Technical University of Denmark

Assessment of chemical emissions in life cycle impact assessment - focus on low substance data availability and

Larsen, Henrik Fred

Publication date:
2004

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Larsen, H. F. (2004). Assessment of chemical emissions in life cycle impact assessment - focus on low substance data availability and.

Assessment of chemical emissions in life cycle impact assessment

- focus on low substance data availability and ecotoxicity effect indicators

Henrik Fred Larsen

Thesis for the degree of Philosophiae Doctor

Ph.D. Thesis, October 2004
Department of Manufacturing, Engineering and Management
Technical University of Denmark

Supervisor:

Associate professor, Ph.D., Michael Z. Hauschild

Department of Manufacturing, Engineering and Management
Innovation and Sustainability
Technical University of Denmark
Kgs. Lyngby, Denmark

Assessment of chemical emissions in life cycle impact assessment
- focus on low substance data availability and ecotoxicity effect indicators

Cover: IPL
Printed by: IKON Document Services
ISBN: 87-91035-22-8

Innovation and Sustainability
Department of Manufacturing, Engineering and Management
Produktionstorvet, DTU-Building 424, Technical University of Denmark
DK-2800 Kgs. Lyngby
Phone: +45 45 25 48 00
Fax: +45 93 34 35
E-mail: info@ipl.dtu.dk

External examiners:

Senior Scientist, Ph.D., Peter M. Chapman

EVS Environmental Consultants
North Vancouver, Canada

Associate professor, lic.scient., K. Ole Kusk

E&R DTU
Department of Environment and Resources
Technical University of Denmark
Kgs. Lyngby, Denmark

Professor, Ph.D., Sverker Molander

Environmental Systems Analysis
Chalmers University of Technology
Göteborg, Sweden

Foreword

This Ph.D. thesis is a result of a Ph.D. study carried out in 2001 – 2004 at the Department of Engineering and Management, IPL, at the Technical University of Denmark with associate professor Michael Hauschild as supervisor. The Ph.D. study is part of KEMI (Centre for Chemicals in Industrial Production), which is a Danish joint know-how centre with the overall aim to promote the development of better products meeting technical quality requirements regarding health and the environment. KEMI is supported financially by the Danish Ministry of Science, Technology and Innovation.

The Ph.D. work has been carried out in close relation to the EU project OMNIITOX (Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments) seeking European consensus on how to assess toxic impact from chemical emissions in the context of life cycle assessment (LCA). Besides this thesis and the publications on which it is based, the Ph.D. study also comprises a production of a number of scientific reports, several oral presentations and poster presentations at international conferences/meetings (see Appendix). Furthermore, a two month stay at one of the academic OMNIITOX partners the Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland has been part of the Ph.D. study.

October 2004

Henrik Fred Larsen

In deep gratefulness to my beloved ones Anna, Celine and Lisbet

Acknowledgement

Michael Hauschild is gratefully acknowledged for his support and guidance throughout the entire Ph.D. study. Thanks to colleagues at IPL and IPU, especially Morten Birkved and Stig Irving Olsen, for discussions on scientific issues and help with PC software. The discussions and input from colleagues associated with the OMNIITOX project and from colleagues at DHI Water & Environment, especially Finn Pedersen, Jens Tørsløv and Gitte Pedersen, is also acknowledged.

Thanks to Olivier Jolliet and his LCA group, especially Jerome Payet, for organising my stay at EPFL.

The fruitful discussions and input from the steering committee members of the project "Ecolabelling of printed matter" (included in this thesis as a case study) is acknowledged. Thanks especially to Ninna Johnsen and Carsten Bøg, both from the Graphics Association of Denmark, Flemming Skovlund Schultz Grafisk A/S, Per K. Hansen Stibo graphic A/S and Jesper Gruvmark the Danish Environmental Labelling Secretariat.

The financial support of the Danish Ministry of Science, Technology and Innovation given via KEMI and the financial support from the Danish Environmental Protection Agency given via the project "Ecolabelling of printed matter" are acknowledged.

Finally, but not least, thanks to Christine Molin for English corrections of this thesis.

Summary

Life cycle assessment (LCA) studies on products or services seem generally to be carried out without a proper inclusion of potential toxic impacts from emissions of chemicals. The first goal of the thesis is to investigate this statement and to clarify whether or not the outcome of an LCA can be significantly dependent on the inclusion of toxicity- or chemical-related impact categories. The two main reasons for poor coverage of potential toxic impacts from chemical emissions in LCA studies are lack of available data on upstream emissions (e.g. emissions during production of raw materials) and lack of substance data on known emissions. To be able to characterize the potential toxic impacts on humans and the environment of chemical emissions, substance data on fate and effect are needed. The second goal of this thesis is to investigate how to deal with low substance data availability on especially effect data within the context of LCA, when the aim is to improve the inclusion of toxicity- or chemical-related impact categories.

The first goal regarding the significance of potential toxic impacts in LCA is investigated by carrying out a full LCA case study on printed matter and putting special emphasis on the inclusion of chemical emissions. The second goal regarding low data availability is addressed in two ways. First by introducing selection methods, which are chemical screening methods designed to select the most significant chemical emissions on a low to very low data availability. Secondly by developing a low data demand ecotoxicity effect indicator to be used together with a fate indicator, when estimating the potential impact of chemical emissions.

The results of the case study document that for LCAs on printed matter, the inclusion of chemical-related impact categories can be decisive for the outcome, and it shows that chemical-related impact categories are poorly or not at all included in previous studies. The share for the total environmental impact of for example the printing process in the case study is reduced from 41% to 10%, if the chemical-related impact categories are excluded. So, the basis for defining for example ecolabelling criteria (typically based on life cycle thinking) on printed matter is substantially different depending on whether or not the chemical-related impact categories are (properly) included.

The investigation on selection methods shows that only three chemical screening methods, associated with a characterisation method, and therefore here defined as selection methods, actually exist to day. Selection method performance criteria are developed including demands on consistency in prioritisation with associated characterisation method, applicability to different chemical groups, high data availability combined with low data demand, data useable in characterisation, user friendliness and transparency. A mainly qualitative evaluation of the existing selection methods against these performance criteria shows that none of these score high on all criteria, and this indicates the need for development of new selection methods. Recommendations on which components to include, which issues to address and general principles for developing selections methods are therefore given. A quantitative evaluation of the consistency in chemical ranking between the existing selection methods (EDIP-selection, Priofactor and CPM-selection), the risk ranking method EURAM, and the characterisation methods EDIP97 and CPM, is performed. The result of this evaluation shows a good correlation between the ranking of all the tested methods, but strongest between the EDIP97 method and its two associated selection methods EDIP-selection (revised version) and Priofactor. A statistical test of correlation in ranking between EDIP97, Priofactor, CPM and EURAM shows significant correlation in all cases. The main reason for this result is that a common perception of what makes a substance ecotoxicologically problematic

underlies all four methods. Nevertheless, some outliers as compared to the EDIP97 ranking are identified. These outliers are due to specific characteristics of each of the methods which for certain combinations of substance properties may result in false negatives or false positives as compared to EDIP97. These characteristics include the influence of data availability on the size of assessment factors for conversion of acute effect data to chronic values, and whether or not mode of entry is taken into account in the fate modelling. Further, the reversing of the effect of toxicity on ranking by negative logKow values is observed when logKow is a direct factor in the expression, and there is a significant influence of the way in which the BCF is estimated and included.

The second part of the second goal of this thesis, which deals with low availability of substance effect data, is addressed by carrying out an inventory of existing ecotoxicity effect indicator approaches, including a qualitative evaluation based on developed performance criteria. Both impact approaches, and damage approaches, which are all at an early development stage, are included. The evaluation of the existing impact approaches, i.e. the assessment factor-based PNEC approach and the PAF-based approach, shows pros and cons for both. However, taking the comparative nature of LCA and its aim for best estimate into account, and combining this with the possibilities for reducing the data demand of an EC_{50}-based PAF approach, and further including the (at least theoretical) connection to damage approaches, leads to the choice of an effect-based average PAF ecotoxicity effect indicator expressed by $0.5/HC50_{EC50}$ for further development. The most reasonable way to estimate the hazardous concentration for 50% of the included species (HC50) based on only three acute laboratory effect data is hereafter investigated by testing and discussing different ways of estimating averages (e.g. median and geometric mean), different data selection strategies and different ways of estimating uncertainty (confidence) limits around the $HC50_{EC50}$ value. The results of this investigation show that the geometric mean is the most robust estimator for small data sets. Seeking the coverage of many chemicals in LCA and considering the fact that the main part of the useable single species laboratory test data (EC_{50}) is on algae, crustacean and fish, which in practice represent the trophic levels primary producers, primary consumers and secondary consumers, the use of a minimum of three acute EC_{50} values from each of these three throphic levels is recommended when estimating $HC50_{EC50}$. Due to the comparative nature of LCA, the possible bias from severe unequal species representation and inclusion of erroneous data, due to bad non-standardised test conditions, should be avoided by only including tests on standard organisms fulfilling certain defined test criteria on durations and endpoints. Further, in order to avoid the effect of possible haphazard or regulatory determined species representations in the data set used, which may be decisive for the weighting of each trophic level in the estimation, the geometric mean based on the average of the averages within each trophic level is chosen for the ecotoxicity effect indicator GM-troph. Hereby, it is consciously chosen to put equal weight on each throphic level. The statistical confidence limits around the GM-troph are in most cases too wide, because the average is based on only three data values, making a statistically significant differentiation between the different toxicants nearly impossible. However, test on fictitious three data value test sets based on combinations of max and min values from a larger ‘mother’ data set indicates that the use of the min and max value among the three data value GM-troph data set (i.e. average within algae, average within crustacean and average within fish) as max-min limits around GM-troph gives a reasonable (and as good as confidence limits) certainty that the ‘true’ GM-troph value (based on the full ‘mother’ data set) lies within the interval.

The inclusion of the toxicity-related impact categories in LCA at a similar level as the better established impact categories, like global warming, is far from achieved yet. This thesis point at relatively well functioning selection methods and defines the framework including performance criteria and recommendations on how to improve existing selection methods and how to develop new ones. By introducing the GM-troph this thesis contributes with a robust, low data demanding effect part of the ecotoxicity characterisation factor. The GM-troph has the potential of facilitating a high number of characterisation factors which are robust with relatively low uncertainty if combined with a ‘fate part’ of equal strength. The way for further improvement of the involvement of toxicity-related impact categories in LCA is hereby facilitated.

Resumé

Livscyklusvurderinger (LCV) af produkter gennemføres i dag i mange tilfælde uden at toksiske effekter af kemikalie-emissioner inddrages. Hvis der tages hensyn til disse, er inddragelsen typisk mangelfuld. Et af målene med denne ph.d. afhandling er at belyse denne påstand samt undersøge systematisk om inddragelse af de kemikalie- eller toksicitets-relaterede påvirkningskategorier kan have afgørende betydning for resultat af et LCV studie. De to vigtigste årsager til mangelfuld inddragelse er manglen på data vedrørende opstrøms-emissioner (f.eks. emissioner i forbindelse med produktion af råvarer) og mangel på stofdata for de kendte emissioner. At kunne karakterisere den potentielle toksiske påvirkning på mennesker og miljø kræver nemlig at stofdata vedrørende skæbne og effekt er tilgængelige for de pågældende kemikalie-emissioner. Et andet mål for denne ph.d. afhandling er at undersøge hvordan begrænset tilgængelighed af specielt effektdata håndteres bedst i en LCV sammenhæng, når målet er at forbedre inddragelsen af kemikalie-relaterede påvirkningskategorier.

Det første mål vedrørende betydningen af kemikalie-relaterede påvirkningskategorier undersøges ved at udføre en fuld LCV på tryksager med speciel fokus på inddragelse af mulige toksiske påvirkninger af kemikalie-emissioner. Det andet mål behandles på to niveauer. Først ved at introducere selektionsmetoder, som er kemikalie-screeningsmetoder, der anvendes til at screene for betydende kemikalie-emissioner blandt typisk flere hundrede. Dernæst ved at udvikle en økotoksicitetseffektindikator, som er i stand til at fungere på basis af kun tre akutte laboratorium effekt data.

Resultatet af livscyklusvurderingen på tryksager dokumenterer at inddragelse af kemikalie-relaterede påvirkningskategorier kan have afgørende betydning for udkommet af et LCV studie, og at mulige toksiske påvirkninger fra kemikalie-emissioner kun i begrænset omfang eller slet ikke er inddraget i tidligere LCV studier inden for denne produktgruppe. F.eks. viser det sig, at betydningen af trykkeprocessen for den samlede miljøbelastning i hele tryksagens livsforløb reduceres fra 42% til 10%, hvis de kemikalie-relaterede påvirkningskategorier udelades. Grundlaget for at definere miljømærkekriterier på tryksager, som typisk er baseret på en livscyklustankegang, kan derfor være vidt forskellig afhængig af om de kemikalie-relaterede påvirkningskategorier er (forsvarligt) inddraget eller ej.

