OMNIITOX: LCA Case Studies

Comparison between Three Different LCIA Methods for Aquatic Ecotoxicity and a Product Environmental Risk Assessment

Insights from a Detergent Case Study within OMNIITOX

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Abstract

Background and Objective. In the OMNIITOX project 11 partners have the common objective to improve environmental management tools for the assessment of (eco)toxicological impacts. The detergent case study aims at: i) comparing three Procter & Gamble laundry detergent forms (Regular Powder-RP, Compact Powder-CP and Compact Liquid-CL) regarding their potential impacts on aquatic ecotoxicity, ii) providing insights into the differences between various Life Cycle Impact Assessment (LCIA) methods with respect to data needs and results and iii) comparing the results from Life Cycle Assessment (LCA) with results from an Environmental Risk Assessment (ERA).

Material and Methods. The LCIA has been conducted with EDIP97 (chronic aquatic ecotoxicity) [1], USES-LCA (freshwater and marine water aquatic ecotoxicity, sometimes referred to as CML2001) [2, 3] and IMPACT 2002 (covering freshwater aquatic ecotoxicity) [4]. The comparative product ERA is based on the EU Ecolabel approach for detergents [5] and EUSES [6], which is based on the Technical Guidance Document (TGD) of the EU on Environmental Risk Assessment (ERA) of chemicals [7]. Apart from the Eco-label approach, all calculations are based on the same set of physico-chemical and toxicological effect data to enable a better comparison of the methodological differences. For the same reason, the system boundaries were kept the same in all cases, focusing on emissions into water at the disposal stage.

Results and Discussion. Significant differences between the LCIA methods with respect to data needs and results were identified. Most LCIA methods for freshwater ecotoxicity and the ERA see the compact and regular powders as similar, followed by compact liquid. IMPACT 2002 (for freshwater) suggests the liquid is equally as good as the compact powder, while the regular powder comes out worse by a factor of 2. USES-LCA for marine water shows a very different picture seeing the compact liquid as the clear winner over the powders, with the regular powder the least favourable option. Even the LCIA methods which result in the same product ranking, e.g. EDIP97 chronic aquatic ecotoxicity and USES-LCA freshwater ecotoxicity, significantly differ in terms of most contributing substances. Whereas, according to IMPACT 2002 and USES-LCA marine water, results are entirely dominated by inorganic substances, the other LCIA methods and the ERA assign a key role to surfactants. Deviating results are mainly due to differences in the fate and exposure modelling and, to a lesser extent, to differences in the toxicological effect calculations. Only IMPACT 2002 calculates the effects based on a mean value approach, whereas all other LCIA methods and the ERA tend to prefer a PNEC-based approach. In a comparative context like LCA the OMNIITOX project has taken the decision for a combined mean and PNEC-based approach, as it better represents the 'average' toxicity while still taking into account more sensitive species. However, the main reason for deviating results remains in the calculation of the residence time of emissions in the water compartments.

Conclusion and Outlook. The situation that different LCIA methods result in different answers to the question concerning which detergent type is to be preferred regarding the impact category aquatic ecotoxicity is not satisfactory, unless explicit reasons for the differences are identifiable. This can hamper practical decision support, as LCA practitioners usually will not be in a position to choose the 'right' LCIA method for their specific case. This puts a challenge to the entire OMNIITOX project to develop a method, which finds common ground regarding fate, exposure and effect modelling to overcome the current situation of diverging results and to reflect most realistic conditions.

Keywords: Aquatic ecotoxicity; case studies; detergents; ecotoxicity; LCIA; OMNIITOX; surfactants; toxicity

Introduction

Research context. The overall objective of the OMNIITOX project is the further development of models and environmental management tools for the assessment of (eco)toxicological impacts [8]. More specifically, the OMNIITOX-project addresses five main issues of importance for the improvement of methods used in toxicological and ecotoxicological characterisation of chemicals:

1. Analysis of similarities and differences between the toxicological characterisation of chemicals in Life Cycle Impact Assessment (LCIA) and (environmental) risk assessment ((E)RA), leading to recommendations regarding their domain of application.

2. Analysis of similarities and differences of current methods for toxiclogical characterisation of chemicals within LCIA in order to allow harmonization and possibly identify a best practice.
3. Expansion of the scope of these methods used within LCIA.
4. IT-facilitated LCIA/ERA due to increased availability of data and tools.
5. Background for possible inclusion of LCA of chemicals into the regulatory risk assessment context.

As a test case with real products, the P&G detergent case study within the OMNIITOX project focuses on the evaluation of the toxic effects on the aquatic environment that can be triggered by the release of detergent ingredients into water. The stated OMNIITOX goals one, two and four are specifically relevant to this detergent case study.

The tools LCA and ERA are both used for evaluating (potential) toxicological impacts on the environment. They use some common data, but there are also significant differences between the tools [9–11]. ERA usually is looking at the emission of one specific substance taking into account all possible sources or, in the case of a product ERA, at the emission of all ingredients contained in a product [12]. LCA usually has a much wider scope, taking into account all kinds of emissions originating along the life cycle of a product and a range of potential environmental impacts from emissions of greenhouse gases, potential toxicity to resource consumption. All emissions and potential impacts are only taken into account if they are related to the product or service under investigation (functional unit approach). LCA deliberately disregards all other potential sources of the emission of substances [13,14].

These differences were illustrated by the results of an earlier P&G case study in which two detergent products were compared with Ecological Risk Assessment (ERA) and Life Cycle Assessment (LCA). This earlier case study showed that the tools may give conflicting answers to the question concerning which product is preferable from an environmental perspective, as they provide different insights [15].

Research objectives. To better understand the differences between the LCA results and the ERA results, both the results and the methodologies of the two tools have to undergo an in-depth comparison. The specific objectives of the detergent case study are threefold:

i) to compare three Procter & Gamble laundry detergent forms regarding their environmental burdens for the impact category of aquatic ecotoxicity,
ii) to provide insights into the differences between various LCIA methods with respect to data needs and results, and
iii) to prepare the comparison of the tools LCA and ERA.

Research approach. To answer our research questions, it was a key to achieve consistency in the technical design of the LCIA studies and the ERA:

- The chosen life cycle stage must be the same, e.g. as the ERA is conducted for the discharge of detergent ingredients after waste water treatment, the LCIA – or a part of it – also focuses on this disposal stage only. Results from a comprehensive LCA, including all life cycle stages, may deviate significantly due to the impact of environmental interventions at other life cycle stages, particularly the use stage with the energy consumption for heating-up water [16].
- The input data for LCIA and for the PEC/PNEC calculations in the ERA must be consistent. For example, as only acute ecotoxicity values with application factors of 1000 are used for calculating predicted no effect concentrations (PNECs) in the first tiers in the selected ERA method, the same values are applied in the LCA for the calculation of the Life Cycle Impact Assessment characterisation factors (CFs).

1 Material and Methods

1.1 Three laundry detergent types and their ingredients

Three types of laundry detergent products were chosen for this case study. The product formulas are based on data of the United Kingdom for the year 2001. They represent a Regular Powder (RP), a Compact Powder (CP) and a Compact Liquid (CL).

