available in the LCA database SPINE, started by CPM. CPM, a Competence Centre for Environmental Assessment of Product and Material Systems was established at Chalmers University of Technology in Gothenburg, Sweden in 1996. Reported figures are based on a combination of data from a LCI-study performed at ETH, Zürich and Paul Scherrer Institut, Villigen, ''Ökoinventare von Energiesystemen'', 3rd edition 1996 and of data from a LCI-study performed at Vattenfall AB, Life-cycle Assessment for Vattenfall's Electricity Generation, 1996 and adapted to the demands of the EPD-guidelines (Environmental Product Declaration guidelines in Sweden).

Data about the fuel chain i.e. fuel production and transports of fuel have been acquired from ETH and data about power plant operation has been provided by Vattenfall's study. Only the operation emissions to air of the studied plant and the amounts of ashes generated are included in Vattenfall's set of figures. ETH's LCI-results comprise all parameters received during inventory and calculation, i.e. no selection has been made by ETH.

The purpose of the ETH study was to examine a number of energy systems quantitatively and to the same extent with respect to environmental issues during their life cycles. The results

can be used in life cycle assessments, as basis information in decision-making regarding environmental optimisation or in working with municipal energy plans.

Vattenfall's purpose with LCA for their electricity generation was to provide customers with data about the environmental impact of the electricity they buy, to create a basis for comparisons between energy systems and for decisions about future energy systems.

Vattenfalls purpose - as a commissioner of putting ETH:s data (and in this case also Vattenfall's data) into Spine format with metadata - is to supply EPD-practitioners with general LCA-data for electricity generation to be used in absence of specific data in accordance with the directions of Miljöstyrningsrådet (The Swedish Environmental Management Council) and the Swedish EPD-guidelines. Data is supposed to be used together with IEA statistics about electricity generation mixes in the OECD countries/regions. (SPINE)

Electricity mixes
Datasource is Energy statistics of OECD countries, a publication from International Energy Agency, IEA. The data is based on information provided in annual OECD questionnaires completed by the national administration of the OECD member countries (IEA statistics 2006). The OECD (Organisation for Economic Co-operation and Development) groups 30 member countries sharing a commitment to democratic government and the market economy (OECD).

The International Energy Agency (IEA) acts as energy policy advisor to 26 member countries in their effort to ensure reliable, affordable and clean energy for their citizens. Founded during the oil crisis of 1973-74, the IEA's initial role was to co-ordinate measures in times of oil supply emergencies. As energy markets have changed, so has the IEA. Its mandate has broadened to incorporate the "Three E's" of balanced energy policy making: energy security, economic development and environmental sustainability. Current work focuses on climate change policies, market reform, energy technology collaboration and outreach to the rest of the world, especially major producers and consumers of energy like China, India, Russia and the OPEC countries. With a staff of around 150, mainly energy experts and statisticians from its member countries, the IEA conducts a broad programme of energy research, data compilation, publications and public dissemination of the latest energy policy analysis and recommendations on good practices. (IEA)

6.2.2 Transport data

Emission data, emission from different types of vehicles, is taken from the Swedish organisation NTM, the Network for Transports and the Environment (in Swedish: Nätverket för Transporter och Miljön). NTM is a non-profit organisation, founded 1993 to work for common bases of calculation of the environmental impact of transport. NTM offer method for calculation of emissions from transports, up to date environmental data and tools for evaluation of suppliers.

Energy use and emissions refer to the transportation of 1 ton goods 1 kilometre for an utilisation level of 50% for delivery vans and medium-sized lorries in local distribution traffic and 70 % for long distance transport with heavy trucks. An utilisation level of 70 % is considered to be representative for Swedish domestic long-distance traffic if empty trips are

not included. Only regulated emissions to air are included. The parameters that are presented are:
-regulated emissions for diesel engines: NOx, HC, particles and CO
-fuel regulated SO2
-tax regulated CO2

Data have been put together for NTM by a group of manufacturers and hauliers, i.e. Volvo, Scania, BTL, ASG, Swedish Hauliers Association (NTM 2005).

The data presentation is suitable for LCA purposes. SCA has recalculated the data to fit their products, since they are bulky with relatively low weight.

6.2.3 Plastics Europe

Plastics Europe assembles detailed environmental data on the processes operated by its member companies with the intention of making the information available for public use.
The organisation aims at placing robust data in the public domain to meet the external demand for such information for use in product life-cycle studies. Since this must be done without compromising the need of companies to keep confidential their own data on quantities of energy and raw materials used in their processes, industry averages are produced. One of the objectives of the Plastics Europe Eco-profile work is to facilitate internal company benchmarking that can lead to a reduction in environmental impact (Plastics Europe).

The bases of all eco-profile studies are data collected from the participating companies for the performance characteristics of their plants. Most of the information that is supplied is derived from the records that are already kept by companies and plants. Few companies have the resources available to carry out new measurements on their plants. Plastics Europe regard that this does not usually pose any serious problems since the monitoring of most plants in the industrialised world is sufficiently detailed to allow the extraction from existing records of the information needed for eco-profile calculations. But they state that it is still difficult to obtain reliable primary data for air and water emissions. Usually organisations monitor air and water emissions as concentrations because this is the way that the statutory limits, with which they must comply, are expressed. However, in eco-profile studies, information is needed on the total mass of each emission per unit output of product and this is seldom measured. However there is a trend within industry as a whole to report total emissions per time period so in future the data needed for eco-profile analysis should be more readily available. The situation is further complicated by the complex structure of many industrial plants. An industrial plant often produces a number of products simultaneously, and different plants can share common facilities, for example water treatment plants (Boustead 2005).