Undersøgelsen af selektionsmetoder viser, at der i dag kun eksisterer tre kemikaliescreeningsmetoder, som er tilknyttet karakteriseringsmetoder og derfor kan betegnes som selektionsmetoder. En hovedsagligt kvalitativ vurdering af disse metoder baseret på et sæt af udviklede vurderingskriterier (f.eks. graden af konsistens med den tilknyttede karakteriseringsmetode mht. rangordning af kemikalie-emissioner) viser, at ingen scorer højt for alle kriterier, hvilket indikerer et behov for udvikling af nye selektionsmetoder. Der opstilles derfor generelle principper for udvikling af selektionsmetoder, herunder hvilke komponenter der bør indgå. Herudover er der gennemført en kvantitativ test af overensstemmelse i kemikalie-rangordning mellem de tre eksisterende selektionsmetoder (UMIP-selektion, Priofaktor og CPM-selektion), risikoscreeningsmetoden EURAM, og de to karakteriseringsmetoder UMIP og CPM. Resultatet af denne test viser rimelig god overensstemmelse i rangordning mellem de testede metoder men stærkest imellem UMIP og de to associerede selektionsmetoder UMIP-selektion og Priofaktor. En statistisk test af korrelation mellem rangordning af UMIP, Priofaktor, CPM og EURAM viser signifikant korrelation i alle tilfælde. Hovedårsagen til dette er, at estimeringsprincipperne i alle disse metoder afspejler en fælles opfattelse af, hvad der gør et stof økotoksikologisk problematisk, nemlig det såkaldte PBT princip

(Persistent, Bioaccumulative, Toxic). Hvis rangordningen af de testede kemikalier for de øvrige metoder sammenlignes med UMIP's rangorden kan flere outsidere dog konstateres. Disse afvigelser skyldes specifikke egenskaber ved den enkelte metode, som ved bestemte kombinationer af iboende egenskaber hos de testede kemikalier kan resultere i falsk negative eller falsk positive udfald i forhold til UMIP. Disse egenskaber omfatter blandt andet betydningen af datatilgængelighed på størrelsen af den vurderingsfaktor (assessment factor), der anvendes ved konvertering af akutte effekt data til kroniske, og hvorvidt der er taget hensyn til hvilket medie kemikaliet udledes til ("mode of entry").

Målet vedr. den lave effektdata tilgængelighed behandles i første omgang ved at kortlægge eksisterende økotoksicitetseffektindikatorer og evaluere disse på basis af et opstillet sæt af vurderingskriterier omfattende bl.a. videnskabelig validitet og data krav. Kortlægningen omfatter både indikatorer, der er defineret tidligt i miljømekanismen (midpoint or impact indicators) og derfor udtrykkes som påvirkning af miljøet, og indikatorer, der er forsøgt defineret sent i miljømekanismen (endpoint or damage indicators) og derfor forsøger at udtrykke skade på miljøet. Den sidstnævnte type er dog stadig på et tidligt udviklingsstadie. To hovedtyper af økotoksicitetseffektindikatorer baseret på påvirkning (impact indicators) eksisterer, nemlig de vurderingsfaktorbaserede PNEC tilgange og de artsfølsomhedsfordelingsbaserede PAF tilgange. Begge viser fordele og ulemper, når de holdes op imod de opstillede vurderingskriterier. Dog vurderes en EC_{50} baseret PAF tilgang at være den mest fornuftige, når det bl.a. tages i betragtning at LCV er baseret på en relativ sammenligning (ikke absolut) af de forskellige kemikalie-emissioner, hvor der søges et bedste estimat og ikke et konservativt estimat som typisk i risikovurdering. Herudover sikres endvidere, i hvert fald i teorien, muligheden for at modellere hele vejen til skade i miljømekanismen. Den valgte indikator kan udtrykkes som $0,5/HC50_{EC50}$, hvor $HC50_{EC50}$ er den koncentrationsstigning i miljøet forårsaget af en given kemikalie-emission, der antages at have effekt (f.eks. 50% reduktion af reproduktionsevne) på 50% af de forekommende arter. Den mest fornuftige måde at estimere HC50 på basis af minimum tre akutte EC_{50} værdier undersøges herefter ved både teoretiske overvejelser og test på konkrete data. Herudover undersøges forskellige datavalgstrategier og forskellige måder at estimere usikkerhedsintervaller omkring HC50. Resultatet af disse undersøgelser viser at den mest robuste estimator for små data sæt er geometrisk gennemsnit. Hvis det tages i betragtning, at vi i LCV søger at dække så mange kemikalie-emissioner som muligt og at hovedparten af brugbare enkeltarts laboratorium test resultater er udført på alger, krebsdyr og fisk, som i praksis repræsenterer tre trofiske niveauer i et ferskvandsøkosystem, nemlig primær producenter, primær konsumenter og sekundære konsumenter, anbefales det at minimum i alt tre EC_{50} værdier fordelt på hver af disse trofiske niveaur benyttes ved estimering af $HC50_{EC50}$. Det anbefales at kun EC_{50} værdier fra test på standard organismer, der lever op til bestemte krav, hvad angår endpoint (f.eks. mortalitet) og tid, anvendes, for at undgå skævhed i estimeringerne af $HC50_{EC50}$ for de enkelte kemikalier, forårsaget af bl.a. uens kvalitet af de anvendte EC50 værdier. Endvidere anbefales det at anvende de geometriske gennemsnit inden for hvert trofisk niveau som de tre data værdier der anvendes ved estimering af $HC50_{EC50}$, der herved benævnes GM-troph. Dette gøres for at undgå mulig skævvridning på grund af tilfældigt bestemt antal EC50 værdier på hvert trofisk niveau, f.eks. voldsom dominans af fiske data som konsekvens af myndigheders fokus på fisk for visse stoffer. Ved at anvende GM-troph vælges bevidst at vægte de tre trofiske niveauer ens. Konfidens intervallerne omkring $HC50_{EC50}$ er i de fleste tilfælde meget vide på grund af få data, hvilket gør differentiering mellem de enkelte værdier næsten umulig. For GM-troph anbefales det at anvende max-min værdier defineret ud fra de tre geometriske gennemsnit fra hver af de trofiske niveauer, således at den højeste værdi anvendes som max værdi og den laveste værdi som min værdi.

Endnu er vi langt fra at de kemikalie-relaterede påvirkningskategorier inddrages på samme niveau, som de mere etablerede påvirkningskategorier (f.eks. drivhuseffekt), når der udføres LCV studier. Denne ph.d. afhandling peger dog på relativt velfungerende selektionsmetoder og beskriver hvordan nye kan udvikles. Ved at introducere GM-troph bidrages endvidere med en robust økotoksicitetseffektindikator med lavt data behov. Hvis GM-troph kombineres med en skæbne indikator med tilsvarende styrke, vil et stort antal robuste karakteriseringsfaktorer for økotoksicitet kunne estimeres. Denne ph.d. afhandling har hermed bragt os et skridt nærmere muligheden for at inddrage toksiske effekter af kemikalie-emissioner i livscyklusvurderinger på en behørig måde.

Contents

1 Introduction 1
  1.1 Goal and scope of the thesis 1
  1.2 Life Cycle Assessment 2
    1.2.1 Life Cycle Impact Assessment 4
  1.3 The importance of chemical related impact categories in LCIA 8
    1.3.1 Results of the case study 8
    1.3.2 Conclusions on the case study 11
  1.4 Selection methods – qualitative evaluation and framework 11
    1.4.1 Results of the qualitative evaluation of selection methods 12
    1.4.2 Conclusions on the qualitative study on selection methods 13
  1.5 Selection methods – quantitative evaluation 14
    1.5.1 Results of the quantitative evaluation of selection methods 15
    1.5.2 Conclusions on the quantitative study on selection methods 16
  1.6 Ecotoxicity effect indicators – inventory and evaluation 17
    1.6.1 Results of the inventory and evaluation of EEIs 18
    1.6.2 Conclusions on the inventory and evaluation of EEIs 21
  1.7 Development of a low data demanding EEI: GM-troph 22
    1.7.1 Results of the development of GM-troph 23
    1.7.2 Conclusions on the development of GM-troph 31
  1.8 Discussion and conclusion 33
  1.9 References 38
2 Importance of chemical-related impact categories - a case study 45
3 Selection methods 75
4 Ranking performance of selection methods 91
5 Ecotoxicity effect indicators 109
6 GM-troph: An ecotoxicity effect indicator based on three data values 137

Appendix: Publications, posters and oral presentations 167

Glossary

Acronyms

ACR	Acute-to-Chronic-Ratio
AF	Assessment Factor
AOX	Absorbable Organic Halogens
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BDF	BioDegradation Factor
BM	Base Model
CA	Concentration Addition
CART	Classification And Regression Tree analysis
CDF	Cumulative Distribution Function
CF	Characterisation Factor
COD	Chemical Oxygen Demand
CPM	Competence Centre for Environmental Assessment of Products and Materials Systems
CRS	Chemical Ranking and Scoring
EC$_{50}$	Effect Concentration (50% of test organism affected)
ECOSAR	Name of Ecotoxicological estimation (QSAR) program
EDIP	Environmental Design of Industrial Products
EEI	Ecotoxicity Effect Indicator
EPA	(US.) Environmental Protection Agency
EURAM	EU Risk Ranking Method
EUSES	European Union System for the Evaluation of Substances
fu	functional unit
GM	Geometric Mean
HC5	Hazardous Concentration for 5% of included species
HC5$_{NOEC}$	HC5 based on NOEC values
HC50	Hazardous Concentration for 50% of included species
HC50$_{NOEC}$	HC50 based on NOEC values
HC50$_{EC50}$	HC50 based on EC$_{50}$ values
HDT	Hasse Diagram Technique
HU	Hazard Units
IPA	Isopropyl alcohol
K$_d$	Soil adsorption coefficient
K$_{oc}$	Adsorption coefficient for organic carbon
LC$_{50}$	Lethal concentration (50% of test organism dead)
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LOEC	Lowest Observed Effect Concentration
LogK$_{ow}$	The logarithm of the Octanol/Water partition coefficient
LowEC$_{50}$	Lowest EC$_{50}$
MET	Mean Extinction Time
mPE	milli-person-equivalents
mPET	milli-person-equivalents-targeted
mPET$_{WDK2000}$	mPET based on World and Danish WFs with target year 2000
mPE$_{WDK90}$	mPE based on World and Danish NRs for the year 1990
mPR	milli-person-reserves
msPAF	multi-substance PAF
N.C.	Not Classified

NMVOC	Non Methane Volatile Organic Carbon
NOEC	No Observed Effect Concentration
NR	Normalisation Reference
OECD	Organisation for Economic Co-operation and Development
OMNIITOX	Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments
PAF	Potentially Affected Fraction of species
PBT	Persistence, Bioaccumulation and Toxicity
PDF	Probability Distribution Function
PE	Person Equivalents
PET	Person Equivalents Targeted
PVF	Potentially Vanished Fraction of species
pKa	Dissociation constant for acids (and bases)
PNEC	Predicted No Effect Concentration
PR	Person-Reserves
QSAR	Quantitative Structure Activity Relationship
RA	Response Addition
R-phrases	Risk phrases
SAR	Structure Activity Relationship
SBM	Simple Base Model
SETAC	Society of Environmental Toxicology and Chemistry
SM	Selection method
SSD	Species Sensitivity Distribution
$T_{1/2}$	Half-life
TGD	Technical Guidance Document
TMoA	Toxic Mode of Action
TOC	Total Organic Carbon
USES	Uniform System for the Evaluation of Substances
VOC	Volatile Organic Carbon
WF	Weighting Factor
WMPT	Waste Minimization Prioritization Tool
WWTP	Waste Water Treatment Plant

Definitions

Category indicator	“Quantifiable representation of an impact category” (ISO 2000a).
Characterisation factor	“Factor derived from a characterisation model which is applied to convert the assigned LCI results to the common unit of the category indicator “ (ISO 2000a).
Characterisation method	A method or model used to derive characterisation factors.
Chemical-related impact categories	Impact categories on ecotoxicity and human toxicity.
CRS-method	A tool to provide practical information on human health and environmental hazard, exposure, and/or risk of chemicals for risk management decisions (Davis et al. 1997).
Energy-related impact categories	Global warming, acidification and nutrient enrichment, and in many cases photochemical ozone formation.
Impact category	“Class representing environmental issues of concern to which LCI results may be assigned” (ISO 2000a). For example ecotoxicity and human toxicity.

Selection method	A method to select (prioritise) those emissions (chemicals) from the inventory of a specific LCA-study that are most likely to contribute - according to a specific characterisation method - significantly to the impact categories on ecotoxicity and human toxicity.
Toxicity-related impact categories	Impact categories on ecotoxicity and human toxicity.
β	Scale parameter.
γ	Slope factor.

1 Introduction

For a person, especially in the Western world, an acceptable living standard today is closely connected to the possession of, or access to, services or products, products; which may all be defined by the service they provide, e.g. cars for transport and newspapers for printed communication. However, the procurement, use and final disposal of products does in all cases have a more or less severe impact on the environment. But how does society meet the need for products in an optimal way if protection of the environment has to be taken into account. One of the tools or approaches to reach this goal is (product) life cycle assessment (LCA), serving as a decision supporting tool. LCA is a holistic analytical tool looking at the total environmental impact of a product from extraction of raw materials over production and use, and ending up with the final disposal. In other words the life cycle of the product is covered from ‘cradle to grave’. By comparing the LCAs of different ways to procure, use and dispose products serving the same service (e.g. glass bottles and tin canes for containing soft drinks), the optimal way from an environmental point of view may be found.

The overall frame of this thesis is LCA but within this frame the focus is on chemical emissions occurring during the life cycle of a product. These emissions contribute to toxic impacts on humans and the environment, which in the LCA terminology are categorized in impact categories on human toxicity and ecotoxicity respectively. The part of the LCA procedure where the potential impacts from the emissions are estimated and evaluated is called life cycle impact assessment (LCIA). LCIA is the frame of this thesis.

The main results of this Ph.D. study are presented as verbatim versions of five papers submitted to or published in international peer-reviewed journals in Chapter 2 – Chapter 5. The main results of the research described in these chapters are summarized below in this introduction (Section 1.4 - Section 1.7). In Section 1.1 the goal and scope of the thesis is presented, and in the following two sections the frame of this thesis, i.e. LCA and LCIA, is shortly described. A discussion and conclusion relating the results of this Ph.D. study to the goal and scope of the thesis can be found in Section 1.8. Finally, a full overview of the publications, posters, oral presentations and other outputs from this Ph.D. study may be found in the Appendix.

The terms ‘toxicity-related impact categories’ and ‘chemical-related impact categories’ are used synonymously in the thesis. They both cover the ecotoxicity and human toxicity-based impact categories to which emissions of specific chemicals exclusively contribute.