The release data on the ingredients used were taken from market data on the overall use of detergents in the UK in the year 2001 and adapted to assume a 100% market share for each of the three products. To be consistent with the approach in EUSES, the release data for the ERA were calculated for 20 million inhabitants. **Table 1** summarizes the assumptions for the release of the three products Regular Powder (RP), Compact Powder (CP) and Compact Liquid (CL).

Based on the total consumption per capita and year, and the product formulation for the three detergent types in the UK in the year 2001, the release data for the single ingredients contained in the three products is calculated. A list of the ingredients contained in the three detergent types is provided in **Annex 1** together with the results of the LCI.

1.2 Data requirements and availability

Internal P&G databases and external databases, such as IUCLID and AQUIRE from the US Environmental Protection Agency (US EPA), were searched to obtain the necessary data. If no measured data could be obtained, Quantitative Structure Activity Relationship (QSAR) values were derived via available software packages. Most data gaps were encountered for physico-chemical data, fewer for acute ecotoxicity. The availability of three or more data points on chronic toxicity from 3 different taxonomic groups was limited to the more important and well-studied compounds.

Table 1: Assumptions for the calculation of the amount of products consumed

	Regular Powder	Compact Powder	Compact Liquid
Number of washes/(year*capita)	85	85	85
Recommended dosage [g/wash]	121.5	75	78
Total consumption [kg/(year*capita)]	10.3	6.4	6.6

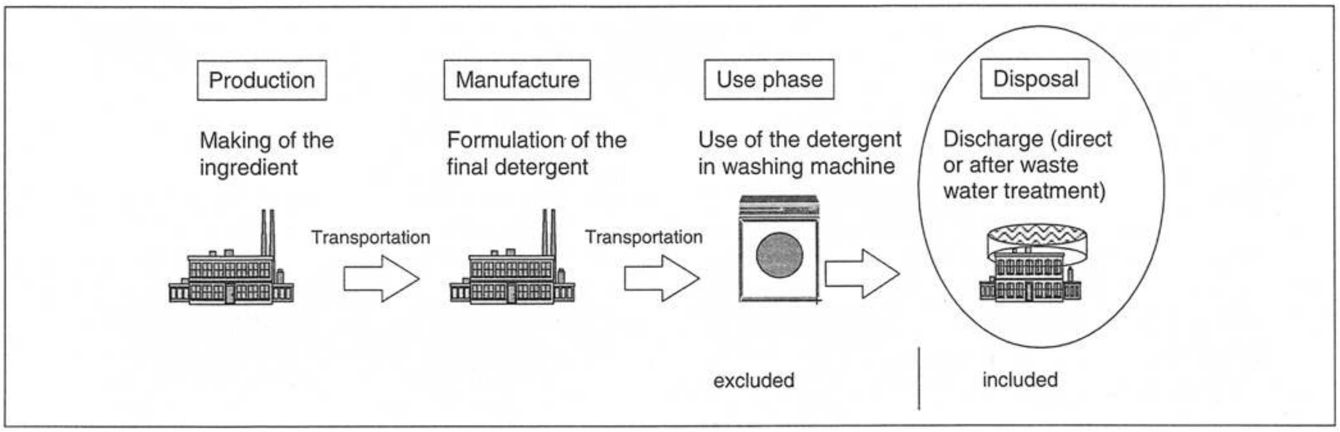

Fig. 1: Limited system boundaries for the LCIA and ERA in this case study

1.3 Approach for the LCA/ERA comparison

1.3.1 Goal and Scope definition

1.3.1.1 Description of the system boundaries and the functional unit

For this case study, the system boundaries for the LCIA and the ERA have been set identically and do not cover the entire life cycle of detergents but the disposal stage only, see **Fig. 1**. This is to enable a better comparison between the tools ERA and LCIA. For the same reason, only emissions into water (direct discharge or after waste water treatment) were taken into account.

The functional unit was chosen in a way that the LCIA results with the ERA (85 washes per year and capita for 20 million inhabitants in the UK in the year 2001) are compatible. For the ease of reporting, the functional unit for the LCA is chosen as 1 wash cycle in the UK, using the recommended dosage of the different detergent products.

1.3.2 The tiered approach to comparative product ERA

The ERA was designed for different conditions within the EC and was performed using a tiered approach:

Tier 1: On a local scale: EU Eco-label method and Detergent Ingredient Database [5]

- Comparably simple model developed in the context of eco-labelling of detergent products in the EC, not for use in safety assessments
- PEC calculation: Loading Factors (LF) based on removal factors derived from activated sludge tests, assuming 100% connection to sewage treatment
- PNEC calculation: In contrast to the ERA with EUSES, in the Detergent Ingredient Database the given Long Term Effect (LTE) factors are based on chronic data where available, in other cases on acute toxicity data and expert judgement [5]
- Here, used for screening purposes to determine the most relevant ingredients for a more in depth evaluation in the next tier. As the Detergent Ingredient Database is widely accepted by different stakeholders within the EU, it may be assumed that it appropriately reflects the toxicity of the relevant ingredients and is thus suitable as a screening and selection tool.

Tier 2: On a regional scale: The European System for Evaluating Substances (EUSES)

- ERA approach according to the legal requirements in the EC [6,7]
- PEC calculation: based on a unit world approach for fate and exposure modelling (200 x 200 km² region, allowing for losses from the region in air and water)
- PNEC calculations: Here, based on acute toxicity data with application factor (AF) 1000

According to the EU Eco-label approach a critical dilution volume (CDV tox) for aquatic toxicity is calculated for each ingredient i in the product formulation according to Eq. (1)

$$\text{CDV tox (ingredient i)} = \frac{weight\,/\,wash(i) \times LF(i)}{LTE(i)} * 1000 \qquad (1)$$

CDV tox: Critical Dilution Volume-toxicity [L/wash]
LF: Loading Factor (reflecting removal in waste water treatment)
LTE: Long Term Effect (reflecting data on chronic and acute ecotoxicity)
i: ingredient i

The CDV tox of the product is the sum of all ingredients CDV tox in L/wash.

EUSES is based on the Technical Guidance Document (TGD) that is valid in the European Union (25 countries) for ERA and provides default emission scenarios for both regional and local risk assessment of detergent and household cleaning substances. These emission scenarios are designed to be conservative. The regional scenario was chosen due to the similarity with the conditions and many of the methods in LCA approaches.

For the EUSES standard scenario, the volume of ingredients released into the environment was based on the assumption of 85 washes per capita and year, and the recommended dosage for the respective detergent type. The obtained volumes were extrapolated to 370 million inhabitants in Europe. 10% of the release of detergents by these 370 million inhabitants is assumed to happen in the EUSES 200 x 200 km² region with 20 million inhabitants (default value in EUSES).

This is to assume a 'reasonable worst case region', where *per capita* detergent consumption is higher than the EU average. A sewage flow per capita and day of 200 L and a connection rate to the sewer of 70% were assumed.

To be consistent with the LCA approach, only emissions due to the detergent products have been taken into account disregarding other potential non-detergent emission sources in the modelled region of these ingredients.

1.3.3 Comparative product ERA versus assessment of safety of ingredients

The conducted ERA does not have the objective to assess the safety of the ingredients, but is to be used in a comparative product ERA. The difference of these approaches has to be acknowledged to understand the different meanings of the achieved results.