Since the original Eco-profile reports were issued, many technological and commercial changes have taken place within the industry, and some plants have been upgraded whilst others have closed. Much new technology has been implemented and the fuel infrastructure in many countries has changed; for example, moves away from coal to cleaner burning gas fuels. The quality of data reporting by companies has improved as a consequence of benchmarking programmes and more factual information has become available. These changes have

combined to render the data in the earlier reports less representative of the polymers manufactured and marketed today. Therefore are the eco profiles updated (Plastics Europe).

6.2.4 EDANA the European Disposables and Nonwovens Association

In 2001 the trade association of EDANA started life cycle analysis project on incontinence products. Life cycle analysis of materials used in diapers, among others super absorbants, were done. Questionnaires were delivered to seven companies converting incontinence products and to 57 companies supplying the raw materials. Each participant of the EDANA incontinence product LCA has been asked to fill in the requested data as far as those data are available and relevant concerning the process.

Information of main input/output flows, transports, electricity demand, heat demand, process water demand, flue gas from process - combustion and waste respectively are collected. Waste should be specified concerning type, mass and way of disposal or recovery. Inventory data shall be given as yearly averages and be representative for the production. Factory buildings and infra structure is not included in the life cycle.

In the LCA, processes and activities that together are not considered to contribute more than 1 % to each environmental impact category are cut-off.

According grid electricity usage, country specific data is used. Different partition of electricity generation systems in different countries is taken into account. Data concerning electricity is taken from ETH (see 6.2.1). Emission data from transports is taken from NTM.

It is stated that generic plastics data is taken from APME, Association of Plastics Manufacturer in Europe (present Plastics Europe) and packaging data from FEFCO (European Corrugated Packaging Association), www.fefco.org.

Since permanent technological progress is made the basic data of the processes involved in producing a diaper is changing. Environmental improvements of production related resource use and emissions is made, as well as for auxiliary processes like transportation and energy generation. As a consequence an update of the basic data sets could lead to quite important changes (IFEU 2004).

6.3 Toxicological assessment

The toxicological assessment is carried out on production of elastic film. The data set on production of elastic film that is used originates from Plastics Europe. The TA is carried out on a half year usage of a specific diaper, this functional unit is often used in the LCAs made at SCA Personal Care.

Methods applied are the EDIP method and Simple estimation of effect factors for toxicity used for screening LCA, a method based on the EDIP methodology but which uses risk phrases as toxicity information.

The methods are applied to the inventory report of elastic film. The toxicity impacts are expressed in m^3 of air, water or soil into which the emission should be diluted for its concentration to be so low that no toxicological effects could be expected.

6.4 Results of the case study

Toxicity would be an interesting aspect in the comparing LCAs. The study does not show that some toxic substances have to be supervised because of their relatively big impact. But if recommendations on LCA practice should be followed toxicity should be included as an impact category to fulfil the requirement completeness. The list of impact categories should cover all environmental problems of relevance. Inclusion of toxicity as an impact category would mean five impact categories in the LCAs:

- Global warming
- Acidification
- Aquatic oxygen depletion
- Photochemical ozone creation
- Toxicity

Substances relevant to the impact category toxicity are among others heavy metals, chloro-organic substances, Polynuclear Aromatic Compounds (PAH) , carcinogenic substances and substances that affect hormonal status. Emissions of these substances are not accounted for in the other impact categories.

Toxicological assessment performed with the EDIP methodology ends up in six different categories; Human toxicity with the exposure routes air, water and soil respectively and ecotoxicity water chronic, water acute and soil.

Different data bases use different names on the same substance. For the practicality it is important to have *one* name for a substance in Ecolab. For the already calculated characterisation factors in the EDIP method and the risk-phrase method the substances are specified with both name and CAS number. When searching already calculated characterisation factors you use CAS numbers.

Groups of substances, like PAH, are often encountered in the datasets. Within these groups are different substances with different toxicity and consequently different characterisation factors. Often it is not known which substances the emission refers to, but in some cases it is specified. One way to handle the groups is to use characterisation factors for the substance within the group having the largest toxicity. In this case the cautious principal is used; the values represent a worst case.

There are a lot of substances lacking already made characterisation factors. There are different ways to handle these substances. Characterisation factors can be calculated, a characterisation factor for another very similar substance can be chosen or the substance can be excluded from the assessment.

Characterisation factors was found for 69 (EDIP) resp. 74 (the risk-phrase method) flows in the data set of emissions from production of elastic film. More than 60% of the characterisation factors of the risk-phrase method used in the TA had data quality notion 1. This notion means that no risk-phrase related to human toxicity was assigned to this substance and a toxicity value corresponding to the lower end of the criteria for risk-phrase R22 was used to calculate effect factor for human toxicity.

The characterisation factors of the risk-phrase method has a big uncertain interval, therefore it is not interesting to compare the sizes of the impact between the EDIP and the risk-phrase method. The relative ranking order is interesting though. There is fairly good agreement about which substances having significant impact. A noteworthy discrepancy is the assessment of mercury emissions (see appendix 3).

The emissions contributing the most to the impact category toxicity are presented in the annex with confidential data, belonging to SCA Personal Care.