1.1 Goal and scope of the thesis

When dealing with toxicity-related impact categories in LCIA the main problem today, besides problems with lack of data on especially upstream emissions, seems to be the low availability on substance data for the emitted chemicals. Inventories on products like printed matter and textiles may include several hundred different chemical emissions. Many of the chemicals emitted during the life cycle of a product may be important in an environmental context for only a few products and therefore not considered as important in traditional societal regulation focusing on high production volume chemicals and known very toxic and/or persistent chemicals. This seems to be one of the reasons why data on fate and potential effects on humans and the environment of many of the chemicals involved in an LCA are few or non-existing. So, estimation of impact potentials for the toxicity-related impact categories becomes very difficult or impossible and in many cases these impacts are only included in an incomplete way, if at all.

The goal is to investigate whether or not this is a problem for LCA and in the affirmative case to contribute to a solution. The aim is to answer the following questions:

1. Can the outcome of an LCA (i.e. the impact profile) be significantly dependent on whether or not toxicity related-impact categories are included?
2. If the inclusion of toxicity-related impact categories can be decisive, how is the problem with low data availability solved the most optimal way?

Question 1 is investigated by use of a case study on printed matter comprising a life cycle including many chemical emissions. Question 2 is sought answered at two levels. First, at the chemical screening level by defining the framework for selection methods to be used for selecting only significant chemical emissions to be included in the characterisation step of LCIA. Second, at the level of potential impacts on the ecosystem by the development of an ecotoxicity effect indicator (EEI) able to work on only three acute ecotoxicity data.

Development of a new selection method is not part of the thesis. This work is covered by co-workers within the OMNIITOX project on the basis of the framework described here.

The thesis includes both human toxicity and ecotoxicity but a focus on ecotoxicity effects means that only this issue is included in the last part dealing with EEIs.

In order to provide the reader with the context within which this thesis has been developed, the concepts of LCA and LCIA are described shortly below.

1.2 Life Cycle Assessment

Life cycle assessment (LCA) is a holistic approach to assess potential environmental impacts of human activities involved in providing a product or service described and quantified in the functional unit. In its most comprehensive form, LCA includes all exchanges, i.e. emissions and resource consumptions, in the whole life cycle of a product, from extraction of raw materials to final disposal ('cradle to grave'). An LCA study may, thus, include several decades in time and exchanges occurring all over the world.

Important uses of LCA are product development and ecolabelling. In product development it is typically used for comparing the life cycle-based environmental performance of one product (or service) against one or more alternatives all providing the same functional unit. So, in this case it may support the management decision on which alternative to chose. In ecolabelling it may be used to identify the stages or processes with highest potential impact (i.e. 'hot spots') in the life cycle of a product or product group. In this way it may deliver important documentation for ecolabel criteria development, i.e. where to focus or put weight in the criteria set.

An example of a life cycle for printed matter is shown in Figure 1. For the sake of clarity only the raw material stage for the main material paper is shown in the figure. Other raw materials like printing ink have comparable steps. The printing company in Figure 1 is illustrated as heavily polluting because this is traditionally the focus point when looking at the potential impact from providing the service of printed communication to the society.

However, at each stage in the life cycle resources are consumed and emissions of e.g. chemicals occur, and this is actually what the holistic LCA approach is taking into account.

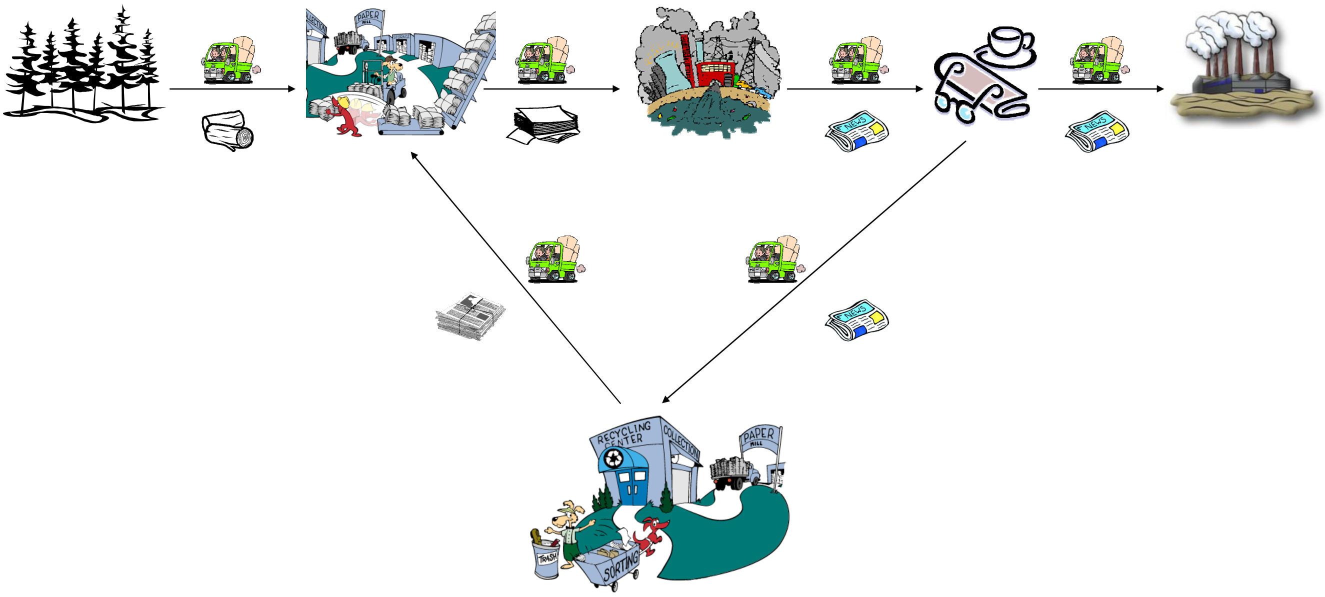

Figure 1. Life cycle of printed matter

The different types of resources used and emissions occurring are many and varied in a life cycle like the one depicted in Figure 1. Fuel consuming machinery used in forestry emits air contaminants, and consumption of bleaching chemicals at the paper mill gives rise to water emission of chlorinated organic substances, just to mention a few. In an LCA all these exchanges with the environment are quantified and related to the product, in this case the printed matter, e.g. one newspaper. Further, the fuel may have been produced some years ago in the Middle East, the forestry done in Eastern Europe, the bleaching chemicals produced in South America and the paper mill placed in Scandinavia. So, the time and geographical extent may be large. In most cases, all temporal and spatial details of the processes are not known, and this leads to a frequent use of generic data. The LCA approach is therefore quite different from the traditional way to assess environmental and health impacts of human activities by use of risk assessment, typically focusing on the (local) impact of a specific chemical emitted under more or less well defined conditions in time and space.

The methodological framework for LCA is described in ISO 14000-series (ISO 1997, 1998, 2000a, 2000b) and further elaborated upon for the impact assessment part in Udo de Haes & Lindeijer (2002). The main steps in LCA include:

1. Goal and scope definition
2. Inventory
3. Impact assessment
4. Interpretation

The first challenge to deal with when starting up an LCA study is to define the framework of the study, i.e. the goal and scope definition. During this step the goal and intended use of the study is described, the functional unit is defined and the scope of the technological level included, the time period covered, and the geographical extent is described.

Having the study well defined the next step is the inventory, where all resource consumption and emissions for the processes in the life cycle of the product is mapped and related to the functional unit, taking the scope of the study into account.

The third step comprises the impact assessment where the potential impacts or damages from the emissions, and in some cases also the resource consumption, are assessed.

The last step is the interpretation where the results are held up against the goal of the study, discussed and conclusions made. Sensitivity analyses to test the robustness of the results and uncertainty analysis are typically involved. The study may be externally peer-reviewed in order to strengthen the reliability of the conclusions in this kind of complex environmental assessment.

It must be emphasized that an LCA study is an iterative process where results and experience achieved at one step may lead to revisions at another (previous) step, e.g. revision of the scope, and several iterations of the LCA procedure may be involved in an LCA study.

This thesis deals almost exclusively with the impact assessment step, which is therefore described separately in the next section.

1.2.1 Life Cycle Impact Assessment

Several LCIA methods exist today, covering types where the modelling of toxicity-related impact categories are based on modification of tiered generic risk assessment, like EDIP97 (Wenzel al. 1997) and USES-LCA (Huijbregts et al. 2000) and methods trying to avoid the conservative approach in risk assessment like Eco-Indicator 99 (Goedkoop & Spriensma 2001a, 2001b) and Impact 2002+ (Jolliet et al. 2003). Methods comprising monetarisation of environmental impacts also exist like EPS (Steen 1999) based on the principle of ‘willingness to pay’. Some of these methods like the EDIP97 (Wenzel et al. 1997) also include instructions on how to deal with the other steps in the LCA procedure described in Section 1.2., i.e. goal and scope definition, inventory and interpretation.

The goal of a life cycle impact assessment (LCIA) is to give an assessment of the potential impact (or damage) from the whole life cycle of a given product on the chosen ‘areas of protection’ (or ‘safeguard subjects’) of the LCA, i.e. the properties on which the LCA is performed in order to help us protect against unwanted damages, i.e. human health, natural environment, natural resources, man-made-environment and life support functions (Udo de Haes & Lindeijer 2002). Natural environment and human health are typically included in terms of impact categories comprising both potential global impacts like global warming and ozone depletion, and potential regional impacts like acidification, nutrient enrichment, photochemical ozone formation and chronic toxicity to humans and ecosystems. Some LCIA methods like the EDIP97 (Wenzel et al. 1997) also include local impacts like acute toxicity to humans and ecosystems. Relatively newly developed impact categories on for example land use and coming ups like desiccation may also be included.

The potential effects modelled within each of these impact categories are in most cases (e.g. Huijbregts et al. 2000, Wenzel et al. 1997) only modelled to the level of midpoint or impact along the environmental mechanism or impact chain (ISO 2000a, Udo de Haes & Lindeijer 2002). However, some attempts have been done to model all the way to damage or endpoint, for example the Eco-indicator 99 (Goedkoop & Spriensma 2001a, 2001b) using the endpoints human life years lost (actually disability adjusted life years) for damage to humans and potentially disappeared fraction of species for damage to ecosystems.

LCIA comprises two steps, i.e. classification and characterisation, which are mandatory according to ISO 14042 (ISO 2000a), but it may also include the optional steps normalisation and valuation (weighting).

During *classification* the impact categories to be included are chosen and the emissions mapped in the inventory are assigned to the relevant impact categories, e.g. carbon dioxide (CO_2) and methane (CH_4) emissions are assigned to global warming potential (gwp), and the CH_4 emission is also assigned to photochemical ozone formation.

Then during *characterisation* a category indicator result (CIR) is calculated for each impact category, by summing up the results of each assigned emission quantity (Q) multiplied by its corresponding characterisation factor (CF) within that impact category:

$CIR_{\text{impact category A}} = Q_1 * CF_{1A} + Q_2 * CF_{2A} + \ldots\ldots\ldots$

For example for global warming:

$CIR_{gwp} = Q_{CO2} * 1 + Q_{CH4} * 25 + \ldots\ldots\ldots$

In this example CF_{CO2} has the value 1 gram CO_2 per gram CO_2 emitted and CF_{CH4} the value 25 gram CO_2 per gram CH_4 emitted, so the resulting CIR_{gwp} is given in the unit gram of CO_2. As is indicated by this example, all the characterisation factors for the emitted substances contributing to global warming are expressed in units of CO_2 equivalents.

A characterisation factor expresses the potential effect on the actual area of protection per emitted amount of the substance in question. The effect may be expressed indirectly if only modelled to the midpoint, i.e. CO_2 equivalents in the example above, or directly if modelled to damage, e.g. human life years lost as a consequence of global warming.

The collection of category indicator results for all the impact categories included in a study represents the characterised LCIA profile of the product. This profile can be presented as such, see Table 1, but may be further elaborated by use of normalisation and further by valuation to assist comparisons across impact categories.

The aim of *normalisation* is to provide an impression of the relative magnitude of the potential impacts and resource consumptions. The category indicator results are related to reference information, typically the background impact from society’s total activities. In for example the EDIP97 method (Wenzel et al. 1997), this reference information consists in the total impact potential or resource consumption in the reference region divided by the number citizens in that region. For example for global warming the reference information or normalisation reference (NR) for the year 1990 is 8,700 kg CO_2-equivalents/person/year, meaning that in 1990, greenhouse gases equivalent to 8,700 kg CO_2 was emitted to air on average for each citizen worldwide. The NR therefore represents the annual impact of an average person. Also for the other global impact categories, and for all resource consumptions, the NR is based on global values whereas for the regional ones, it may be based on values for Europe or another region.

Table 1. Simplified example of an LCIA profile showing the category indicator results for the functional unit of one ton printed matter. Only four impact categories included.

Impact category	Amount	Unit
Global warming	1,400,000	gram CO_2-equivalents
Photochemical ozone formation	1,600	gram C_2H_4-equivalents
Acidification	4,000	gram SO_2-equivalents
Nutrient enrichment	5,400	gram NO_3^--equivalents

The normalized category indicator results and normalized resource consumptions are calculated by dividing the category indicator result or resource consumption by the corresponding NR. The normalised results are, thus, expressed in units of person-equivalents (PE) or typically multiplied by 1000 and designated milliperson-equivalents (mPE) in the EDIP97 method. An example of a normalized LCIA profile is shown in Figure 2.