Due to the given data set in the Eco-label approach, a mixed set of acute and chronic toxicity data was used. The ERA with EUSES is based on acute toxicity data applying an application factor of 1000 even for substances where a data set on chronic ecotoxicity is available. This is to avoid that products, which largely consist of ingredients without chronic ecotoxicity data, would be generally 'punished' for the lack of this type of data by multiplying with this high application factor. This so-called 'reasonable worst case approach' which is conservative in the vast majority of cases is understandable for safety purposes. However, it could seriously flaw the results of a comparative study, as products consisting of ingredients with a comprehensive chronic dataset are likely to look preferable versus products with a lot of ingredients where only an acute dataset is available. Nevertheless, it should be noted that a comparison using acute data implicitly assumes that the ranking of the chronic and acute data sets for the different chemicals will be similar.

1.3.4 Mixture toxicity in a comparative product ERA

Evaluating the environmental profile of products that are inherent mixtures of chemicals means that sooner or later one has to address the questions of 'mixture toxicity': What is the effect of the sum of all chemicals present in the environment? Are their effects additive or synergistic or antagonistic? Here, a product risk assessment indicator, adding up all the risk scores of the ingredients of a product, is used to allow a comparison between the detergent types.

According to ECETOC [17], mixtures of substances that are chemically related or have the same mode of action are generally found to be additive in acute toxicity tests. When large numbers of substances are present in mixtures at low concentrations relative to their individual acute toxicities, additivity of acute toxic effects can be observed. Also according to ECETOC [17] this holds true even when the substances are not related chemically, or exhibit different modes of action when acting as acute toxicants alone. Thus, their toxicity can be captured using the concept of 'baseline toxicity' or narcosis.

The risk scores for ingredients are based on the results of the EUSES standard scenario.

$$Riskscore = PEC / [EC50 * 1000] \qquad (2)$$

PEC: Predicted Environmental Concentration (based on EUSES multimedia model)

*EC*50: Effect Concentration at which 50% of test organisms show an effect

The Risk scores of the single ingredients are then added up to a product risk score assuming toxicity additivity.

Compared to the algorithm introduced by Saouter et al. [15], here the effect calculation is based on acute data on aquatic ecotoxicity (EC50 values) multiplied by an Application Factor of 1000 for all ingredients, whereas Saouter et al. used PNECs based on chronic toxicity data where available. As stated above, we deliberately chose to disregard data on chronic toxicity to evenly treat all ingredients and calculate PNECs based on the same data set, i.e. data on acute toxicity. Therefore, the generated risk scores are not the most appropriate to be used for safety assessment [18]. A safety assessment has to make use of the highest tier data available, including data on chronic toxicity and multi-species tests.

1.3.5 Life Cycle Impact Assessment (LCIA)

As described, the LCIA is not applied to a cradle to grave LCI, but limited to the end of use stage where the emission of detergent ingredients into the aquatic environment takes place. Results for cradle to grave LCIAs on detergent products are published elsewhere [16,19].

The results of the following LCIA methods are presented in this paper:

- EDIP97 (chronic aquatic ecotoxicity)
- USES-LCA (freshwater aquatic ecotoxicity, marine water ecotoxicity)
- IMPACT 2002 (aquatic ecotoxicity)

The selection of the LCIA methods has been conducted in close cooperation with the OMNIITOX partners, especially the academic partners. IMPACT 2002 and USES-LCA are based on multimedia fate and exposure models, while EDIP97 consists of a key property approach (selected parameters weighted to provide an indicator) often demanding much less data input than the multimedia models.

The ecotoxicological characterisation factor of IMPACT 2002 describes the Potentially Affected Fraction (PAF) of a species per kg emission. The fresh water Aquatic EcoToxicity Potential in USES-LCA assesses substance released to a specific compartment in 1,4-dichlorobenzene (DCB) equivalents. EDIP expresses a potential aquatic ecotoxicity with an Equivalency Factor for acute and one for chronic ecotoxicity in water based on a few parameters with a comparably high data availability. A more detailed comparison of the LCIA methods can be found in Guinée et al. [20].

2 Results and Discussion

2.1 Screening with the EU Eco-label approach

Due to the considerable work involved in conducting the full ERA with EUSES for all ingredients, it was necessary to focus on the most relevant ingredients. As a cut-off criterion, it was decided that the chosen ingredients have to cover at least 90% of the toxicity score according to the screening tool based used in the EU Eco-label methodology, in order to ensure consideration of the most likely relevant ingredients in the further ERA. The number of the selected ingredients for further evaluation in the tiered ERA is relatively similar for all products, 10 for regular powder, 11 for compact powder and 9 for compact liquid (**Table 2**). The covered product formula in weight % (excluding water) by these selected ingredients varies from 44% for compact powder over 48% for regular powder to 74% for compact liquid. The high value for compact liquid is mainly due to the fact that it has by far the highest content of water of the three product forms and the water content has been subtracted from the product formula for the calculation. But the far more relevant figure is the share of the toxicity score according to the Eco-label methodology attributable to the selected ingredients. Here, the figures are similar with 91% of the toxicity score covered for the compact powder, 95% of the toxicity score covered for the regular powder and 98% of the toxicity score covered for compact liquid.

A direct comparison of the other results with the EU Eco-label approach has to take into account that the EU Eco-label results are based on a different effect data set than the results for EUSES and the LCIA methods.

2.2 EUSES

Fig. 2 provides a comparison of the risk scores with Regular Powder having the lowest score closely followed by Compact Powder and Compact Liquid with the highest score. If the result for regular powder is set to 1, compact powder scores 1.24 and compact liquid 3.14. The ingredients dominating the results are surfactants with a low influence of inorganic substances, as only carbonates have a significant impact. It has to be mentioned that the score for compact powder is to a large extent due to a single very low acute toxicity (LC50) value for C12-15 alkylsulphate (0.54 mg/L). Acute toxicity (LC50) values for C12-18 alkylsulphate, which is contained in the RP, are more than an order of magnitude higher.

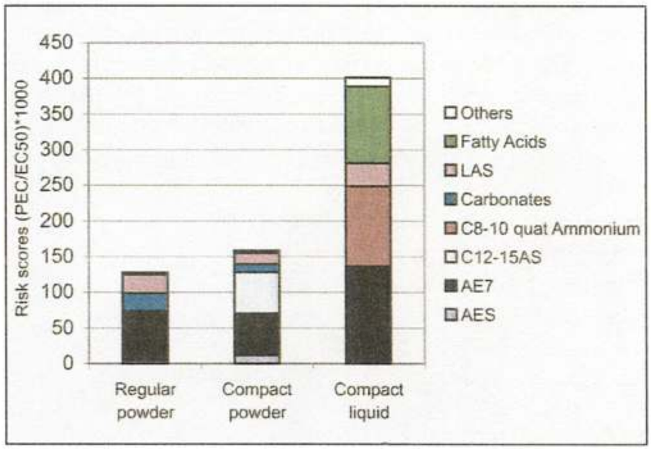

Fig. 2: Risk scores (PEC/EC50)*1000 with EUSES standard scenario

Table 2: Selected ingredients for further evaluation in next tier ERA

	Regular Powder	Compact Powder	Compact Liquid
Linear Alkyl Benzene Sulphonate, Na salt	X	X	X
Alkyl Sulphate (C12-C15), Na		X	
Alkyl Sulphate (C12-C18), Na	X	X	
Alkyl Ethoxy Sulphate (C12-C15)	X	X	
C12-15 Alcohol Ethoxylate AE7	X	X	X
C8-10 Quarternary Ammonium Compound			X
Carbonates (including Percarbonate)	X	X	
Hydrogenated fatty acid	X	X	
Topped Palm Kernel Fatty Acid			X
Orthoboric acid			X
Monoethanolamine			X
Perfume Compound 1	X	X	X
Perfume Compound 2	X	X	X
Brighteners	X	X	X
Quarternary Ammonium Compounds	X	X	
Number of ingredients selected for further ERA	10	11	9
Covered share of the product formula (excl. water) [weight %]	~48	~44	~74
Covered share of the total toxicity score according to the Eco-label approach [%]	~95	~91	~98

2.3 Life Cycle Inventory

The results of a cradle to grave LCI of detergent products have been published in [15]. The inventory results for the emission of detergent ingredients into freshwater after wastewater treatment are presented in Annex 1.