6.5 Interpretation of the results

Toxicological assessment in LCA is an environmental analysis tool to reduce emissions of potentially toxic substances. Substances that are ranked high in the result, i.e. have highest influence on the impact category toxicity, should be paid special attention. Effort of reducing emissions should be made on these substances.

The impact category toxicity functions as the other environmental impact categories in the LCA. It shows which substances that contribute most to the impact category and it shows differences in impact between different products in a comparing LCA.

For toxicity, there is often a threshold value where toxicological effects occur. Most often this is not accounted for in the models. It is difficult to measure or predict. But there is also reason to count all flows regardless size at the emission site, since background concentrations are not accounted for in the model. Toxicity can occur as a consequence of an emission regardless size, since it can be summed with emissions from other sources. That is why potential toxicity is calculated in the toxicological assessment models.

Toxicological assessment performed with the EDIP methodology ends up in six different categories; Human toxicity with the exposure routes air, water and soil respectively and ecotoxicity water chronic, water acute and soil. All these categories are relevant as different substances have different properties and have their effect through different mechanisms. I recommend that each one is compared independently in the comparing LCA. The results, percentages showing the increase or decrease of impact to the categories in relation to the reference product, can not be summed up resulting in one figure. A 2 % decrease in impact for one tox category does not correspond to a 2 % decrease in impact for another tox category. Partly, because the categories are expressed at different scales, m^3 of air, water and soil. Partly, because the impacts to the different categories expressed at same scale can be of different magnitude, a 10% decrease can be from 1000 to 100 but it can also be from 100 to 10. A reduced toxicity impact of great magnitude is of course more valuable for the environment. Comparisons between the different impact categories are obviously not easy.

6 categories for toxicity in the LCA are not desirable. In the LCAs at SCA Personal Care there is currently one effect category for each environmental problem. From a logical point of view it should be one impact category also for toxicity. As the different impact categories for toxicity in the EDIP method can not be summed, the only way to reduce impact categories is to exclude some. It seem reasonable to suggest that the impact categories for toxicity in a comparing LCA would came out with the same result about which product having the least impact to toxicity. But it does not have to be that way.

I would recommend using the category Ecotoxicity water chronic in the comparing LCA. It is easier to find toxicity data to this category than the others and the data is relevant, it does not have to be a big extrapolation. Moreover it includes a long time perspective which means that degradation mechanisms and bioaccumulation are considered. But if the TA would solely rely on eco tox water chronic, substances that end up in the air compartment would not be included in the impact calculation. This is true since the eco tox calculation according the EDIP method only comprise the final compartments water and soil. An illustrative example is the carcinogenic substance benzo(a)pyren, an air emission of this substance stays in the air compartment. The EDIP characterisation factors for air emissions of benzo(a)pyren are zero, unless for human toxicity air. For human toxicity air the characterisation factor is $5\ 10^7$ m^3/g, which means that $5\ 10^7$ m^3 air is needed to dilute an air emission of 1 g benzo(a)pyren to a non hazardous concentration. To include impact from toxic substances that ends up in the air compartment human toxicity air has to be included in the LCA.

7 Discussion concerning relevance of implementation of toxicological assessment

The strength with LCA is its ability to show the entirety. LCA can be used to get a total overview of the company's environmental impact. Substances relevant for the impact category toxicity will be added to the LCA database if toxicological assessment is implemented. In this way there will be a more complete view of the life cycles. Since the life cycles with associated substances are established to show environmental impact of the products, substances hazardous to the environment should be present. Therefore it is to be regretted to leave out substances that are toxic.

Toxicological assessment is a good instrument to keep an eye on chemical substances in the lifecycles of products. It is interesting from an internal company view to have a good documentation of hazardous substances appearing in the life cycles and their environmental impact. TA would be a good incentive for use of easy degradable substances with low toxicity and with low tendency to bio-accumulate.

The LCA work is also an instrument to catch up on suppliers. To get a trustworthy comparison between products and suppliers it is important to have a complete view of the negative environmental impacts caused by the suppliers' activities. Often you don't know more than you ask for. Inputs and outputs of toxic substances in the steps in the products life cycle is important information. Information needed to be able to say that a company do not use this and that in the production of their products.

For most companies, as for SCA, there is a product safety department whose responsibility is to secure that the products are safe to use. Their task is to secure that hazardous substances, not acceptable to be present in the products according different directives, are not present in the products produced. The safety department is not securing that toxic substances are not used at the process level. Toxicological assessment shows the presence of toxic substances throughout the whole life cycle of the product and it is a valuable tool for straight forward work for use of more harmless substances and in the extension, production of more environmentally friendly products.

Then there is the consumer perspective. As long as there are people that worry about chemical substances in the products and their life cycles there are an incentive for assessment of toxic substances. If there is knowledge about which substances appear and to which extent, the worried voices can be answered with facts and that is something really important for the company and its ability to survive and be a large, important company also in the future. Consumers get more and more conscious of environmental concerns and become more likely to use their power in their choice of products. A mistake can be expensive, negative publication spread rapidly and sales figures can fall dramatically fast. This is especially important in this business where the companies are sensitive for the powers of the market economy.

Against all these advantages stands the cost. To benefit from implementation of toxicological assessment it is crucial to have a simple administration of the TA

8 Discussion

There is a need for a common LCIA nomenclature. The present toxicological assessment methods use different names for the same thing, which is very confusing and makes it hard to compare different models.