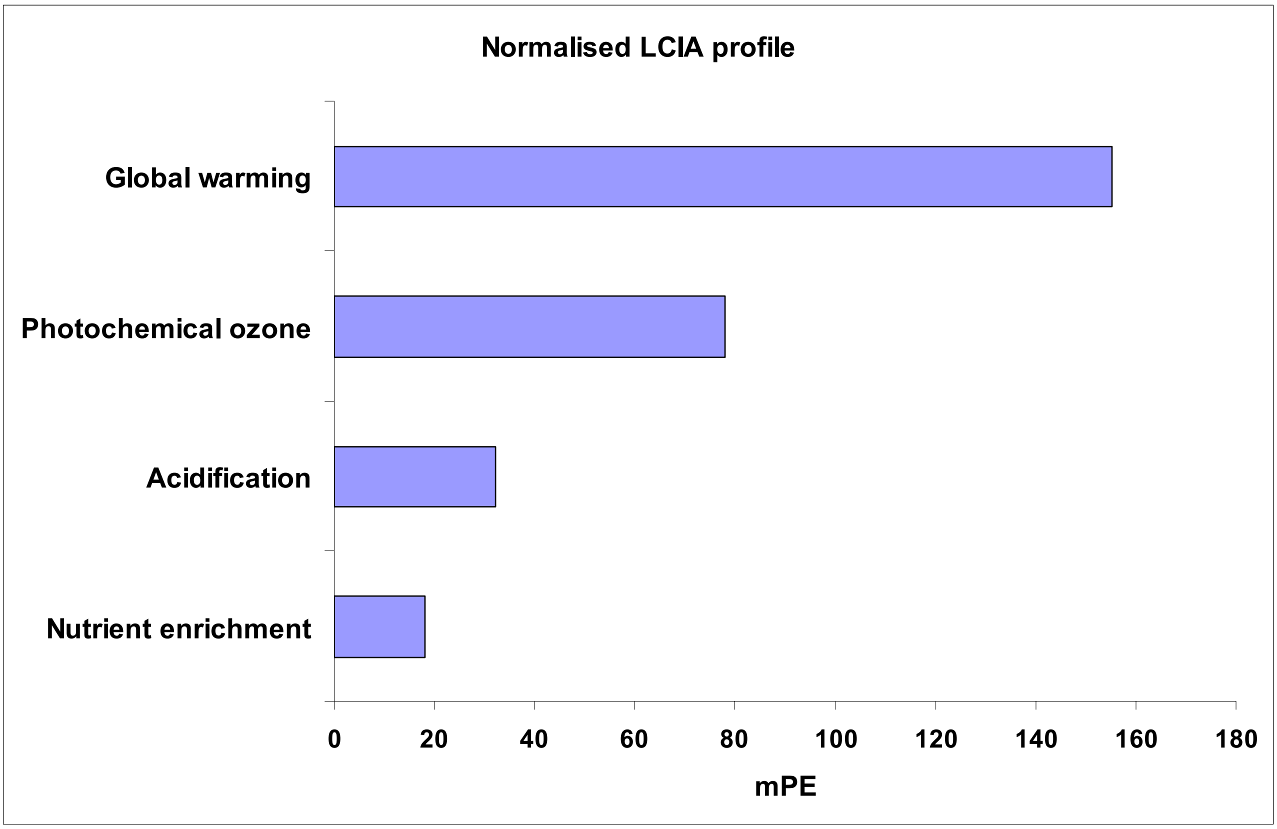

Figure 2. Simplified example of a normalized LCIA profile showing the normalized category indicator results for the functional unit of one ton printed matter. Only four impact categories are included and normalisation references from EDIP97 (Wenzel et al. 1997) are used.

By normalisation the different potential impacts from the product system in question (i.e. the functional unit) are expressed relative to the impacts from an average person in for example 1990. However, we have no indication of how serious (as related to the goal of the study) the different normalized category indicator results are compared to one another. This may be achieved by *valuation*, typically based on subjective preferences and stakeholder values, and involving the use of scores or weighting factors.

Weighting factors (WFs) for the potential environmental impacts may be based on ‘revealed preference approaches’ like for example ‘distance to political reduction targets’ (Wenzel et al. 1997) and ‘willingness to pay’ (Steen 1999), based on governmental and international conventions on reduction targets, and the willingness in the society to pay for restoration of impacts on ‘areas of protection’ respectively. WFs may also be based on a ‘panel approach’, i.e. direct questioning of a representative group in society, like in the Eco-indicator 99 method (Goedkoop & Spriensma 2001a, 2001b). The possibilities of using sustainability as grounds for weighting have been discussed (e.g. Hauschild & Wenzel 1998) but a method has never been developed. For the resource consumption the WFs may be based on the scarcity of the resource expressed as supply horizon.

In the EDIP97 method (Wenzel et al. 1997) the WFs for the individual impact categories are based on the Danish political targets for the reduction of impact within regional and local impact categories, whereas weighting of the global impact categories is based on international conventions and plans of action for reduction. The reference year is 1990 and the target year is 2000 meaning that if the political target is to reduce the impact within a certain impact category by 50% during that period the WF becomes 2 (100/50 = 2).

The weighted normalized category indicator results are calculated by simply multiplying the normalized category indicator results by the corresponding weighting factor and in for example the EDIP97 method expressed in targeted milliperson-equivalents (mPET).

For normalized resource consumption the supply horizon for non renewable resources is calculated by dividing the known reserves by the annual global consumption. The WF is afterwards calculated as the reciprocal of the supply horizon. The normalized resource consumption is multiplied by the corresponding weighting factor giving rise to the weighted normalized resource consumption expressed in for example units of milliperson-reserves (mPR).

By weighting we have the opportunity to aggregate all the environmental impact category indicator results into one common impact score and similarly all the individual resource consumptions into another common score. In the EDIP97 method the WFs are 1.3 for both global warming and acidification and 1.2 for both nutrient enrichment and photochemical ozone formation. So, the normalized profile shown in Figure 2 will only undergo minor changes if weighted. If we weight and calculate the total impact score for the example in Figure 2, we end up with about 400 mPET.

The framework of LCIA including new developments is most recently described by Hauschild (2004).

1.3 The importance of chemical related impact categories in LCIA

It is one of the aims of this thesis to elucidate whether or not the inclusion of chemical-related impact categories can be decisive for the outcome of an LCA study. This issue is dealt with in terms of a case study on printed matter in Chapter 2, which is further documented in the background report by Larsen et al. (2004a). In the following is a short description of the main findings from this study.

The LCA case study on printed matter produced at a hypothetical model printing company is performed in the context of ecolabelling. Besides elucidating the relative importance of the chemical-related impact categories, the goal of the case study is to identify the hot spots in the life cycle of the product. The functional unit is one ton generic sheet fed offset printed matter, and the results of the study are to be used for ecolabelling criteria development on printed matter covering both Scandinavia and the rest of Europe. All life cycle stages are covered, but due to the ecolabelling context and data availability the focus is on the production stage. The technological scope is defined as modern (below state of the art) technology used in Europe for production during the time span of 1990 – 2002.

The midpoint LCIA methodology EDIP97 (Wenzel et al. 1997) including a key property-based impact assessment part on ecotoxicity and human toxicity is used. The ‘areas of protection’ chosen are human health, natural environment, natural resources, and only indirectly man-made environment due to inclusion of the natural environment related impact category on acidification (damage to concrete constructions like buildings etc.). The impact categories included are: Global warming, ozone depletion, acidification, nutrient enrichment, photochemical ozone formation, chronic human toxicity via water and soil, chronic ecotoxicity in water and soil, acute human toxicity via air, acute ecotoxicity in water, hazardous waste, nuclear waste, slag and ashes, and bulk waste. Furthermore, resource consumption is included. All steps of the LCIA are performed, i.e. classification, characterisation, normalisation (person-equivalent) and valuation (weighting, based on political reduction targets and for resources supply horizon).

In order to highlight the importance of including chemical emissions, a distinction is made between the chemical(or toxicity)-related impact categories comprising the categories on ecotoxicity and human toxicity, and the energy-related impact categories comprising global warming, acidification and nutrient enrichment.

1.3.1 Results of the case study

The major part of former LCA case studies focuses on the energy-related impact categories and if chemical-related impact categories are included, it is typically done in an incomplete way. Looking at earlier case studies on printed matter (Dalheilm & Axelsson 1995, Axelsson et al 1997, Drivsholm et al. 1996 and 1997, INFRAS 1998, Johansson 2002) it is found that one study does not look at chemical-related impact categories at all, another study only includes emissions of two chemicals, and the rest of the studies include chemical emissions to a limited and for some studies opaque degree, and especially inclusion of specific organic substances seems very restricted.

One of the reasons for this low coverage of chemical-related impact categories in former studies is that the impact categories on ecotoxicity and human toxicity differ from all the other impact categories because a very large number of chemical emissions may contribute to potential toxicological impact. Substances contributing to other impact categories such as global warming, nutrient enrichment and acidification are limited in number and well defined, and characterisation factors are already available. However, for the chemical-related impact categories, a sufficient number of characterisation factors are not at all available to day to cover even the most important contributors. Furthermore, many of the existing characterisation factors for the chemical related impact categories are based on poor data availability and/or poor data quality, particularly for the effect data. In order to compensate for this, assessment factors are typically used when the effect part of the characterisation factors is estimated. For example assessment factors between 10 and 1000 are used in the EDIP97 method when characterisation factors for chronic ecotoxicity are estimated. This estimation principle has the consequence that the value of the characterisation factor for a given substance may vary a factor of 10 or even 100 depending on the data available and used (this issue is further dealt with in Chapter 5 and Chapter 6). The characterisation factors and the normalisation references for the chemical related impact categories should therefore be considered as having a higher uncertainty than those of the energy related impact categories.

In this case study, a better coverage of the chemical-related impact categories is achieved, than what is typically the case in LCA studies, by including characterisation factors from recent work in other industry sectors and by calculating new factors for chemical emissions expected to contribute significantly. By choosing the EDIP97 methodology, relatively many characterisation factors on emissions of industrial chemicals already exist (e.g. about 200 for chronic ecotoxicity in water), and the key property-based estimation principles and moderate data demand makes it easier, as compared to e.g. multi media-based methods, to estimate new ones. In this study eleven new characterisation factors for emission to water have been estimated.

Looking at emissions to air the total number of substances mapped in the inventory of this case study is 99, excluding emission of CO_2 and water. Among these, 33 emissions have characterisation factors for human toxicity corresponding to 33% and 26 have characterisation factors for ecotoxicity corresponding to 26%. The emissions from the disposal stage and particularly the material stage include emission categories like VOC, NMVOC and unspecified dust for which more specific information of actual content is not available. In the printed matter study 48% of the total emitted quantity (kg) consists of substances which are covered by characterisation factors for human toxicity and for the ecotoxicity part 21% is covered. If we exclude the amount coming from some of the emissions which contribute most to the total emitted quantity (SO_2, NO_x, unspecified dust, COD, calcium, Cl^- and suspended solids), for which at least the main part typically does not contribute significantly to the potential ecotoxicity impact, the coverage becomes 64% for the ecotoxicity impact category.

In total 123 emissions to water are included in the study. 31 waterborne emissions are covered by characterisation factors for human toxicity corresponding to 25% and 45 emissions are covered by characterisation factors for ecotoxicity corresponding to 37%. Also in this case the emissions from the material and disposal stage include unspecific types like COD, TOC, VOC and suspended matter, for which information of the actual content is not available. Only 3.1% of the total emitted quantity (by weight) to water is covered by characterisation factors for human toxicity, and only 3.4% is covered for ecotoxicity. If we exclude the amount coming from the in quantity highest contributing emissions (SO_4^{--}, Tot-P, Na^+, COD, calcium, Cl^- and suspended solids), for which at least the main part typically does not contribute significantly to the toxicity impact categories, the coverage becomes 48% for human toxicity and 53% for the ecotoxicity part.

In this case study the main part of the specific known individual emissions to water, for which characterisation factors are lacking, consists of inorganic salts (e.g. disodium silicate, sulphates), polymers (e.g. acrylates, modified phenol resin) and acids/bases (e.g. NaOH, HCl). In general, these substances/mixtures have a low toxicity and are not expected to contribute significantly to the toxicity-related impact categories, if not emitted in high quantities. In the latter case they will typically contribute only to acute ecotoxicity (e.g. reactive monomers from binders, acids or bases causing low or high pH), and only if not treated in a waste water treatment plant (WWTP) before emission to the water recipient. Most of them have been assessed on the basis of hazard assessments and/or generic risk assessments in Larsen et al. (1995, 1998, 2000, 2002a) and Nielsen et al. (2000) for potential effects if emitted to WWTP or directly to a water recipient.

Known emissions from the production stage, which are not covered by characterisation factors, and which may contribute significantly to the toxicity impact categories, include emissions of components occurring in small quantities in the raw materials (typically well below 5%) like siccatives (organic metal compounds), softeners (phthalates), antioxidants (aromatics) and “wetteners” (surfactants). Due to lack of readily available knowledge of their exact identity and/or lack of readily available data on their inherent environmental properties, it has not been possible to include them in this study.