2.4 Life Cycle Impact Assessment

The following LCIA results are limited to the release of ingredients after use and waste water treatment (disposal stage).

2.4.1 EDIP97 chronic aquatic ecotoxicity (ETWC)

The picture for chronic toxicity potential according to EDIP97 in **Fig. 3** shows regular powder and compact powder are assigned very similar toxicity potentials, whereas compact liquid has a slightly higher potential than the other types. The surfactants are the main contributing factor to all detergent types. Sulphates also contribute a large share (up to more than 25%) to the toxicity potential. Other inorganic substances and perfumes play only a minor role.

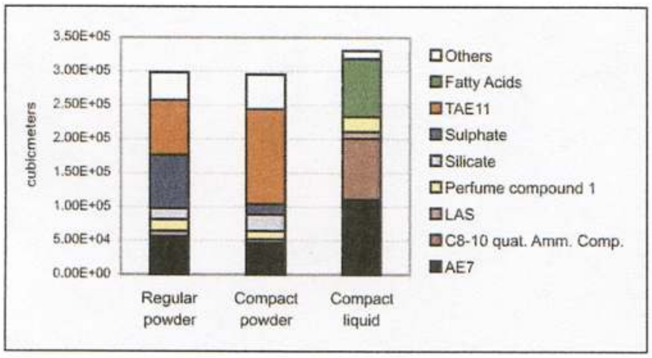

Fig. 3: EDIP97 results for chronic aquatic ecotoxicity (ETWC)

2.4.2 USES-LCA

The results for the different detergent types according to the USES-LCA method are presented in **Fig. 4** for freshwater and in **Fig. 5** for marine water.

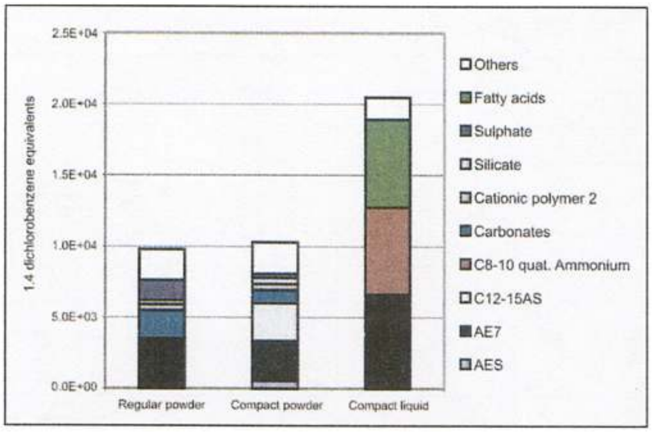

Fig. 4: USES-LCA Results for freshwater ecotoxicity

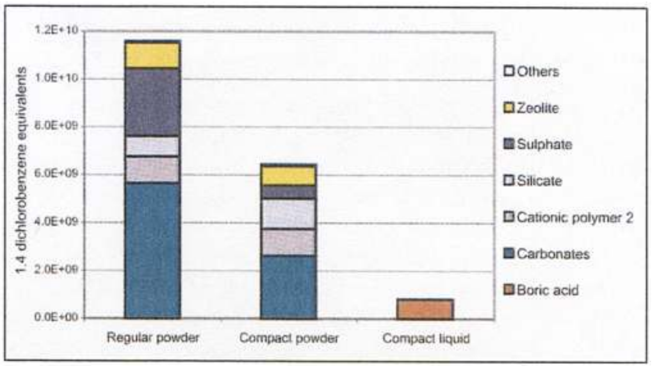

Fig. 5: USES-LCA results for marine water ecotoxicity

According to USES-LCA freshwater toxicity there is no clear preferable option as regular powder and compact powder are very similar in their potential environmental impacts. compact liquid is with more than a factor of 2 the least favourable option. A range of ingredients is contributing significantly to the toxicity score with surfactants as the overall drivers.

Fig. 5 shows that the toxicity potential scores for marine water according to USES-LCA are on a different scale compared to the freshwater results. Compact liquid is clearly preferable compared to compact powder and regular powder, but the results need some further attention and interpretation regarding the main contributing substances. The results for all products are dominated by a very limited set of substances, mainly by water-soluble inorganic substances, which are by definition non-biodegradable or by substances, which are not readily biodegradable. This reflects that only these substances will accumulate in the marine water compartment as a final sink (they are lost from freshwater by advection, which relatively limits their influence in freshwater systems). At least the results for sulphate, carbonate and boric acid are questionable with respect to their scientific relevance as the natural background concentrations in marine water for those substances are much higher than any human contribution and the marine species are fully adapted to those high natural concentrations. A review of the model calculations would suggest elimination of these from further consideration.

The reasons for the questionable results are mainly twofold:

- On the predicted environmental concentration side, the residence time for many inorganic substances and persistent organic chemicals in the marine compartment is much higher than in the other compartments. The marine compartment essentially acts as a sink. CFs are derived by comparing the PEC/PNEC ratios of the substances. The PEC is calculated from the steady state concentration in a compartment resulting from a constant emission in a certain compartment. This approach means that a high residence time for a substance in a compartment results in a high PEC and hence high CF for the substance in the compartment.
- On the effect side, the data provided for calculation of the marine toxicity potentials. The reported effect data were only measured against freshwater species. No

ecotoxicity values for marine water were provided. This leads to a situation where the effect data does not necessarily reflect the adaptation of marine species to some of the ingredients and, in this case, the derived PNEC will be very much on the conservative side. This indicates that a simple extrapolation from freshwater ecotoxicity results to marine water ecotoxicity potential is not a viable option as it is not meaningful for all substances. As the data availability for marine toxicity is not expected to increase significantly in the foreseeable future, it was decided that the marine ecotoxicity will not form a part of the OMNIITOX Base Model, but will be covered for fewer chemicals in the Model Options [20].

2.4.3 IMPACT 2002

The results with IMPACT 2002 in **Fig. 6** show distinct differences between the detergent types with compact powder and compact liquid as the preferred options, followed by regular powder as the least favourable one. Although the overall results might look comparable to most of the other LCIA methods and the ERA results, the main contributing substances are very distinct from the other methods, apart from USES-LCA marine water. Only a very limited set of inorganic substances are dominating the impact scores for all detergent types. For regular powder and compact powder, carbonate, sulphate and silicate are dominating the profile, while other substances, including surfactants, only have a minor impact. For compact liquid, boric acid dominates the picture and only chlorides have further significant impacts.