Since SCA Personal Care is converters, it is hard to get detailed data since they have to rely on data from sources outside the company. There are data from suppliers and there are data from other type of sources, e.g. LCA studies performed by organisations. It is important to use up to date values in the inventory and the LCAs, because technical changes often affect environmental impact. It could be useful to let an LCA data base used for toxicological assessment comprise CAS numbers.

You should keep in mind, when analysing the results that the inventory and the toxicological assessment are done in a limited case study. The inventory showed that there are sufficient data to be able to do a reliable toxicological assessment. That conclusion is only valid for production of the three materials included in the inventory.

To get a better inventory, transport data comprising toxic emissions should be collected. This is not easily done, since the data has to be applicable for LCA use. Transport data is today taken from NTM (see 6.2.2). This data is ready to use since it is adopted for LCA use.

A complicated model is not a good help searching a fairly good estimate of environmental impact. The idea of doing a model is often to do a simplification of something. When you try to do it more and more precise and accurate, more alike the reality, it becomes more intrinsic and less clear. It also gets more data demanding, which often is a big disadvantage. If more data is needed to calculate flows in the model, the model gets less user-friendly and it becomes time consuming to use. Another strength with a simple and well documented model is that lacking characterisation factors can be calculated by the LCA practitioner. In addition it is more easy done to calculate characterisation factors for groups of substances (eg PAH) and mixtures of substances (eg oil) if an easy model is used for the calculation. It becomes easier to do reasonable estimations and get a value.

Emissions of metals constitute a significant group of emissions that contribute to the impact category toxicology. Therefore it is a serious problem that current methods for toxicological assessment have been criticised for how they handle toxicological assessment of metals. It is evident that further research on toxicological assessment of metals is needed. EDIP uses a simple toxicity estimation and therefore the assessments of metals is not a big problem in this model.

For ecotoxicity, there are more relevant data available than for human toxicity where there is a bigger extrapolation. Because of the big extrapolation there are big assessment factors. This means that the human toxicity characterisation factors are more uncertain than the ones for ecotoxicity.

The two different methods applied in the toxicological assessment had characterisation factors for quite the same number of flows in the inventory list. This was a little bit surprising as there are a lot more calculated characterisation factors for the risk phrase method than for the EDIP method. The lack of relevant risk-phrases assigned to many of the substances makes a

big problem for the risk-phrase method. Toxicity values that are guesses make not a good base for a serious toxicological assessment. The big uncertainty connected to the result of the TA using the risk-phrase method render the result of the assessment less interesting, as it is not trustworthy.

Toxicological assessment can be used to reduce flows of potentially toxic substances in a company's production. Implementation of toxicological assessment in the LCA practice means one further impact category to consider in the evaluation of the environmental impact of two different products. In the evaluation of environmental impact of different products all parameters in the LCA are considered. It is not possible to compare different impact categories with each other. The different impacts are not on the same scale. You may consider some environmental problems more relevant than others. This sort of evaluation between impact categories is a subjective step.

9 Conclusion

I would recommend using a simple screening method to investigate which substances that have noteworthy impacts on the impact category Toxicity. Later, when doing a toxicological assessment on those substances a more reliable method should be applied. I recommend EDIP. It is an advantageous method; well developed, simple, easy to use and well documented. EDIP includes a screening method that can be applied. Another alternative is to use the method "simple estimation of effect factors for toxicity used for screening LCA" for the screening. It is though important that the toxicological assessment can be carried out easily. Otherwise it will be too expensive to have toxicological assessment as an integrated part in the LCA practice.

References

Baird C. & Cann M. (2005) *Environmental chemistry*. 3rd ed. New York: W.H. Freeman and Company.

Baumann H.& Tillman A-M. (2004). *The Hitch Hiker's Guide to LCA*. Lund: Studentlitteratur.

Baumann H. & Rex E. (2004). *Expanding the green practice of LCA: The first decade of life cycle assessment activity in the Swedish forest product industry*. Göteborg: Chalmers University of technology. (CPM-report 2004-1)

Boustead I. (March 2005) *Methodology -Ecoprofiles of the European Plastics Industry*. Brussels: Plastics Europe. <http://www.plasticseurope.org/content/default.asp?PageID=392#> (2006-11-08)

CAS Registration criteria overview. <www.cas.org/Support/regcriteria.pdf > (2006-11-13)

de Koning A., Guinée J., Pennington D., Sleeswijk A., Hauschild M., Molander S., Nyström B., Pant R. & Schowanek D. (2002). *OMNIITOX –inventory and classification of LCA characterisation methods for assessing toxic releases*.(OMNIITOX project: D11 part A) <www.omniitox.net/results>

Effect Factor Calculator -calculation tool in MS Access format (last modified 2005-11-30) <www.norden.org/pub/sk/showpub.asp?pubnr=2006:549>

Effect Factors calculated for 23.029 substances based on toxicity data derived from risk-phrases in MS Excel format. <www.norden.org/pub/sk/showpub.asp?pubnr=2006:549>

Gloria TP., Russell AJ., Atherton J., Baker SR. & Cook M. (2006) Ecological Toxicity Methods and Metals. *The international journal of Life Cycle Assessment*, vol. 11: 1, ss. 26-33.

Hemond HF. & Fechner-Levy EJ. (2000) *Chemical fate and transport in the environment*. 2nd ed. San Diego: Academic press.