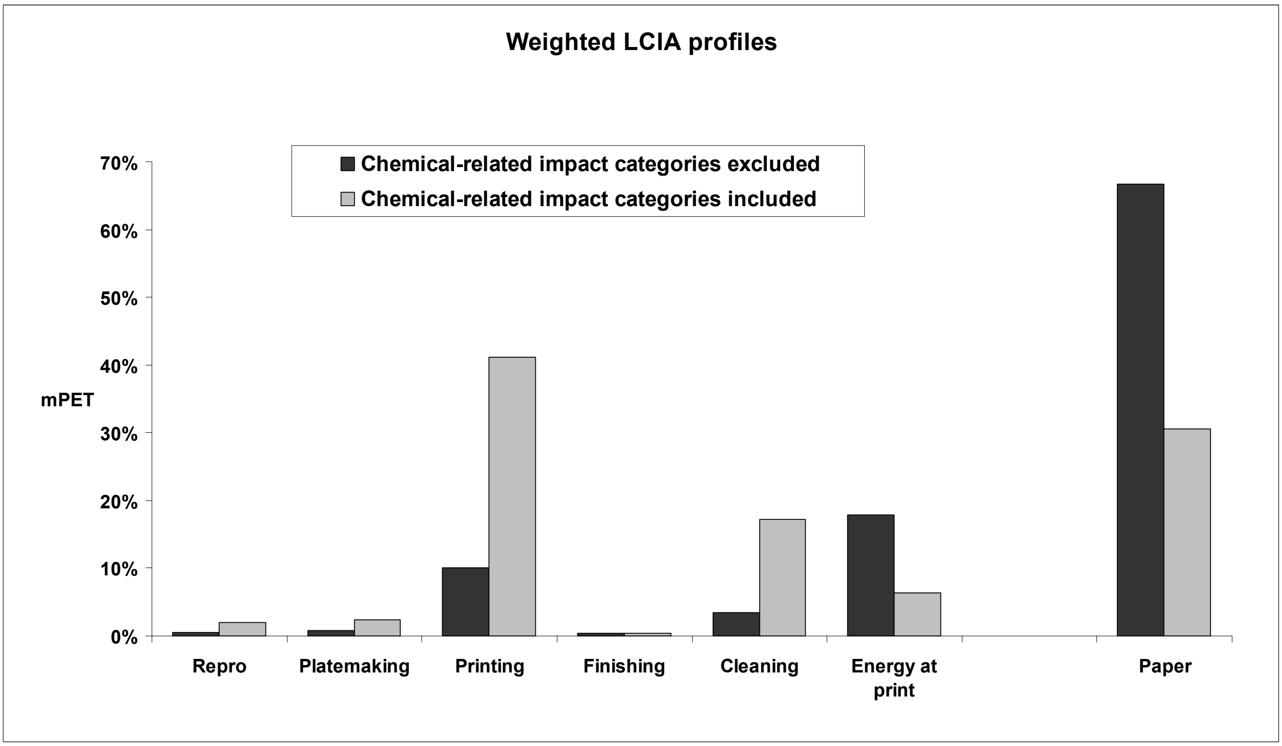

Figure 3. Weighted profiles with or without chemical-related impact categories included. Weighted potential impact (mPET) scores shown as relative values of the total aggregated value. Due to the ecolabelling context the profile is divided into the production steps at the model printing company (repro, platemaking etc.). The energy consumption at the model printing company (‘Energy at print’) and the entire life cycle of the paper (‘Paper’) are shown separately.

From the material and the disposal stage, known emissions, which are not covered by characterisation factors but which may contribute significantly to the toxicity impact categories, include, for example, emissions of unspecified metals, AOX, unspecified oil and unspecified detergents. The emission of AOX from paper production is suspected to be the most potent among these and it is dealt with by sensitivity analysis. The results show that inclusion of emission and toxicity data for individual components of the AOX (not available to day) would probably not change the overall outcome of the LCA study.

The final result of this case study expressed as a comparison between a weighted LCIA profile with chemical-related impact categories included and one without is shown in Figure 3.

1.3.2 Conclusions on the case study

The effect of excluding chemical-related impact categories in this case study is substantial, as shown in Figure 3. The importance of paper for the total impact is raised from 31% to 67% and that of printing reduced from 41% to 10% if the chemical-related impact categories are excluded.

The case study shows that, even though this is a special case where the potential fate and toxicity of relatively many of the chemical emissions are known, making it possible to characterize or exclude them as potential significant contributing, only 25% - 37% of the total number of emissions is characterized. For many of the non-characterized emissions sufficient data to estimate characterisation factors do not exist. Depending on the scope, this fact seems to be of general validity in LCA studies – at least for those including many chemical emissions like studies on all types of printed matter and textiles – and this weakens the credibility of the results. This problem calls for a method that is able to come up with characterisation factors based on a poor database or perhaps more realistically a screening method able to work on a very poor database and prioritize those emissions in the inventory, which potentially contribute significantly and which therefore are worth putting characterisation effort into. Such methods are here called selection methods and are dealt with in the next section.

1.4 Selection methods – qualitative evaluation and framework

One way to go, in the attempt, to break the barrier against inclusion of chemical-related impact categories in LCA at the same level as the more well-established impact categories like global warming, is to use selection methods (SMs). The aim of these methods is to point out those emissions which contribute significantly to the overall toxicity impact and thereby normally exclude the (main) part as unnecessary to characterize. An inventory and evaluation of existing SMs and other Chemical Ranking and Scoring (CRS) methods assessed to be relevant for the development of new SMs are described in Chapter 3 and in further details in the report “Inventory of LCIA selection methods for assessing toxic releases” by Larsen et al. (2002b). Furthermore, a framework for developing SMs is described. The main results from this study are described in the following.

1.4.1 Results of the qualitative evaluation of selection methods

The concept of a selection method has been created within OMNIITOX in order to differentiate from the wider and more ambiguous group of methods covered by the phrase ‘LCA screening method’. The latter has been used for concepts with the same purpose as defined for an SM, but the phrase can also mean something quite different, e.g. simple screening level LCA methodology including other impact categories than the toxicity related.

An SM is a method for prioritising chemical emissions to be included in an LCIA characterisation on the impact categories covering ecotoxicity and human toxicity. So, this kind of method serves for the step classification (i.e. assignment of emissions to impact categories) in the LCIA procedure. An SM is therefore a classification rather than a characterisation method but the purpose of an SM is to focus the effort within characterisation. However, a simple characterisation method may serve as an SM to support a more sophisticated characterisation method. SMs are used within LCIA to select those chemical emissions (mapped in the inventory part of the LCA case in question) that are expected to contribute significantly to the characterisation and exclude the insignificant ones. In this way only significant emissions (i.e. the selected ones) are included in the typically more data demanding and more time demanding characterisation step.

The need for SMs are underlined by the fact that the existing mostly used 8-10 LCIA characterisation methods covering toxic impacts each only include characterisation factors for 30 – 450 chemicals (de Koning et al. 2002) of which a major part are well known substances like metals and pesticides. A life cycle inventory (LCI) can include several hundred to thousands of chemical emissions (depending on the scope) including a lot of industrial chemicals. According to for example the EU White Paper on Chemicals Policy (EU 2001) 30,000 substances are marketed on the European marked in a quantity above 1 ton and totally about 100,000 substances are registered today.

Very few SMs have been developed to this day. Only the EDIP-selection method (Wenzel et al. 1997) and the Priofactor (Larsen et al. 1999a, 1999b), which are both associated with the EDIP97 method (Wenzel et al. 1997), and the CPM-selection method, which is associated and described in connection with the CPM-characterisation method (Eriksson 1999), are ‘true’ selection methods in the sense that they have been developed to support a characterisation method. So, other relevant chemical ranking and scoring (CRS) methods have been included in this study, i.e. the EURAM method (Hansen et al. 1999) and the WMPT method (US EPA 1997, 1998). Two statistical/mathematical methods, i.e. the Hasse diagram technique (Brüggemann et al. 2001) and the CART analysis (Bennett et al. 2000), have also been included. The study thus covers the only existing selection methods (i.e. EDIP-selection, Priofactor and CPM-selection), the dominating Chemical Ranking and Scoring (CRS) method in Europe (i.e. EURAM) or in USA (i.e. WMPT), and methods presenting novel approaches which can be valuable in development of new selection methods (i.e. CART and Hasse diagram technique) or as baseline when comparing ranking by different SMs (i.e. Hasse diagram technique).

An SM can be considered as a CRS method with some special constraints, the most important being the requirement for consistency with the associated characterisation method for which it is supposed to identify the most important emissions. A set of criteria for the performance of an SM has been developed. A good SM is one that:

- Is consistent with the associated characterisation method in ranking and methodology. The required substance data should also be applicable in the characterisation method
- Is transparent
- Is applicable to different chemical groups (in principle all)
- Has a data requirement that can be characterized by
  - low demand on scope and quality of data
  - subset of data needed for calculation in characterisation step
  - high availability of data and prediction methods (e.g. QSARs)
- Is user friendly, i.e.
  - practicable - easy in use, end-user software existing
  - time demand low as compared to the characterisation method
  - skilled scientific background not needed

The included methods (except for the Hasse diagram technique and CART, both representing frameworks rather than operational methods) are evaluated against the performance criteria. The result is shown in Table 2.

Table 2. Results of the evaluation of the SMs and the two other CRS methods

Criteria	**EDIP-selection**	**Priofactor**	**CPM-selection**	**EURAM**	**WMPT**
Consistency in prioritization (validity)	+	+++	n.a.	n.r.	n.r.
Applicable to different chemical groups	++++	+	+++	+	++
High data availability	+++	++	++	+	+++
Low data demand	++++	++	++	+	+
Data useable in characterisation	+	+++	+++	n.r.	n.r.
Low in time demand and easy to use	+++	++	++	+	(++)
Skilled scientific background not needed	+++	++	++	+	+

++++:	Very high degree of fulfilment	+:	Low degree of fulfilment
+++:	High degree of fulfilment	n.a.:	Not assessed
++:	Moderate degree of fulfilment	n.r.:	Not relevant

In addition to this evaluation, principles on how to develop and select CRS systems, as described in the SETAC guide “Chemical Ranking and Scoring” the by Davis et al. (1997), have been included and applied to SMs in general and as relevant to the methods included here.

1.4.2 Conclusions on the qualitative study on selection methods

As shown in Table 2, none of the existing methods evaluated achieve a high degree of fulfilment for all performance criteria in this qualitative evaluation. The development of new SMs is therefore recommended, and the following main issues should be taken into account:

- ➢ Emitted amount should be included (improve the consistency with characterisation method considerable)

- ➢ Very high data availability for the underlying substance data should be sought (e.g. based on R-phrases and/or QSARs)

- ➢ The method should be low in false positives and create no false negatives or false negatives should only account for an insignificant amount of the impact potential as calculated by the associated characterisation method

Furthermore, the principles described in Chapter 3 on how to develop and select chemical ranking and scoring systems as applied to selection methods should be consulted

In the further research on SMs it is recommended to focus on the following questions:

- ✓ Is it possible to use simple data with very high availability (e.g. R-phrases, QSAR calculations) and simultaneously achieve high consistency with the associated characterisation method?

- ✓ What are the key parameters (e.g. persistence, bioaccumulation, toxicity and emitted amount) to include in a selection method and how? Can it be done without subjective value choices (e.g. Hasse diagram technique) or must value choices be included?

- ✓ Is multimedia fate modelling necessary (and desirable) or is a simple key parameter approach sufficient to achieve high consistency with the associated characterisation method?

- ✓ Will a statistical approach (e.g. CART analysis or linear regression) be appropriate to achieve high consistency with the associated characterisation method?

Due to lack of existing quantitative evaluations this study is primarily based on qualitative assessments. However, the evaluation of the consistency in prioritization (validity) of the EDIP-selection method and the Priofactor (see Table 2) is actually based on quantitative data from the only known quantitative validation, viz. a validation on a single case study (Larsen et al. 1999a). In order to achieve experience with performance of SMs in practise, there is a need for quantitative validations. This is the issue of the next section.

1.5 Selection methods – quantitative evaluation

For an SM its consistency in chemical ranking with the associated characterisation method is crucial for its performance. But how consistent is chemical ranking actually between existing SMs and associated characterisation methods, and between these and a dominating CRS method, used within tiered risk assessment/screening, which may be a good candidate as the basis for a new selection method? Furthermore, what are the causes of significant differences in ranking, if such appear? These questions are sought answered by testing the ranking of the two characterisation methods EDIP97 and CPM, the three SMs EDIP-selection, Priofactor and CPM-selection, and the risk ranking method EURAM, all against each other. For the EDIP-selection method a modified version is used excluding the (conservative) use of risk-sentences (R-phrases) for the soil compartment because these R-phrases are not yet assigned to any substances (N-CLASS 2003) due to the fact that no official criteria have yet been defined. This study is described in details in Chapter 4 and the main results presented in the following.

1.5.1 Results of the quantitative evaluation of selection methods

This comparative analysis is focusing on aquatic ecotoxicity and the chemicals used for testing belong to the amphiphilic (e.g. surfactants) and dissociating substances (e.g. acids/bases). A total of 27 chemicals are included which are part of a test set of around 80 substances (Margni et al. 2002, de Koning & Guinée 2002) developed within OMNIITOX for a structured comparison between characterisation methods and SMs. Due to the fact that this comparison is not based on a case study, the emitted amount is not included (only relevant for EDIP97, Priofactor and EURAM).

The 27 chemicals have been ranked according to the principles of each of the included methods and the results (not shown here but in Table 2 in Chapter 4) show for example that the ranking of the EDIP-selection method (ranking in four levels) is in accordance with the 12 substances ranking highest by the associated EDIP97 method, and with two exceptions, this is also the case for the Priofactor (ranking in 27 levels). The CPM-selection method (ranking in three levels) also ranks the same way as the associated CPM method for the 18 substances ranking highest by the CPM method, but the substance given the lowest rank (27) and the substance given the rank 22, by the CPM method, are both given the highest rank (1) by the CPM-selection method.

For those methods which rank in 27 levels, a test for significant differences in ranking by use of Spearman Rank Correlation Coefficient has been performed. The result of this test is shown in Table 3.

Table 3. Spearman's Rank Correlation Coefficient (R^2) and significance levels in brackets

Method	EDIP97	Priofactor	CPM	EURAM
EDIP97	1	0.77 (< 0.001)	0.86 (< 0.001)	0.68 (< 0.001)
Priofactor	0.77 (< 0.001)	1	0.56 (< 0.01)	0.71 (< 0.001)
CPM	0.86 (< 0.001)	0.56 (< 0.01)	1	0.43 (< 0.05)
EURAM	0.68 (< 0.001)	0.71 (< 0.001)	0.43 (< 0.05)	1

As the EDIP97 method is the most comprehensive characterisation method, as compared to the CPM method, and broadly accepted among LCA practitioners, the result from the EDIP97 ranking may be used as a reference in a comparison with the other methods. The ranking of the CPM method, the Priofactor and EURAM are therefore held up against the ranking of the EDIP97 method in order to identify outliers and create the basis for analysing the causes to differences in ranking. This comparison is shown in Figure 4.