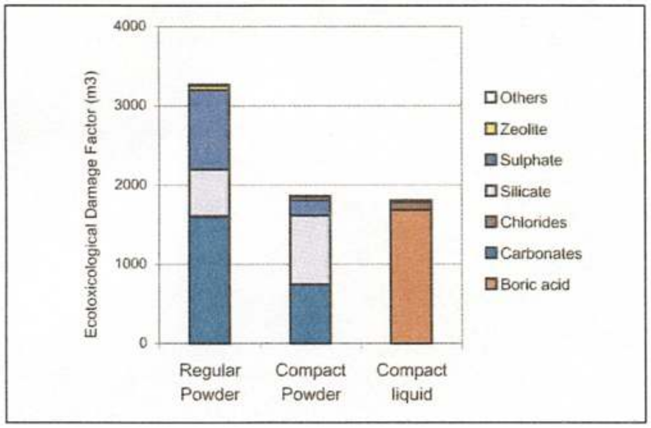

Fig. 6: Impact 2002 results for aquatic ecotoxicity

IMPACT 2002 uses an average surface water residence time for Western Europe. This is dominated by the residence time of freshwater in lakes, as these constitute most of the European freshwater volume. These higher residence times are therefore more similar to those in the oceans than in rivers. As the inorganic substances don't degrade, they are only lost from surface waters via advection or intermedia transport. As most are not lost at an intermedia transport rate greater than the advective rate, advection will dominate. Inorganic substances will therefore be among the most persistent types of compounds found in surface waters when considering residence times in lakes.

3 Comparison of the methods

3.1 Comparison of characterisation factors between the LCIA methods

To enable a better comparison of the LCIA methods, the CF of LAS, a compound with intermediate toxicity, is set to 1 in all LCIA methods and the CFs for all other ingredients are expressed in relation to the CF for LAS.

Table 3 provides an overview on how the different LCIA methods attribute CFs to the various ingredients of the detergent case study. It can be seen that the CFs from EDIP97 for chronic aquatic ecotoxicity and from USES-LCA for freshwater ecotoxicity have a similar pattern. The CFs for IMPACT 2002 are significantly different. In IMPACT 2002, inorganic substances have a much higher CF compared to the other LCIA methods, the top three ingredients are inorganic substances and all inorganics are attributed a higher CF than LAS. This pattern is comparable only to USES-LCA for marine water for the reasons highlighted above.

If we take a closer look at some of the ingredients that are most relevant to the detergent products under investigation, the following comparison can be made if LAS is set to 1 for all methods (**Fig. 7**).

Bars above 1 indicate a higher CF compared to LAS, inverted bars indicate a CF lower than the CF for LAS. The differences in the CFs for the majority of the surfactants lie

Table 3: Overview on the CFs in relation to LAS for the different LCIA methods

	EDIP97 (chronic toxicity)	**USES-LCA freshwater**	**IMPACT 2002**	**USES-LCA marine water**
Substances with higher CF than LAS Maximum Factor between highest CF and CF for LAS Kind of substances with higher CF than LAS	17 300 1 inorganic only	12 500 no inorganics	16 3500 includes all inorganics	20 10E+08 includes all inorganics
Top 3 substances	Perfume 1 TAE11 ZnPhtalocyan. sulf.	ZnPhtalocyan. sulf. C8-10 quat amm com Cationic polymer 2	Chloride Boric acid Silicate	ZnPhtalocyan. sulf. cationic polymer 2 Brightener 49
Substances with lower CF than LAS Maximum Factor between CF for LAS and lowest CF	24 2000	22 700	22 880	12 700
Bottom 3 substances	Citrate Ethanol Enzyme	Citrate Starch Enzyme	Citrate Starch Fatty acids	Citrate Starch Enzyme

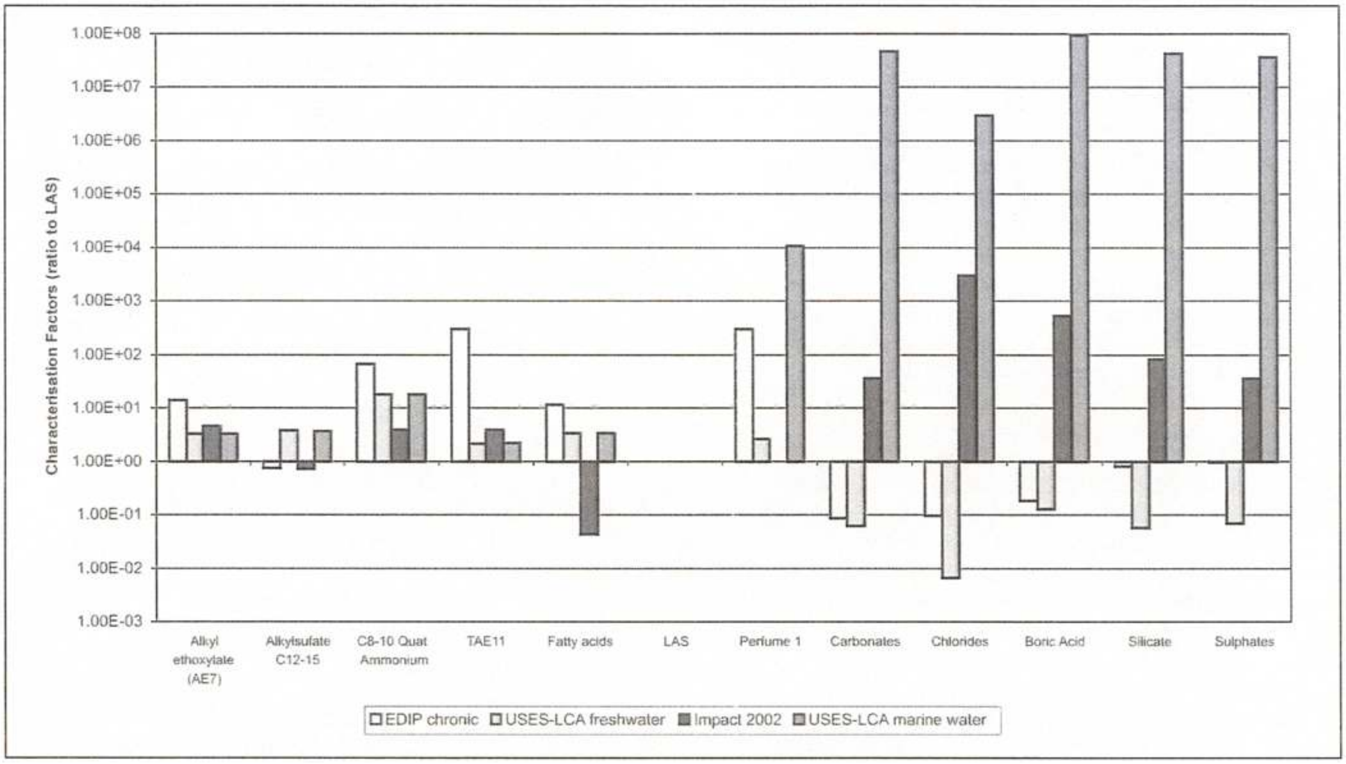

Fig. 7: Comparison of the characterisation factors for key ingredients

in between a range of factor 300. The differences in the CFs for non-biodegradable organic substances and particularly for inorganic substances are very high and are in need of further evaluation. There is a clear distinction between the EDIP97 chronic aquatic and USES-LCA freshwater methods on the one hand and IMPACT 2002 and USES-LCA marine water on the other hand. The EDIP97 chronic ecotoxicity method and USES-LCA freshwater attribute a lower CF compared to LAS to almost all inorganic substances, whereas IMPACT 2002 and USES-LCA marine water attribute a much higher value to the inorganic substances.