Hertwich EG., Jolliet O., Pennington DW., Hauschild M., Schulze C., Krewitt W., Huijbregts M. (2002) Fate and exposure assessment in the life-cycle impact assessment of toxic chemicals. In Udo de Haes HA. et al. *Life-cycle impact assessment: Striving towards best practice*. Brussels: SETAC press.

Huijbregts M. (2006) Multimedia toxic pollutants: Toxic equivalency factors for multimedia pollutants. Radboud University Nijmegen: Department of environmental studies. <http://www.ru.nl/environmentalscience/research/life_cycle/multimedia_toxic/>

Huijbregts M., Struijs J., Goedkoop M., Heijungs R., Hendriks J. & van de Meent D. (2005) Human population intake fractions and environmental fate factors of toxic pollutants in

life cycle impact assessment. *Chemosphere* 61 (2005), ss. 1495-1504 <http://www.ru.nl/environmentalscience/research/life_cycle/multimedia_toxic/>/ useslca_fate_extern.zip

International Energy Agency, IEA <http://www.iea.org/Textbase/about/index.htm> (2006-10-16)

IEA statistics (2006). *Energy statistics of OECD countries 2003-2004*, IEA International Energy Agency

IFEU (Institut für Energie und Umweltforschung) (March 2004). *Life Cycle Data for Incontinence Products: Data Report for the EDANA Communication Project*. Heidelberg: IFEU

IMI OMNIITOX project site (last updated 2005-07-07). <http://www.imi.chalmers.se/Projects/Finalised/OMNIITOX/default.htm> (2006-10-01)

Integrated pollution prevention and control (IPPC) (December 2001). *Reference document on best available techniques in the pulp and paper industry.* European commission.

Landis WG. & Yu MH. (1999) *Introduction to environmental toxicology: Impacts of chemicals upon ecological systems*. 2nd ed. Boca Raton, Fla: Lewis publishers

LCA-center <www.lca-center.dk>/ LCA Software (2007-01-11)

LCA-center <www.lca-center.dk>/ LCA Data/ EDIP Factors (2007-01-11)

McKone TE., Kyle AD., Jolliet O., Olsen SI. & Hauschild M. (2006) Dose-Response Modelling for Life Cycle Impact Assessment. *The international journal of Life Cycle Assessment*, vol 11: 2, ss. 137-140.

Molander S. (2002) *Refined problem definition for the OMNIITOX project*. Göteborg: Chalmers University of technology. (OMNIITOX project: D8) <www.omniitox.net/results> (2006-09-19)

Murray W. (1992). *Pulp and paper: the reduction of toxic effluents*. Government of Canada: Science and Technology Division. (BP-292E) <http://dsp-psd.pwgsc.gc.ca/Collection-R/LoPBdP/BP/bp292-e.htm> (2006-09-21)

Nätverket för Transporter och Miljön, NTM (last updated 2005-09-07) <http://www.ntm.a.se/index.asp>/ Om NTM (2006-10-16)

OECD <http://www.oecd.org/about/> (2006-10-16)

OMNIITOX Information System (IS) <http://omniitox.imi.chalmers.se/> (2006-10-06)

OMNIITOX project website <http://omniitox.imi.chalmers.se/OfficialMirror/default.htm> (2006-10-01)

Plastics Europe <www.plasticseurope.org> (2006-11-08)

Plastics Europe. Ecoprofiles of the European plastics industry. <www.plasticseurope.org>/ Plastics and environment/ Eco-profiles/ the Eco-profile reports

Rosenbaum R. (2005) *Short overview of the interpretation of intermediate and final results produced by the system*. http://omniitox.imi.chalmers.se/documents/short_overview.htm

Spak B. (2006) *LCA: Product ecology discussion concerning incontinence product X*. Göteborg: SCA Personal Care.

SPINE@CPM CPM member access database < http://databases.imi.chalmers.se/> (2006-10-16)

Stora Enso (2005) *EMAS miljöredovisning 2005 Skutskärs Bruk*. Skutskär: Stora Enso publication paper.

The Danish EPA (miljøstyrelsen) <http://www.mst.dk/activi/08020000.htm>

Wegener Sleeswijk A. (2005) GLOBOX. Leiden University: Institute of Environmental Sciences (CML) <http://www.leidenuniv.nl/cml/ssp/software/globox/index.html>

Wenzel H., Hauschild M. & Alting L. (1997) *Environmental Assessment of products*. 1st ed. London: Chapman & Hall.

Willum O. *Simple estimation of effect factors for toxicity used for screening LCA*. (2006) Copenhagen: norden. (TemaNord 2006:549) <www.norden.org/pub/sk/showpub.asp?pubnr=2006:549> (2006-10-26)

Appendix 1

The OMNIITOX project: Minimum requirement list of substance properties

Minimum requirement list for Base and Simple Base model.