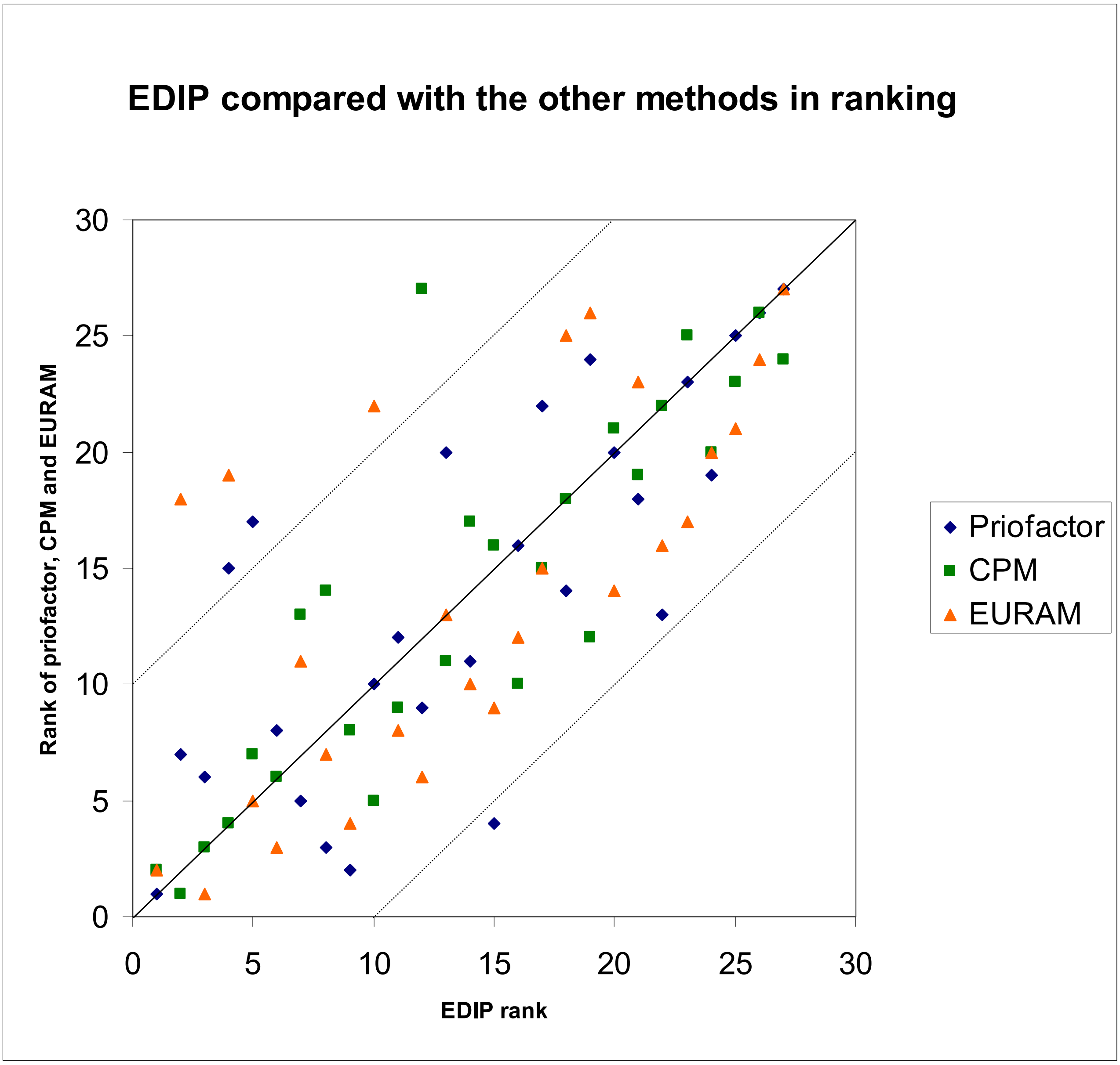

Figure 4. Ranking of the key property-based characterisation method EDIP97 as compared to the associated selection method Priofactor, the simple key property-based characterisation method CPM and the risk ranking method EURAM. The limits for a deviation of more than 10 in rank are indicated by the two thin lines.

1.5.2 Conclusions on the quantitative study on selection methods

The results of this study indicate that for these special groups of substances, viz. amphiphilics and dissociating substances, there is a good correlation between the ranking of the characterisation method EDIP97 and its associated selection methods, the EDIP-selection (revised version, i.e. terrestrial labelling excluded) and the Priofactor, see Table 2 in Chapter 4 for details. Anyway, a larger dispersion among the scores of the substances in the EDIP-selection would be desirable (e.g. by multiplying with emitted amount) in order to differentiate better between emissions to include and emissions to exclude in the characterisation step. The correlation between the simpler characterisation method CPM and its associated selection method, i.e. CPM-selection, is also good for the highest CPM ranks, but not so good for the lowest ranking substances (see Table 2 in Chapter 4 for details). Also in this case, a larger dispersion in the scores is desirable. Despite the differences in ranking it is not possible by using Spearman's Rank Correlation Coefficient to come up with any statistical significant (at the 0.05 level) difference in the ranking obtained by the four tested methods which all rank in 27 levels, see Table 3. However, the correlations between the EDIP97 method and all of the methods Priofactor, CPM and EURAM are stronger ($\alpha < 0.001$) than the correlation between the CPM method and the EURAM method ($\alpha < 0.05$). These results indicate that even though CPM and EURAM have not been designed to act as selection methods for the EDIP97, a common perception of what makes a substance ecotoxicologically problematic underlies all three methods. This is also revealed in the expressions of these three methods which all include similar combinations of biodegradability (or persistence), bioaccumulation potential and toxicity (PBT). Nevertheless, some outliers, as shown in Figure 4, have been identified, and through analysis of these, characteristics of the individual methods have been identified which for certain combinations of substance properties may result in false negatives or false positives as compared to EDIP97. These characteristics include:

- The influence of data availability on size of assessment factors for conversion of acute effect data to chronic values

- Whether or not mode of entry (i.e. the environmental compartment, e.g. air or water, to which the chemical is emitted) is taken into account in the fate modelling

- Reversing of the effect of toxicity on ranking by negative $\log K_{ow}$ (logarithm to the octanol-water partitioning quotient) values when $\log K_{ow}$ is a direct factor in the expression

- The way BCF (BioConcentrationFactor) is estimated and included in the calculation of the impact factor or score

It is recommended that the further research on selection method include all types of substances – including inorganics. The amphiphilics and dissociating substances were chosen here because most of the substances typically included in test on CRS methods are inert organic substances (i.e. non-amphiphilic, non-dissociating organic substances).

On the basis of the research result on selection methods contributed by this thesis, the development of selection methods is still ongoing (October 2004) in the OMNIITOX project.

For those chemical emissions which are prioritized by a selection method, and for which characterisation factors do not allready exist, it must be possible to estimate one. As for selection methods we must also in this case face the problem of low data availability. Furthermore, consensus on how to calculate characterisation factors for the chemical-related impact categories has not yet been reached within the international LCA community. The way to estimate ecotoxicity characterisation factors with focus on the effect part (fate part excluded) and data availability is therefore the issue of the remaining part of this thesis.

1.6 Ecotoxicity effect indicators – inventory and evaluation

The calculation of an ecotoxicity characterisation factor involves a fate part and an effect part. In the fate part the destiny of the emitted substance in question is modelled (e.g. by degradation and dispersion models) leading for example to an estimated concentration change in the different environmental compartments (water, soil etc.) for every kilogram emitted. In the effect part, the potential effect or impact of these estimated concentrations on the biota (i.e. plants and animals), or in its most abstract form: on the 'health' of the ecosystem, is modelled. This study deals with the effect part, viz. ecotoxicity effect indicators (EEIs), and focus on method inventory and evaluation: What kind of methods or approaches exist today and how are they performing in the context of LCIA? Which (new) approaches may contribute to the further development? How large are the differences in the estimation principle of the different approaches in practice and what is the key parameter(s)? Which is the direction(s) to go in the further improvement and development of ecotoxicity effect indicators? These are some of the central questions that this study is trying answer. The study is described in details in Chapter 5 and the main findings are outlined below.

1.6.1 Results of the inventory and evaluation of EEIs

Existing EEI approaches fall into two main groups:

- Assessment Factor (AF) based approaches (Predicted No Effect Concentration, PNEC approaches)
- Species Sensitivity Distribution (SSD) based approaches (Potentially Affected Fraction of species, PAF approaches)

For both groups, the EEI is typically only modelled to the level of impact or midpoint in the environmental mechanism or impact chain. However, attempts have been made to model the PAF-approach all the way to damage or endpoint (Goedkoop & Spriensma 2001a, 2001b) and expressing the damage to ecosystem health in terms of Potentially Vanished Fraction of species (PVF). Of potential damage models Chapter 5 identifies the following three:

- Recovery time approach
- Species extinction approach (Mean Extinction Time, MET)
- Changes in genetic diversity

All of these damage approaches are at a rather early stage of development and are today primarily used within for example population biology.

The way the characterisation factor (CF) is estimated when the PNEC approach is used may be expressed by the following equation:

$$\mathrm{CF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{1}{\mathrm{PNEC}} \cdot \mathrm{dC} \qquad (1)$$

In this case the effect indicator equals 1/PNEC (the effect part), and the fate part equals a change in concentration (dC) per emitted quantity of substance (typically per kilogram). Mostly, the PNEC is estimated on basis of acute (e.g. EC_{50}) and/or chronic effect data (e.g. NOECs) from single species laboratory tests by use of conservative AFs (e.g. Hauschild et al. 1998, Huijbregts et al. 2000). This is due to the fact that these approaches have their roots in tiered risk assessment (e.g. EC 2003a). The PNEC approach may, however, coincide with the PAF approach because the hazardous concentration for 5% of the species (HC5) in an

SSD may be used as PNEC (Huijbregts et al. 2000). In this case the effect indicator equals 1/HC5 or 1/HC5$_{NOEC}$. An example of an SSD is shown in Figure 5.

The PAF approaches are based on the principle of SSD which is a statistical distribution describing the variation in toxicity of a certain toxicant among a set of species, see Figure 5. This distribution may be log-logistic defined by a location parameter (α, sample mean that equals HC50) and a scale parameter (β) expressing the steepness of the PAF curve. In order to secure linearity in the estimation of the impact potentials (i.e. the CF multiplied by the emitted amount) the PAF curve is not used directly but a straight line defined by a working point on the PAF curve is used instead (not shown here – but see Figure A3 in Chapter 5). Two main types of PAF approaches exist, viz. the marginal PAF increase approach and the average PAF increase approach.

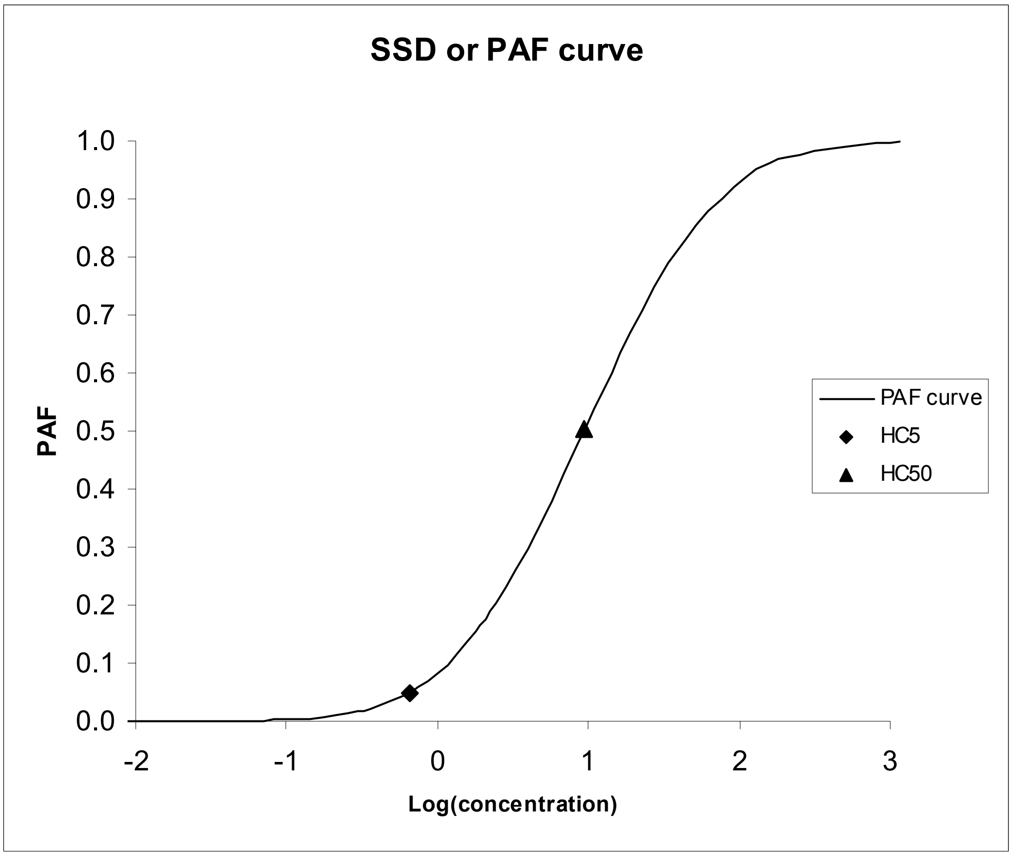

Figure 5. Example of a species sensitivity distribution (SSD) curve or PAF curve illustrating the relationship between the concentration of a toxicant and PAF, i.e. the cumulative probability of exceeding e.g. NOECs for a certain fraction of species in the collection of species included assumed to represent a community/ecosystem. The concentration at which the fraction p of species are having their NOECs exceeded is denoted the Hazardous Concentration at level p, i.e. HCp. In this example the concentration at which 5% (PAF = 0.05) of the species are having their NOEC exceeded (denoted HC5 or HC5$_{NOEC}$) equals $10^{-0.19}$ = 1.5, and the HC50 or HC50$_{NOEC}$ value equals $10^{0.98}$ = 9.5.