According to IMPACT 2002, the CFs for some inorganic substances are up to a factor of 3500 higher than the CF for LAS. With USES-LCA marine water, the differences are even higher with a maximum factor of almost 100,000,000.

The reasons for the differences in the CFs can be found in the varying 'philosophies' of the models regarding fate and exposure modelling as discussed by Margni [21] and to a lesser extent due to different effect calculations. It is interesting to note that the underlying modelling principles of USES-LCA and IMPACT 2002 are similar, suggesting that a lot of the differences will come down to parameterization – in this the case, the residence time of the freshwater bodies are modelled. Also the different way in which the methods make use of biodegradation data for degradable substances could be identified as a major source of the differences.

3.2 Comparison of the ranking of the laundry detergent types

The significant differences of the CFs for the different LCIA methods, especially for inorganic substances, lead to different results in the overall comparison of the detergent products (**Fig.** 8). The high CFs attributed to the inorganic substances are dominating the results for the product comparison for IMPACT 2002 and USES-LCA marine water. Here, regular powder comes out as the worst alternative (due to the highest content of inorganic substances) followed by compact powder and by compact liquid, in which boric acid is the only inorganic substance in significant quantities.

Within the LCIA methods, the results produced by EDIP97 chronic aquatic toxicity and USES-LCA freshwater can be seen as most matching. Both provide nearly exactly the same result for the total product toxicity scores for regular powder and compact powder, whereas USES-LCA freshwater assigns a slightly higher result to compact liquid. However, although the total scores for the powder detergents are the same and both see surfactants as a key group of ingredients, this is fortuitous. The two methods deviate in the identification of the specific main contributing ingredients.

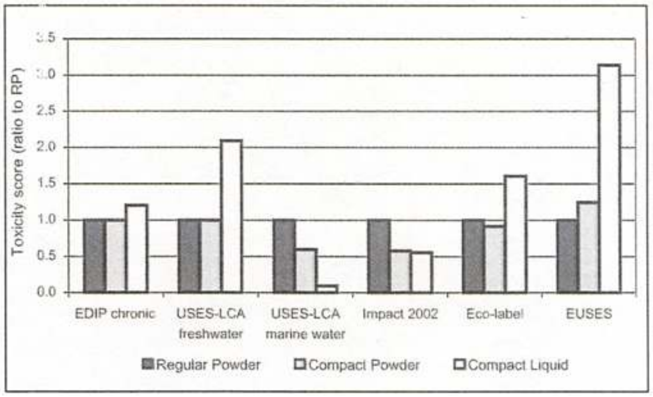

Fig. 8: Comparison of product rankings according to LCIA and ERA

The results of the product risk scores obtained by EUSES and the EU Ecolabel are similar to the LCIA results with EDIP97 chronic ecotoxicity and USES-LCA in terms that all suggest the compact liquid to be the least preferable option and compact powder and regular powder are roughly even. These results are in contrast to the results for USES-LCA marine water and IMPACT 2002. This distinction between the methods also shows up regarding the ingredient groups which contribute most to the final results: For USES-LCA freshwater and EDIP97 chronic ecotoxicity, the most relevant ingredients are surfactants, whereas, according to USES-LCA marine water and IMPACT 2002, inorganic substances clearly dominate the results. Note that the ERA was conducted for freshwater only, based on test results for freshwater organisms. Note also that while the LCIA results and the EU Ecolabel approach include most of the ingredients, the ERA with EUSES has been conducted for only around 10 ingredients per product type.

Table 4 provides an overview of the 3 most relevant ingredients according to the different LCIA and ERA methods. In brackets the percentage share of each ingredient of the total toxicity score is given. Huge deviations exist, especially regarding the relevance of inorganic substances versus surfactants and perfumes. The results for the EU Eco-label approach and EUSES show significant differences, especially regarding the relevance of perfumes. It can be assumed that these differences are due to the use of a separate data set for the Eco-label calculations based on the Detergent Ingredient Database (DID list). The values provided in the DID-list for so-called long-term effects can deviate significantly from the data set for acute toxicity used for calculation of the LCIA and the EUSES results.

Apart from the differences identified by Dreyer et al. [22] regarding inventory coverage, choice of toxicity test results, normalization and weighting this detergent case study shows that the LCIA methods differ significantly, even if the same data set is used for calculating CFs for all LCIA methods. Dreyer et al. [22] state that, in contrast to USES-LCA, EDIP97 does not make a distinction between freshwater and marine water, but it is assumed that the relevant impacts will come from the marine water compartment and that they therefore conduct the comparison of EDIP97 chronic ecotoxicity scores with USES-LCA marine water. For this detergent case study, the product rankings and the main contributors show little (if any) similarity between the results of EDIP97 chronic ecotoxicity and USES-LCA for marine water ecotoxicity. This confirms the conclusion of Dreyer et al. [22] that the results of the different LCIA methods can point into opposite directions. For the detergent case study on aquatic ecotoxicity, the answer to the question posed by Dreyer et al. [22] 'Does it matter which one (LCIA method) you choose?' is a clear and unambiguous 'Yes, it does matter'.

It has to be noted that CFs were not available for all ingredients in IMPACT 2002, whereas they were for the EDIP97 and to a high degree for the USES-LCA methods (compare **Table 5**). As all relevant surfactants and major inorganic substances are covered by all LCIA methods, this different inventory coverage may explain only a minor part of the differences.

Table 4: Comparison of dominating substances according to LCIA and ERA methods

	Top 3 substances (share of the total ecotoxicity score)		
	Regular Powder	**Compact Powder**	**Compact Liquid**
EDIP97 chronic aquatic ecotoxicity	Sulphates (28%) TAE11 (28%) AE7 (20%)	TAE11 (51%) AE7 (17%) Silicate (9%)	AE7 (34%) C8-10 quat. Ammonium (27%) Fatty acids (26%)
USES-LCA freshwater ecotoxicity	AE7 (31%) LAS (19%) Carbonates (18%)	AE7 (27%) C12-15 AS (25%) LAS (12%)	AE7 (30%) Fatty acids (28%) C8-10 quat. Ammonium (27%)
USES-LCA marine water ecotoxicity	Carbonates (49%) Sulphates (24%) Cationic Polymer 2 (10%)	Carbonates (41%) Silicate (20%) Cationic Polymer 2 (17%)	Boric acid (100%)
IMPACT 2002 aquatic ecotoxicity	Carbonates (49%) Sulphates (31%) Silicate (18%)	Silicate (47%) Carbonates (40%) Sulphates (10%)	Boric acid (94%) Chlorides (5%) AE7 (1%)
EU Ecolabel	Perfumes (mix) (45%) LAS (32%) AE7 (11%)	Perfumes (mix) (36%) LAS (21%) C12-15 AS (14%)	Perfumes (mix) (36%) LAS (24%) MEA (14%)
EUSES ERA	AE7 (55%) LAS (21%) Carbonates (20%)	AE7 (37%) C12-15 AS (37%) LAS (16%)	AE7 (34%) C8-10 quat. Ammonium (28%) Fatty acids (27%)