SUBSTANCE PROPERTY PARAMETERS for SBM ECOTOX factors
(Only valid for substances classified as "other")

Mechanism parameter	Unit	Code	Description
Henry's law constant	Pa*m3/mol	C3	One of these is REQUIRED. Henry's law constant is preferred. If not it is estimated from Water solubility, Molecular weight, Vapour pressure.
Water solubility	kg/m	C9	
Molecular weight	g/mol	C4	REQUIRED
Octanol-water partition coefficient	dimensionless	C5	REQUIRED
Partition coefficient between water and solids at steady state/equilibrium	l/kg	C7	Used if available. If not available it estimated from Octanol-water partition coefficient.
Vapour pressure	Pa	C8	REQUIRED
Melting point	K	C10	REQUIRED
Algal growth inhibition expressed in growth rate reduction (EC50)	mg/l	ET4	One of these is REQUIRED. Algal growth inhibition expressed in growth rate reduction (EC50) is preferred.
Algal growth inhibition expressed in biomass reduction (EC50)	mg/l	ET3	
Acute toxicity to fish (LC50)	mg/l	ET1	REQUIRED
Acute toxicity to aquatic invertebrates preferably crustaceans (LC50)	mg/l	ET2	REQUIRED
Reaction half-life in air	day	F10	REQUIRED
Reaction half-life in freshwater	day	F11	REQUIRED

SUBSTANCE PROPERTY PARAMETERS for SBM HUMANTOX factors
(Only valid for substances classified as "other")

Mechanism parameter	Unit	Code	Description
Henry's law constant	Pa*m3/mol	C3	One of these is REQUIRED. Henry's law constant is preferred. If not it is estimated from Water solubility, Molecular weight, Vapour pressure.
Water solubility	kg/m	C9	
Molecular weight	g/mol	C4	REQUIRED
Octanol-water partition coefficient	dimensionless	C5	REQUIRED
Partition coefficient between water and solids at steady state/equilibrium	l/kg	C7	Used if available. If not available it estimated from Octanol-water partition coefficient.
Vapour pressure	Pa	C8	REQUIRED

Melting point	K	C10	**REQUIRED**
Reaction half-life in air	day	F10	**REQUIRED**
Reaction half-life in freshwater	day	F11	**REQUIRED**
ED10 - oral - cancer	mg.kg-1.day-1	HT17	**One of these is REQUIRED for CFs on cancer effect . Priority according to order as listed from top to bottom to the left.**
Cancer oral toxicity to mammal species (q1*)	(mg/kg*day)-1	HT6	
Cancer oral toxicity to mammal species (TD50)	mg.kg-1.day-1	HT5	
ED10 - inhalation - cancer	mg.kg-1.day-1	HT16	**One of these is REQUIRED for CFs on cancer effect . Priority according to order as listed from top to bottom to the left.**
Cancer inhalation toxicity to mammal species (q1*)	(mg/m3)-1	HT4	
Cancer inhalation toxicity to mammal species (TD50)	mg.l-1	HT3	
ED10 - oral - non-cancer	mg.kg-1.day-1	HT19	**One of these is REQUIRED. Priority according to order as listed from top to bottom to the left. Condition "Test species" is also used if available.**
Chronic oral non-cancer toxicity to mammal species - LOAEL	mg.kg-1.day-1	HT8b	
Chronic oral non-cancer toxicity to mammal species - NOAEL	mg.kg-1.day-1	HT8a	
Sub-chronic oral non-cancer toxicity in rodent - LOAEL	mg.kg-1.day-1	HT14b	
Sub-chronic oral non-cancer toxicity in rodent – NOAEL	mg.kg-1.day-1	HT14a	
Sub-acute oral toxicity in rodent - LOAEL	mg.kg-1.day-1	HT12b	
Sub-acute oral toxicity in rodent - NOAEL	mg.kg-1.day-1	HT12a	
ED10 - inhalation - non-cancer	mg.kg-1.day-1	HT18	**One of these is REQUIRED. Priority according to order as listed from top to bottom to the left. Condition "Test species" is also used if available.**
Chronic inhalation non-cancer toxicity to mammal species - LOAEC	mg.l-1	HT7b	
Chronic inhalation non-cancer toxicity to mammal species - NOAEC	mg.l-1	HT7a	
Sub-chronic inhalation non-cancer toxicity in rodent - LOAEC	mg.l-1	HT13b	
Sub-chronic inhalation non-cancer toxicity in rodent - NOAEC	mg.l-1	HT13a	
Sub-acute inhalation toxicity in rodent - LOAEC	mg.l-1	HT11b	
Sub-acute inhalation toxicity in rodent - NOAEC	mg.l-1	HT11a	

SUBSTANCE PROPERTY PARAMETERS for BM ECOTOX factors
(Only valid for substances classified as "other")

Mechanism parameter	Unit	Code	Description
Henry's law constant	Pa*m3/mol	C3	**One of these is REQUIRED. Henry's law constant is preferred. If not it is estimated from Water solubility, Molecular weight, Vapour pressure**
Water solubility	kg/m	C9	
Molecular weight	g/mol	C4	**REQUIRED**
Octanol-water partition coefficient	dimensionless	C5	**REQUIRED**
Reaction half-life in sediment	day	F12	**Used if available. If not available Partition coefficient between water and solids at steady state/equilibrium, or Octanol-water partition coefficient is used for equivalent calculations.**
Partition coefficient between water and solids at steady state/equilibrium	l/kg	C7	**Used if available. If not available Octanol-water partition coefficient is used for equivalent calculations.**
Vapour pressure	Pa	C8	**REQUIRED**
Melting point	K	C10	**REQUIRED**
Reaction half-life in soil	day	F13	**REQUIRED**
Reaction half-life in freshwater	day	F11	**Used if available. Not needed if Photolysis in water and one of Ready biodegradability (%DOC removal), Ready biodegradability (%CO2 production), Ready biodegradability (%O2 uptake).**
Photolysis in water	day-1	F17	**Used if available. Not needed if Reaction half-life in freshwater, and Reaction half-life in air is available.**
Ready biodegradability (%DOC removal)		F15	**Only used if Reaction half-life in freshwater is not available. If no Reaction half-life in freshwater the condition "Exposure duration" must also be available.**
Ready biodegradability (%CO2 production)		F16	
Ready biodegradability (%O2 uptake)		F14	
Reaction half-life in air	day	F10	**Used if available. Not needed if Photolysis in water and Photodegradation rate constant from indirect photolysis with OH-radicals is available**