The marginal PAF increase approach is used in the Eco-indicator 99 method (Goedkoop & Spriensma 2001a, 2001b) and the aim is to express the potential impact from an emitted toxicant by the marginal increase in the number of species having their NOEC values exceeded taking into account the background impact, i.e. the number of species already having their NOEC exceeded. All toxicant concentration scales are normalized and expressed in hazard units (HUs), i.e. each toxicant concentration is divided by the toxicant's

$HC50_{NOEC}$, and concentration addition (CA) is assumed for all toxic modes of action (TMoA). A multi substance PAF (msPAF) curve is made which resembles the one in Figure 5 but with msPAF instead of PAF and log (HU) instead of log(concentration). The background msPAF value and the scale parameter (β) value used in the Eco-indicator 99 method (Goedkoop & Spriensma 2001a, 2001b) are based on environmental monitoring in the Netherlands and equal 0.22 and 0.4 respectively. The background msPAF value of 0.22 defines the working point for the tangent to the msPAF curve and the tangent therefore has a slope of 0.59, see Figure A3 in Chapter 5. The effect indicator is in this case equal to the slope of the tangent divided by $HC50_{NOEC}$ of the toxicant in question, i.e. $0.59/HC50_{NOEC}$.

For the average PAF increase approach two types are described. Pennington et al. (2004) propose the use of HC5 as working point for an average linear gradient. In this case the effect indicator becomes $(0.05*10^{2.94*\beta})/HC50$ and with the known typical variation of β-values for different TMoA among toxicants this expression equals the interval 0.2/HC50 – 43/HC50. The other type, making use of $HC50_{EC50}$ as the working point, is proposed as best available practice by Pennington et al. (2004) and implemented in the AMI method (Payet & Jolliet 2003, Payet et al. 2003). In the AMI method the PAF curve is not based on chronic NOEC values (i.e. no-effect-based) but on chronic EC_{50} values (i.e. effect-based). In this case the effect indicator becomes $0.5/HC50_{EC50}$. Both the HC5 and the HC50-based average PAF increase approaches assume that background impact can be neglected.

Of the damage approaches mentioned earlier for linking impact at midpoint level to endpoint level, the recovery time approach used as media recovery is actually used within the Eco-indicator 99 method (Goedkoop & Spriensma 2001a, 2001b) and the IMPACT 2002+ method (using AMI) (Jolliet et al. 2003) for estimating the potentially vanished fraction of species (PVF). The media recovery model is based on the assumption that the media quality is directly linked with the biodiversity. Species are considered as disappeared as soon as the toxicant concentration in the ecosystem reaches a certain level, and the species reappear when the toxicant disappears by e.g. degradation. So, this model is directly linked to the fate modelling. However, the environmental threats should not cause immediate extinction of a population but shorten the expected time to extinction (Hakoyama & Iwasa 2000). Population models like the Mean Extinction Time (MET) have therefore been developed in order to quantify the expected survival of species exposed to toxic pressure (Lande 1998). The use of genetic diversity instead of biodiversity could solve some of the problems with diversity within species contra diversity between species. A model by Norberg et al. (2001) has been presented linking the phenotypic diversity and the ecosystem functioning expressed in terms of biomass production. These models are all at an early stage of development (especially the last one) and the availability of the data needed is very limited.

The different approaches described above are evaluated against a set of criteria for performance within the framework of LCIA. The result of this evaluation is shown in Table 4 for most of the approaches.

Table 4. Result of the evaluation of the different EEI approaches

Criteria	PNEC-based approaches			PAF-based approaches		Damage-based approaches	
	AF-based PNEC (only acute data)	AF- based PNEC (chronic (preferred) and acute data)	SSD-based PNEC ($HC5_{NOEC}$)	Marginal PAF increase (fixed β value)	Average PAF increase, HC50	Recovery time [a]	Mean extinction time
Scientific validity	++	++	++	+++	++	+(+)	+
Environmental relevance	+	++(+)	+++	+++	+++	++(+)	+++(+)
Reproducibility	++	+(+)	++	++(+)	+++	++	(+)
Transparency	++++	+++(+)	++	+(+)	+(+)	+(+)	+
Low data demand	++++	+++(+)	++	+	++	++	+
High data availability	++++	++++	+(+)	+	+(+)	++	+
Spatial differentiation possible	+	+(+)	++	+++	+(+)	n.a.	n.a.
Quantification of uncertainty included	+	+	++ [c]	+ [c]	++++ [b]	n.a.	n.a.

++++: Very high degree of fulfilment
+++: High degree of fulfilment
++: Moderate degree of fulfilment
+: Low degree of fulfilment

a: As media recovery
b: Implemented in AMI (Payet et al. 2003)
c: Not implemented but possible
n.a.: Not assessed

1.6.2 Conclusions on the inventory and evaluation of EEIs

Based on the result of this study including the evaluation shown in Table 4, different directions to go in the further improvement and development of EEIs may be recommended:

- Improving the assessment factor-based PNEC approach making it less risk assessment based and more suitable for LCIA. The goal will be to come up with some non-conservative assessment factors including uncertainty (confidence limits) and if possible taking toxic mode of action into account.
- For the PAF-based approach the main problem seems to be high data requirements and the fact that in the way this approach has been used till now, it does not represent effects on the ecosystem in a more accurate way than the PNEC-based approach. To achieve higher chemical coverage this approach needs fitting to low data availability if possible. Further, the goal will be to make procedures for a more environmentally relevant application (e.g. more realistic, not haphazard representation of species on each trophic level) and to utilize, improve and develop the inclusion of mixtures and damage modelling.
- Further development of the media recovery damage approach or development of a new damage-based indicator based on the ‘time to extinction’ approach or ‘changes in genetic diversity’.

For damage modelling, the further development of the media recovery approach seems to be the most realistic way to go if a method is to be functional for LCIA in the near future. This approach may also be coupled with the PAF approaches. The two other damage approaches (MET and genetic diversity) are at an even earlier development stage than the media recovery model, and the availability of the data needed is very poor. However, from a theoretical point of view, these two approaches are very attractive and further dealt with in Payet & Larsen (2004).

For the assessment factor-based PNEC approaches the main problem is that they are founded in tiered risk assessment and therefore conservative, which is not compatible with the comparative framework of LCIA. A way to deal with this problem could be to try to develop non-conservative assessment factors taking the huge work on acute to chronic ratios all ready done (e.g. Solbe et al. 1998, Chapman et al. 1998, Länge et al. 1998, Forbes & Calow 2002a) as a starting point and perhaps try to differentiate the assessment factors by TMoA. However, as the PNEC approach is no-effect-based (i.e. NOEC-based) it will still suffer from the uncertainty of measured NOEC values due to e.g. variation in test design (Chapman et al. 1996).

Looking at the PAF approaches, in the practical framework of LCIA, a generalisation is possible for the way the effect indicator is estimated. If we accept to use a fixed β value for the average PAF increase approach based on HC5, which is the most appropriate if the method is going to be functional in a normal LCIA context, then, despite the described differences in theoretical foundation, the effect indicator for all PAF approaches included here may be described by the expression: k/HC50. The constant ‘k’ may be 0.59, 0.5 or 0.2 - 43, as described in Section 1.6.1. So, in the comparative approach applied in LCIA, there will be no difference in practise between the effect indicators based on the different PAF approaches, as long as the same value for HC50 is used. The key element in the effect indicator therefore becomes HC50.

The crucial point in the determination of a PAF-based ecotoxicity effect indicator is therefore the data used and the principles applied for determining the HC50 value of each toxicant. The HC50 may be estimated by use of e.g. NOEC values or EC_{50} values and based on the non-parametric median or the parametric geometric mean. Furthermore, the actual data used may for example reflect haphazard representation of species on each trophic level or a more realistic and consciously chosen representation of the structure of the ecosystem/community in question. The choice of data and estimation principle may have significant influence on the outcome, especially when the number of available data on each toxicant is low, which is the typical case within LCIA handling many chemical emissions. The last part of this thesis addresses these issues.

1.7 Development of a low data demanding EEI: GM-troph

Considering the comparative purpose of LCIA seeking best estimates, and further considering the typically low data availability for many of the substances encountered in LCA, the improvement of an effect-based PAF approach defined by HC50 seems to be the most reasonable way to go in the further development of EEIs. As shown in the previous study (Section 1.6) the key parameter then becomes HC50. This section focuses on the estimation principles and data grounds for HC50 and finally recommends the use of a new EEI able to work on only three acute EC_{50} values, the GM-troph. The following questions, which all should be looked upon in the context of the LCIA framework, cover the main issues of this part of the Ph.D. study: What is the most optimal estimation principle for HC50, if, as typically, only three acute data values are available? Is the aim for a high number of data points in the estimation of HC50 (e.g. for the sake of anticipated low uncertainty), which leads to haphazard species representation, reasonable, or does a consciously chosen representation or weighting of species from selected taxa or trophic levels make more sense? Should only results from standardised tests be used in the estimation of HC50? And if so, what should the criteria for selecting test results be? Is the inclusion of uncertainty limits around an HC50-based on few data reasonable, or is there an alternative? This study is described in Chapter 6 and in further details in the report “Implementation of the OMNIITOX Base Model. Part VIII – Implementation of the ecotoxicological effects module” by Larsen et al. (2004b). The main results of the study are summarised below.

1.7.1 Results of the development of GM-troph

The development of GM-troph is building on recent work done on EEIs and put on top of this some ‘new’ approaches on estimation principles, limits around the HC50 value, data selection and inclusion of ecosystem trophic structure in the theoretical foundation. The general frame for EEIs is recently defined by Hauschild & Pennington (2002) and Pennington et al. (2004). Different ways have been explored for the estimation of average toxicity and its associated uncertainty, using non-parametric statistics (Payet & Jolliet 2003) or using parametric statistics (Payet et al. 2003). Most recently the different EEI approaches have been reviewed and evaluated against performance criteria as part of this thesis work as described in Chapter 5 and summarised in Section 1.6.

The main advantages and disadvantages of choosing an effect-based PAF approach defined by $HC50_{EC50}$ as compared to a no-effect-based (i.e. PNEC) approach are:

Advantages:

- The risk of bias from the laboratory test set-up is low as compared to a no-effect-based indicator, where typically the highest tested concentration, which is not statistically different in toxicity from the control, is used
- The use of a value which is estimated and placed in the centre of the concentration response curve (i.e. HC50) where uncertainty is lowest (see example in Chapter 5, Figure A4)
- The quantification of damage in terms of potential loss of species is possible (at least in theory)

Disadvantages:

- The focus is shifted a way from protection of the function and structure of ecosystems
- The importance of very sensitive species may be neglected

A potential bias between ecotoxicity and other impact categories, which model lower levels of impact, will be removed if normalisation is performed.

For determination of average toxicity, different estimation principles can be (and are) used, i.e. arithmetic mean, geometric mean and median. As variation in biological material often shows a geometrical rather than an arithmetic distribution (Newman & Dixon 1996 citing ref. Bliss 1935), the geometric mean should normally be preferred. In cases of many data points and a wish to avoid any assumption about distribution function, the non-parametric median may be used (Newman et al. 2002). Anyway, the use of the median for estimating average toxicity on few data points (i.e. three) has been proposed (Payet & Jolliet 2003).

The inaptitude of the median as compared to the geometric mean to reflect average toxicity for small data sets is shown in Figure 6 (chemical 1 as compared to chemical 2). Even though chemical 1 is very toxic to algae as compared to chemical 2, which is low in toxicity to all three tested organism (i.e. algae, fish, daphnia), the median shows equal average toxicity of the two chemicals. For comparative reasons the consequence of using a PNEC approach (i.e. lowest EC_{50} value) as compared to the geometric mean is also shown in Figure 6 (chemical 1 as compared to chemical 3).

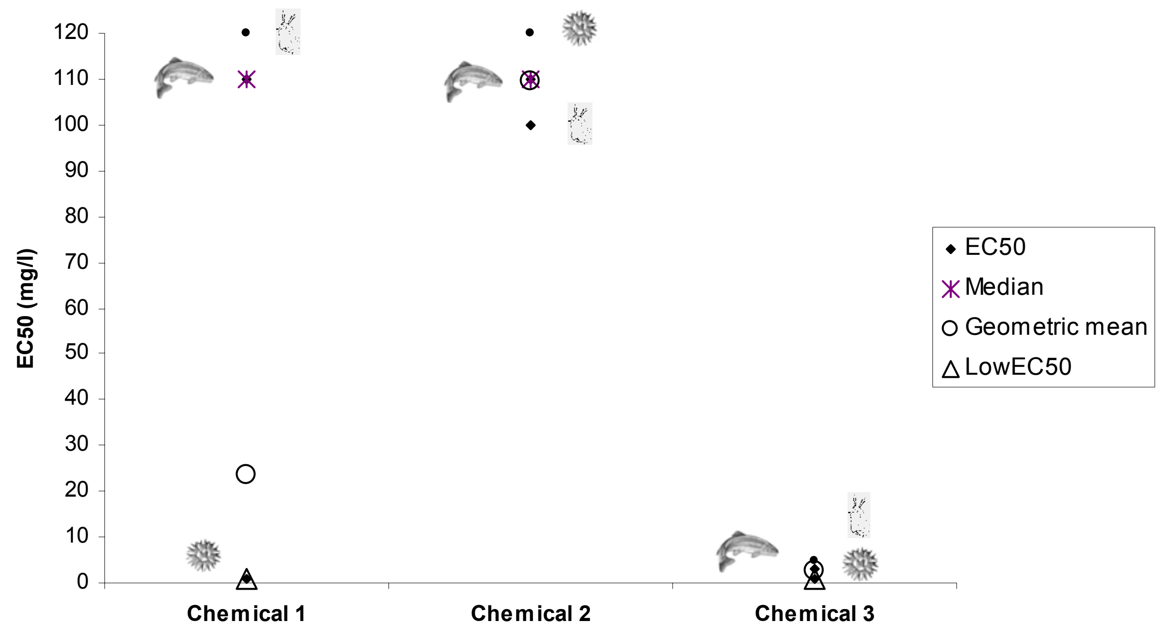

Figure 6. Three theoretical cases. Comparison between chemical 1 and chemical 2 illustrates the inaptitude of the median as compared to the geometric mean to reflect average toxicity of three EC_{50}s. Comparison between chemical 1 and chemical 3 illustrates the inaptitude of lowEC_{50} (used as basis for the PNEC approach) to differentiate between to chemicals having quite different toxicity profiles.