Table 5: Mass% of formula covered by the different LCIA methods

		Share of product formula covered (weight %)		
Method	**Impact category**	**Regular Powder**	**Compact Powder**	**Compact Liquid**
EDIP97	Chronic aquatic ecotoxicity	100%	100%	100%
USES-LCA	Freshwater ecotoxicity	97%	98%	90%
	Marine water ecotoxicity	97%	98%	90%
IMPACT 2002	Aquatic ecotoxicity	94%	93%	76%

4 Conclusion and Outlook

The comparison of results for the different LCIA methods and the ERA tools for the disposal stage of the three detergent products provide the following insights:

- The EDIP97 chronic aquatic ecotoxicity and USES-LCA freshwater toxicity methods lead to similar results regarding the product ranking (regular powder and compact powder similarly good, compact liquid less favourable). Surfactants are dominating the results followed by inorganic substances like sulphate and carbonates and chronic aquatic ecotoxicity for EDIP97, and also for silicate. With that, USES-LCA freshwater and EDIP97 chronic aquatic ecotoxicity provide results comparable to the ERA with EUSES. Nevertheless, EDIP97 chronic and USES-LCA freshwater deviate in defining the most contributing ingredients. As EUSES and USES-LCA are based on the same model with few variations and adaptations, a strong convergence of the results was to be expected.
- The results of IMPACT 2002 and USES-LCA marine water are similar to each other, but very distinct from the other LCIA methods and from the ERA results. According to IMPACT 2002 and USES-LCA marine water, inorganic substances are dominating the results. Surfactants do not have a significant impact on the final scores.
- In contrast to other recently published case studies [22], this detergent case study shows very little (if any) similarity between the underlying results of EDIP97 chronic ecotoxicity and USES-LCA marine water.

From a more methodological point of view, the following can be summarised:

- During the data collection in P&G internal databases and various external databases, some problems regarding data availability were encountered particularly for physico-chemical parameters and for chronic aquatic ecotoxicity. To ensure a broad applicability of the OMNIITOX results, it is therefore a key to keep the data requirements for the Base Model on a realistic level and to make the link to the ongoing REACH efforts in the context of the chemical regulations on an EC level [23] [24]. At the same time, the minimum data requirements must be sufficient to ensure a relevant assessment is feasible.
- As the extrapolation from ecotoxicity tests on freshwater organisms to marine water conditions cannot be easily performed and the data availability for toxicity tests on marine organisms is not expected to improve significantly in the foreseeable future, it was decided that the marine ecotoxicity will not form a part of the OMNIITOX Base Model.
- The differences between the LCIA methods can be considerable with respect to data needs (EDIP97 has the lowest data needs, IMPACT 2002 seems to be more demanding) and results. The difference in the results is likely to be due to different approaches or parameters towards toxicological effects and particularly in the fate and exposure modelling. The residence time in the water is assumed to be much higher in IMPACT 2002 due to lakes. This explains why the IMPACT 2002 results are mainly driven by inorganic substances and similar to those for seawater, whereas the other LCIA methods (and the ERA results) assign a key role to surfactants and, in case of the Eco-label approach, to perfumes. The high characterisation factors attributed to some inorganic substances like carbonates and chlorides according to some LCIA methods can be questioned regarding their environmental relevance, especially in marine systems. The issue of the residence time in the water compartments will be subject to further investigation within the OMNIITOX project.
- The situation that different LCIA methods will come up with different answers to the question concerning which detergent type is to be preferred regarding the impact category aquatic ecotoxicity to freshwater is not satisfactory in the absence of clear and justified reasoning. This hampers practical decision-support, as LCA practitioners usually will not be in a position to choose the 'right' LCIA method for their specific case. This puts a challenge to the OMNIITOX project to develop a method which finds common ground regarding the way to model fate and exposure as well as the effect side to overcome this situation of diverging results and to reflect realistic conditions as far as possible.

Abbreviations of detergent ingredients

AE7	Alkyl ethoxylate
AES	Alkyl ethoxysulfate
C12–15 AS	Alkylsulfate C12–15
C12–18 AS	Alkylsulfate C12–18
C8–10 quat. Ammonium	C8–10 Quaternary Ammonium Compound
LAS	Linear Alkylbenzenesulfonate
MEA	Monoethanolamine
TAE11	Tallow alkyl ethoxylate
ZnPhtalocyan. sulf.	Zinc phthalocyanine sulfonate

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References

[1] Wenzel H, Hauschild M, Alting L (1997): Environmental Assessment of Products. Vol.1 – Methodology, tools and case studies in product development. First edition. Chapman & Hall, United Kingdom, Kluwer Academic Publishers, Hingham, M.A., USA. ISBN 0-412-80800-5

[2] Huijbregts, MAJ (1999): Priority Assessment of toxic chemicals in LCA. Development and application of the multi-media fate, exposure and effect model USES-LCA. IVAM environmental research, University of Amsterdam, Amsterdam, The Netherlands

[3] Guinée JB (ed) (2001): Life Cycle Assessment: An operational guide to the ISO standards; LCA in perspective; Guide; Operational Annex to guide. Centre for Environmental Science, Leiden Univeristy, Leiden, The Netherlands, May 2001

[4] Pennington DW, Margni M, Jolliet O (2003 submitted): Risk-based indicators of cumulative contributions to toxicological effects for LCA. Environ Toxicol Chem[1]

[5] CEC (Commission of the European Communities) (1999): Establishing the Ecological Criteria for the award of the Community Eco-label to Laundry Detergents (1999/476/EC), Official Journal of the European Communities L187/52–68, Brussels, Belgium, 20.07.1999

[6] CEC (Commission of the European Communities) (1996). EUSES, the European System for evaluation of Substances. National Institute of Public Health and the Environment (RIVM), the Netherlands. Available from the European Chemicals Bureau (ECB/JRC), Ispra, Italy

[7] CEC (Commission of the European Communities) (1996): Technical Guidance Documents in support of the Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and the Commission Regulation (EC) 1488/94 on Risk Assessment for Existing Substances

[8] Molander S, Lidholm P, Schowanek D, Recasens M, Fullana P, Christensen FM, Guinée JB, Hauschild M, Jolliet O, Carlson R, Pennington DW, Bachmann TM (2004): OMNIITOX – Operational life-cycle impact assessment models and information tools for life-cycle impact assessment practitioners. Int J LCA 9 (5) 282–288

[9] Udo de Haes A (2002): Life Cycle Assessment (LCA): Its role and future position in SETAC – Don't stretch LCA too far, key note speech at Society of Environmental Toxicology and Chemistry (SETAC) 12th Annual SETAC Europe meeting Vienna (Austria): Challenges in Environmental Risk Assessment and Modelling, 12–16 May 2002

[10] Olsen SI, Christensen FM, Hauschild M, Pedersen F, Larsen HF, Tørsløv J (2001): Life cycle impact assessment and risk assessment of chemicals – A methodological comparison. Environmental Impact Assessment Review 21, 385–404