Photodegradation rate constant from indirect photolysis with OH-radicals	m3/(molec*day)	F9	**Only used if Reaction half-life in freshwater, and Reaction half-life in air is not available.**
Algal growth inhibition expressed in growth rate reduction (EC50)	mg/l	ET4	**One of these is REQUIRED. Algal growth inhibition expressed in growth rate reduction (EC50) is preferred.**
Algal growth inhibition expressed in biomass reduction (EC50)	mg/l	ET3	
Acute toxicity to fish (LC50)	mg/l	ET1	**REQUIRED**
Acute toxicity to aquatic invertebrates preferably crustaceans (LC50)	mg/l	ET2	**REQUIRED**

SUBSTANCE PROPERTY PARAMETERS for BM HUMANTOX factors
(Only valid for substances classified as "other")

Mechanism parameter	**Unit**	**Code**	**Description**
Henry's law constant	Pa*m3/mol	C3	**One of these is REQUIRED. Henry's law constant is preferred. If not it is estimated from Water solubility, Molecular weight, Vapour pressure**
Water solubility	kg/m	C9	
Molecular weight	g/mol	C4	**REQUIRED**
Octanol-water partition coefficient	dimensionless	C5	**REQUIRED**
Reaction half-life in sediment	day	F12	**Used if available. If not available Partition coefficient between water and solids at steady state/equilibrium, or Octanol-water partition coefficient is used for equivalent calculations.**
Partition coefficient between water and solids at steady state/equilibrium	l/kg	C7	**Used if available. If not available Octanol-water partition coefficient is used for equivalent calculations.**
Vapour pressure	Pa	C8	**REQUIRED**
Melting point	K	C10	**REQUIRED**
Reaction half-life in soil	day	F13	**REQUIRED**
Reaction half-life in freshwater	day	F11	**Used if available. Not needed if Photolysis in water and one of Ready biodegradability (%DOC removal), Ready biodegradability (%CO2 production), Ready biodegradability (%O2 uptake).**
Photolysis in water	day-1	F17	**Used if available. Not needed if Reaction half-life in freshwater, and Reaction half-life in air is available.**

Ready biodegradability (%DOC removal)		F15	**Only used if Reaction half-life in freshwater is not available.** **If no Reaction half-life in freshwater the condition "Exposure duration" must also be available.**
Ready biodegradability (%CO2 production)		F16	
Ready biodegradability (%O2 uptake)		F14	
Reaction half-life in air	day	F10	**Used if available. Not needed if Photolysis in water and Photodegradation rate constant from indirect photolysis with OH-radicals is available**
Photodegradation rate constant from indirect photolysis with OH-radicals	m3/(molec*day)	F9	**Only used if Reaction half-life in freshwater, and Reaction half-life in air is not available.**
ED10 - oral - cancer	mg.kg-1.day-1	HT17	**One of these is REQUIRED for CFs on cancer effect .** **Priority according to order as listed from top to bottom to the left.**
Cancer oral toxicity to mammal species (q1*)	(mg/kg*day)-1	HT6	
Cancer oral toxicity to mammal species (TD50)	mg.kg-1.day-1	HT5	
ED10 - inhalation - cancer	mg.kg-1.day-1	HT16	**One of these is REQUIRED for CFs on cancer effect .**
Cancer inhalation toxicity to mammal species (q1*)	(mg/m3)-1	HT4	
Cancer inhalation toxicity to mammal species (TD50)	mg.l-1	HT3	
ED10 - oral - non-cancer	mg.kg-1.day-1	HT19	**One of these is REQUIRED.** **Priority according to order as listed from top to bottom to the left.** **Condition "Test species" is also used if available.**
Chronic oral non-cancer toxicity to mammal species - LOAEL	mg.kg-1.day-1	HT8b	
Chronic oral non-cancer toxicity to mammal species - NOAEL	mg.kg-1.day-1	HT8a	
Sub-chronic oral non-cancer toxicity in rodent - LOAEL	mg.kg-1.day-1	HT14b	
Sub-chronic oral non-cancer toxicity in rodent – NOAEL	mg.kg-1.day-1	HT14a	
Sub-acute oral toxicity in rodent - LOAEL	mg.kg-1.day-1	HT12b	
Sub-acute oral toxicity in rodent - NOAEL	mg.kg-1.day-1	HT12a	
ED10 - inhalation - non-cancer	mg.kg-1.day-1	HT18	**One of these is REQUIRED.** **Priority according to order as listed from top to bottom to the left.** **Condition "Test species" is also used**
Chronic inhalation non-cancer toxicity to mammal species - LOAEC	mg.l-1	HT7b	
Chronic inhalation non-cancer toxicity to mammal species - NOAEC	mg.l-1	HT7a	
Sub-chronic inhalation non-cancer toxicity in rodent - LOAEC	mg.l-1	HT13b	
Sub-chronic inhalation non-cancer toxicity in rodent - NOAEC	mg.l-1	HT13a	
Sub-acute inhalation toxicity in rodent - LOAEC	mg.l-1	HT11b	
Sub-acute inhalation toxicity in rodent - NOAEC	mg.l-1	HT11a	

Appendix 2

“Simple estimation of effect factors for toxicity used for screening LCA"

List of all notes used in the method to characterize the quality of the toxicity data used for the calculation of characterisation factors.

Note No.	Comments characterizing the data quality
1	No relevant Risk-phrase related to human toxicity was assigned to this substance and a toxicity value corresponding to the lower end of the criteria for risk-phrase R22 was used to calculate effect factor for human toxicity. This value is thus intended to serve as a maximum value. This will probably be a correct assumption for many substances but not for all. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
2	No Risk-phrase relevant to ecotoxicity was assigned and an ecotoxicity value corresponding to the lower end of the criteria for risk-phrase R52 was applied. This value is thus intended to serve as a maximum value.
3	The toxicity value used for calculating effect factors for human toxicity to air is estimated as the average of the toxicity criteria for the risk-phrase R23. The real value of the factor is between 0,625 and 2,5 times the presented value.
4	The toxicity value used for calculating effect factors for human toxicity to air is estimated from a representative value of LC50 based on the toxicity criteria for the risk-phrase R26. The real value of the factor could be 10 times lower than the calculated value – but it could also be several decades higher. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
5	The toxicity value used for calculating effect factors for human toxicity to air is estimated as the average of the toxicity criteria for the risk-phrase R20. The real value of the factor is between 0,55 and 5,5 times the presented value.

6	The toxicity value used for calculating effect factors for human toxicity to water and soil is estimated as the average of the toxicity criteria for the risk-phrase R22. The real value of the factor is between 0,55 and 5,5 times the presented value.
7	The toxicity value used for calculating effect factors for human toxicity to water and soil is estimated as the average of the toxicity criteria for the risk-phrase R25. The real value of the factor is between 0,56 and 4,5 times the presented value.
8	The toxicity value used for calculating effect factors for human toxicity to water and soil is estimated from a representative value of LD50 based on the toxicity criteria for the risk-phrase R28. The real value of the factor could be 10 times lower than the calculated value – but it could also be several decades higher. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
9	The ecotoxicity value used for calculating effect factors for ecotoxicity to water is estimated from a representative value based on the toxicity criteria for the risk-phrase R50. The real value of the factor could be 10 times lower than the calculated value – but it could also be several decades higher. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
10	The ecotoxicity value used for calculating effect factors for ecotoxicity to water is estimated as the average of the ecotoxicity criteria for the risk-phrase R51. The real value of the factor is between 0,5 and 5,5 times the presented value.
11	The ecotoxicity value used for calculating effect factors for ecotoxicity to water is estimated as the average of the ecotoxicity criteria for the risk-phrase R52. The real value of the factor is between 0,5 and 5,5 times the presented value.
12	The toxicity value used for calculating effect factors for human toxicity to air is estimated from the risk-phrase defined by oral toxicity criteria.
13	The human toxicity - and ecotoxicity values for calculating effect factors have been estimated from risk-phrases generated by means of computer models, so-called QSAR models (Quantitative Structure-Activity Relationship). This means that the calculated

	effect factors for ecotoxicity represent an uncertain estimate. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
14	No Risk-phrase relevant to ecotoxicity was assigned and an ecotoxicity value corresponding to the lower end of the criteria for risk-phrase R52 was applied. This value is thus intended to serve as a maximum value. This will probably be a correct assumption as sufficient data is available to support this.
15	No Risk-phrase relevant to ecotoxicity was assigned and an ecotoxicity value corresponding to the lower end of the criteria for risk-phrase R52 was applied. This value is thus intended to serve as a maximum value. However there are no data available or available data is insufficient to support this assumption. This means that the calculated effect factors for ecotoxicity represent a very uncertain estimate. This should be taken into consideration when assessing the results of the LCA in question and the importance of the uncertainty should be uncovered by the sensitivity analysis.
16	No relevant Risk-phrase related to human toxicity was assigned to this substance and a toxicity value corresponding to the lower end of the criteria for risk-phrase R22 was used to calculate effect factor for human toxicity. This value is thus intended to serve as a maximum value.

Appendix 3

"Simple estimation of effect factors for toxicity used for screening LCA" and "EDIP"

Comparison of characterisation factors for mercury

Characterisation factors Mercury										
	EF(hta)_air	EF(htw)_air	EF(hts)_air	EF(hta)_water	EF(htw)_water	EF(hts)_water	EF(hta)_soil	EF(htw)_soil	EF(hts)_soil	
risk-phrase	80000	0	0	80000	0	0	80000	0	0	
EDIP	6,667E+06	1,087E+05	8,130E+01	6,667E+06	1,087E+05	8,130E+01	6,667E+06	1,087E+05	8,130E+01	
	EF(etwc)_air	EF(etsc)_air	EF(etwc)_water	EF(etwa)_water	EF(etsc)_water	EF(etwc)_soil	EF(etsc)_soil	Comments on data quality		
risk-phrase	0	0	0	100	0	0	0	See Note 1. See Note 9. See Note 3.		
EDIP	4,000E+03	5,333E+00	4,000E+03	2,000E+03	5,333E+00	4,000E+03	5,333E+00			