[11] Pant R, Schowanek D (2002): LCA and ERA comparison – A detergent case study within the OMNIITOX project, Society of Environmental Toxicology and Chemistry (SETAC, ed) 12th Annual SETAC Europe meeting Vienna (Austria): Challenges in Environmental Risk Assessment and Modelling, 12–16 May 2002, Brussels, 67

[12] Saouter E, Hoof van G, Pittinger CA, Feijtel, TCJ (2001).: The Effect of Compact Formulations on the Environmental Profile of Northern European Ganular Laundry Detergents, Part I: Environmental Risk Assessment. Int J LCA 6 (6) 363–372

[13] Owens JW (1997): Life Cycle Assessment in Relation to Risk Assessment: An Evolving Perspective. Risk Analysis 17 (3) 359–365

[14] Pant R, Hoof van G, Schowanek D, Feijtel TCJ (2003): Comparison of four LCIA methods for ecotoxicity based on a detergent case study within OMNIITOX, presentation at 13th Annual SETAC Europe meeting Hamburg (Germany), Society of Environmental Toxicology and Chemistry (SETAC ed), abstract book, p 18

[15] Saouter E, Feijtel T (2000): Use of Life Cycle Analysis and Environmental Risk Assessment in an Integrated Product Assessment. Environmental Strategies, Nordic Workshop, Vedbaek 1999, in Hauschild M, Olsen SI, Poll C (eds): Risk Assessment and Life Cycle Assessment, TemaNord 2000:545. Nordic Council of Ministers, Copenhagen (Denmark), 81–97

[16] Saouter E, Van Hoof G, Feijtel TCJ, Owens JW (2002): The Effect of Compact Formulations on the Environmental Profile of Northern European Granular Laundry Detergents, Part II: Life Cycle Assessment. Int J LCA (7) 27–38

[17] European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) (2001): Aquatic toxicity of Mixtures, ECETOC report No. 80, Brussels (Belgium), 2001

[18] Pant R, Schowanek D, Hoof van G, Feijtel TCJ (2003): OMNIITOX: Comparative ERA for three detergent products in a tiered approach, poster at 13th Annual SETAC Europe meeting, Hamburg (Germany), May 2003

[19] Hoof van G, Schowanek D, Feijtel TCJ: Comparative Life Cycle Assessment of Laundry Detergent Formulations in the UK, Part I: Environmental Fingerprint of five detergent formulations in 2001. Tenside Surfactants and Detergents (40) 2003, 266–275

[20] Guinée JB, Koning de A, Pennington DW, Rosenbaum R, Hauschild M, Olsen SI, Molander S, Bachmann TM, Pant R (2004): Bringing Science and Pragmatism together in a Tiered Approach for Modelling Toxicological Impacts in LCA. Int J LCA 9 (5) 320–326

[21] Margni M, Pennington D, Jolliet O, Guinée JB, de Koning A (2003): Multimedia Models Comparison: State of the Art in Life Cycle Assessment, presentation at 13th Annual SETAC Europe meeting Hamburg (Germany), Society of Environmental Toxicology and Chemistry (SETAC ed), abstract book, p 18

[22] Dreyer LM , Niemann AL, Hauschild MZ (2003): Comparison of three different LCIA methods: EDIP97, CML2001 and Eco-Indicator 99. Int J LCA 8 (4) 191–200

[23] CEC (Commission of the European Communities) (2001): White paper – Strategy for a Future Chemicals Policy. COM (2001) 88 final (CEC, Brussels, February, 2001)

[24] CEC (Commission of the European Communities; Directorate General Environment and Enterprise) (2003): Consultation document concerning the Registration, Evaluation, Authorisation and Restrictions of Chemicals (REACH). Available via the CEC web pages <http://www.europa.eu.int/comm/environment/index_en.htm> or <http://www.europa.eu.int/comm/enterprise/index_en.htm>

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Annex 1: Inventory results for emission of detergent ingredients at the end of use stage (after waste water treatment)

Ingredient	Unit	Regular Powder	Compact Powder	Compact Liquid
Alkyl ethersulfate (AES)	g	0.0603	0.1905	0
Alkyl ethoxylate (AE7)	g	0.7013	0.585	1.3873
Alkylsulfate	g	0	0.4971	0
Alkylsulfate C12–18	g	0.2262	0.2666	0
C8–10 Quaternary Ammonium Compound	g	0	0	0.2331
Boric Acid	g	0	0	1.5810
Brightener 15	g	0.032	0.0265	0
Brightener 49	g	0	0.0033	0
Brightener 36	g	0	0	0.0503
Carbonates (CO_{3-}, HCO_{3-}, CO_2, as C)+Percarbonate[a]	g	21.956	10.192	0
Carboxymethyl cellulose (CMC)	g	0.0827	0.3510	0
Ethoxylated Methyl Cellulose (EMC)	g	0.7354	0.7183	0
Chlorides	g	0.0021	0	0.0158
Citrate	g	0.5422	0.2516	0.2652
Dieth. triamine pentameth.phosph. (DTPMP))	g	0	0	0.0775
Quaternary Ammonium Compound	g	0.1074	0.1823	0
Dye	g	0.0017	0.0021	0.0005
Enzyme	g	0.2457	0.2576	0.2194
Ethanol	g	0	0	0.3436
Polymer 3	g	0.5986	0.5685	0
Cationic Polymer 1	g	0	0	0.4814
Polymer 2	g	0	0	0.2269
Ethylene diamine disuccinate (EDDS)	g	0.0445	0.0434	0
Hydrogenated fatty acids (Hyfac)	g	0.0048	0.0074	0
Topped Palm Kernel fatty acids (TPK FA)	g	0	0	1.2829
Hydroxyethane diphosphonate (HEDP)	g	0.0652	0.1138	0.0874
Cationic Polymer 2	g	0.0290	0.0292	0
Linear Alkylbenzenesulfonate (LAS)	g	1.4612	0.8760	1.8033
Monoethanolamine (MEA)	g	0	0	1.5521
Silicone	g	0.0286	0.0423	0
Silicone emulsion	g	0	0	0.0009
Perfume 1	g	0.0098	0.0072	0.0128
Perfume 2	g	0.1756	0.1294	0.2285
Polyacrylate	g	0.6728	0	0
Propyleneglycol	g	0	0	1.1620
Silicate	g	3.6098	5.3265	0
Silicon Dioxide (SiO_2)	g	0	0.0002	0
Soap	g	0.1124	0	0
Soil release polymer	g	0.0340	0.0349	0
Sorbitol	g	0	0.0036	0
Starch	g	0	0.1659	0
Sulphates (SO_{4-})	g	14.106	2.7217	0
Tallow alkyl ethoxylate (TAE11)	g	0.0471	0.0814	0
Tetraacetyl ethylenediamine (TAED)	g	0.6759	0.9211	0
Zeolite	g	3.7998	2.8244	0
Zinc phthalocyanine sulfonate	g	0.0003	0.0003	0

[a] For Percarbonate the same toxicity data is taken as for Carbonate. It is assumed that in spite of the formation of hydrogene peroxide due to the release of Percarbonate no hydrogene peroxide will be released into the surface water. Hydrogene peroxide will disappear due to rection with other ingredients in the grey water before it can be released into the environment.