In order to test these estimation principles on real data, 11 substances covering seven different toxic modes of actions (TMoAs) are chosen. Only acute EC_{50} values are included, and a total range of 0.0032 mg/l – 780 mg/l is observed and between 6 and 36 data points (including 'replicates' on the same species) for each substance (see Table 1 and Table 2 in Chapter 6 for details). The comparison is based exclusively on results from test on standard organism as defined by the OECD Detailed Review Paper (OECD 1998) from the three taxa algae, crustacean and fish representing the three trophic levels primary producers, primary consumers and secondary consumers respectively. Restrictions on test endpoints and test durations, as defined in Chapter 5, were also taken into account and the EC_{50} values are mainly extracted from the US EPA database ECOTOX (2003) but also the ECB database IUCLID (2000) and data from RIVM (1999) are included.

The reason for putting these restrictions on the data used is a wish to reduce bias in the estimated $HC50_{EC50}$. In LCIA, we are integrating impacts over time and space, so, in that sense, we are far from ecological realism of the potential effect of the integrated emissions we estimate to be used in a comparative framework. The focus is therefore on issues like reproducibility, robustness and repeatability. As our goal is to treat all chemicals equally, we should aim at choosing a set of tests reflecting the sensitivity of representative 'standard' organism from at least three trophic levels, and besides trying to avoid erroneous data due to bad non-standardised test conditions, also aim at excluding the possible bias due to differences in sensitivity of haphazard test organism included. For most of the chemicals to be modelled by the EEI, we only have access to three acute data values, i.e. $E(L)C_{50}$ values for fish, daphnia and algae, as defined by for example the REACH demands (EC 2003b). Inclusion of non-standardised test result values in the calculation of the effect indicators, in those cases where it is possible, will increase variance and most probably create bias because the type and availability of such data is very variable among chemicals.

A condition for the use of the geometric mean and the arithmetic mean is that the data are either lognormal distributed or normal distributed. This is tested here according to the Anderson-Darling test for goodness of fit (Aldenberg et al. 2002, Stephens 1986) for those data sets equal to or higher than eight in number (excluding 'replicates' on the same species). The test is therefore possible for six out of the eleven included substances and the results show that lognormal distribution cannot be rejected for five of the substances and only in one case can normal distribution not be rejected at a significance level of 0.05 (see Table 2 in Chapter 6 for details). These results confirm the dominance of lognormality as stated above.

In order to examine how robust the different average approaches are to variation in a three-value-data set, eight different fictive three-value-data sets (scenarios) are created for each substance. This is done by combining the highest or the lowest EC_{50} value within each of the taxa algae, crustacean and fish with one another leading to a total of eight combinations (scenarios). We hereby assume that we only know one data point for each of the three taxa which is a typical good case for most chemicals. The scenarios may be realistic in the sense that one can imagine that only the data in one of the scenarios actually exists or are used as a consequence of restricted choice of database by the practitioner doing the average estimation. By choosing the highest and lowest EC_{50} value within each taxa the maximum variation is secured. For a detailed example see Table 3 in Chapter 6.

For each of the scenarios the geometric mean (GM) and the median (Median) are estimated. Furthermore, for each substance the geometric mean of the total number of EC_{50} values on species level (GM-sp.) is estimated (i.e. for 'replicates' within species the geometric mean is used), and the median (Median-sp.) is estimated on the same data. Finally, the geometric mean (GM-troph) of the geometric means within each of the three taxa algae, crustacean and fish is estimated together with the median (Median-troph) estimated on the same data. This is done for all eleven substances and an example of the results is shown in Figure 7.

The 95%, 90% and 80% confidence limits around the different estimates based on the geometric mean are calculated (not shown here – but see examples in Chapter 6). Furthermore, the use of the max-min range as limits around the geometric means are investigated and an example is shown in Figure 8.

In order to have an indication of the robustness of the different average approaches we may estimate the ratio between the highest and the lowest estimated HC50 among the eight scenarios for each substance. This is done for the geometric mean and the median and shown in Table 5.

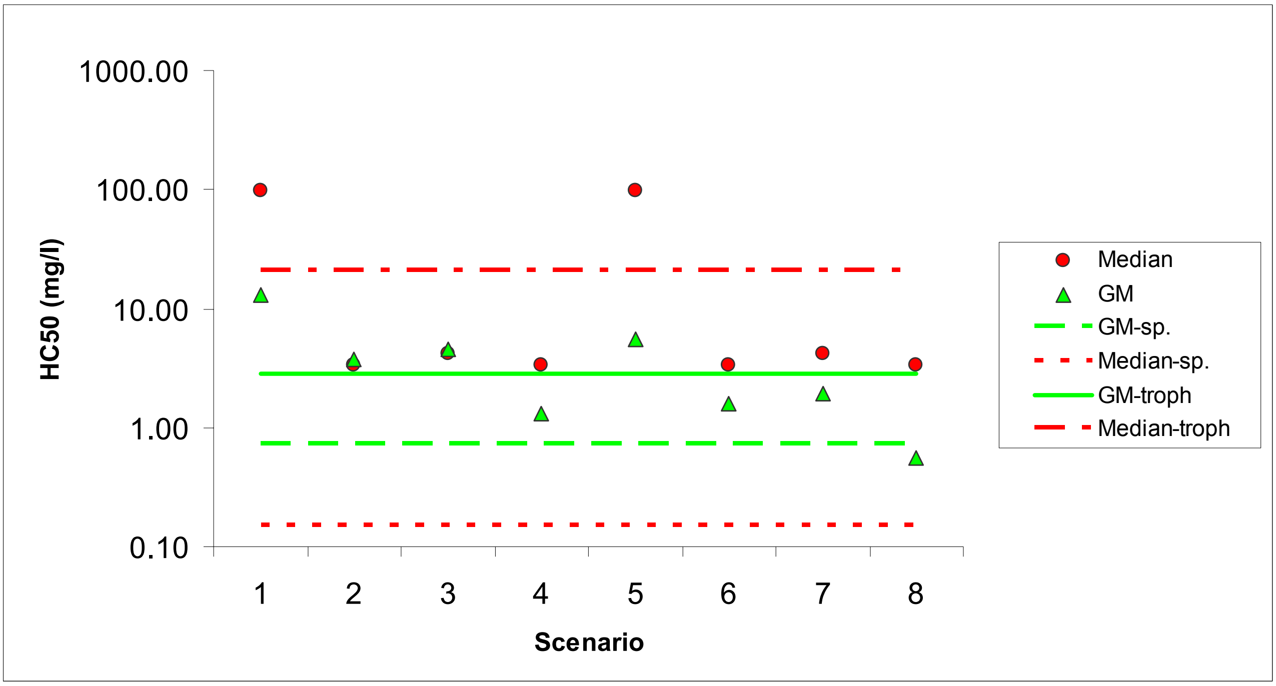

Figure 7. Average estimates of $HC50_{EC50}$ for the substance metribuzin. 'Median' and 'GM' are averages based on the eight fictive three data scenarios. 'GM-sp.' and 'Median-sp.' are averages based on the full data set on the level of species, and GM-troph and Median-troph are averages based on the full dataset on the level of taxa or trophic level.

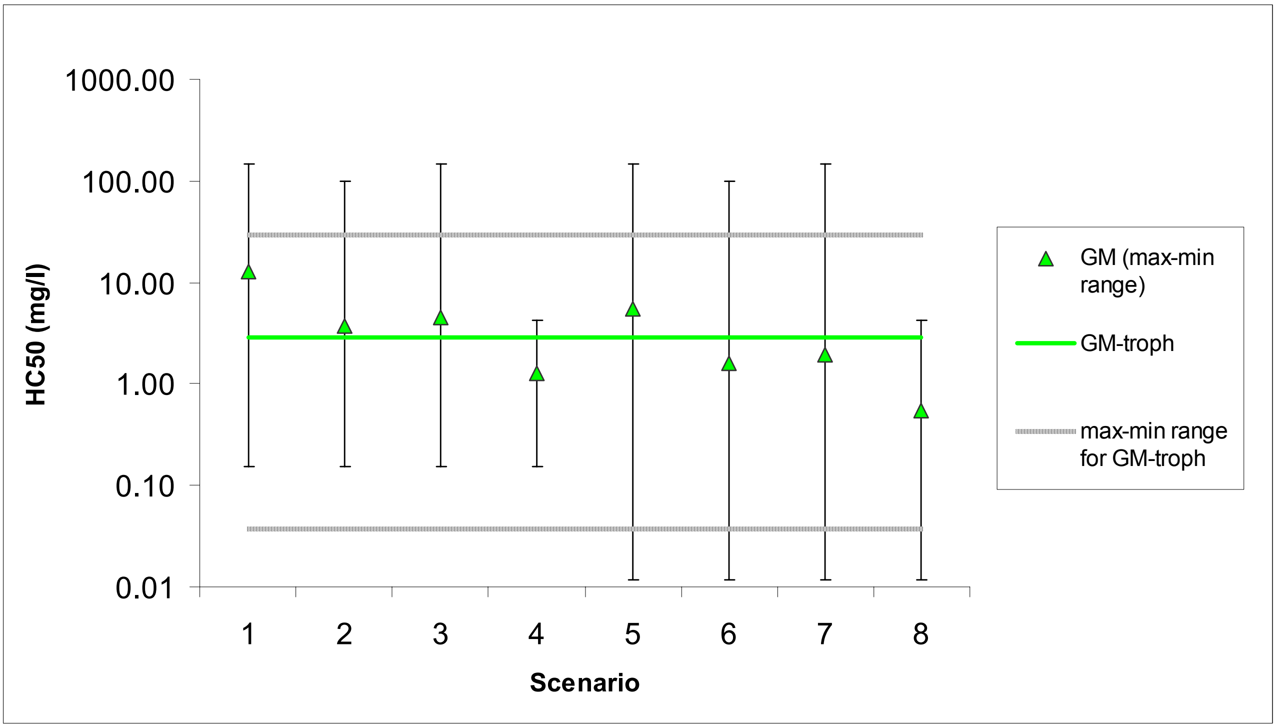

Figure 8. Geometric mean estimates of $HC50_{EC50}$ for the substance metribuzin. 'GM' is the average based on the eight fictive three data scenarios, shown with max-min range, i.e. maximum and minimum values among the three data. GM-troph is the average based on the full dataset on the level of taxa or trophic level.

Table 5. Ratio between the highest and the lowest 'scenario-estimated' HC50$_{EC50}$ for the two average approaches geometric mean (GM) and the median (Median). Furthermore, the ratios between the GM-troph and the GM-sp., and the ratio between the Median-troph and the Median-sp., all based on the full data set, are also shown.

Substance name	Scenario-based ratios (highest HC50/lowest HC50)		Full data set-based ratios	
	GM	Median	GM-troph/GM-sp.	Median-troph/Median-sp.
2,3,4,6-Tetrachlorophenol	7.3	7.8	1.2	0.77
4-Methyl-2-pentanone	1.2	1.0	0.87	0.83
2,4-Dichlorophenol	3.8	6.6	1.1	0.76
2-Chloroaniline	4.2	1.1	0.49	0.29
4-Nitrophenol	10	7.7	0.86	0.94
Dicamba	12	6.4	1.6	1.3
Metribuzin	24	29	3.9	140
Terbutylazine	11	13	1.9	2.7
Pendimethalin	38	37	0.97	1.2
Azoxystrobin	8.5	4.2	0.93	1.1
Dimethoate	85	840	1.2	0.62

The results in Table 5 show that in most cases the variation in the GM and the Median are at the same level, i.e. the ratio of the variation in the median to the variation in the GM lies at a level well below 4, but in one case (dimethoate), the ratio is about a factor of 10 (840/85). This is an example of the sensitivity of the median to a shift in a three value data set from two low values and one high to two high values and one low, i.e. a 'jumping median', see Figure 9 (see also theoretical example in Chapter 6, Figure 2).

A comparison between the GM-troph and the Median-troph for the two substances 4-nitrophenol and metribuzin illustrates the inability of the median to reflect average toxicity for small data sets. On a three value data set, thus representing geometric means at each trophic level (14.6; 12.0; 11.6 for 4-nitrophenol and 30.1; 20.6; 0.038 for metribuzin), the median approach gives the values 12.0 (4-nitrophenol) and 20.6 (metribuzin) indicating that 4-nitrophenol on average is more toxic than metribuzin despite the fact that metribuzin is very toxic to algae. The geometric mean on the other hand gives the values 12.7 (4-nitrophenol) and 2.86 (metribuzin) indicating a higher average toxicity of metribuzin. This kind of problem with the median is theoretically illustrated in Figure 6 (chemical 2 as compared to chemical 1).

Continuing to a comparison of the calculated averages on the species level (GM-sp. and Median-sp.) and on trophic level (GM-troph and Median-troph), which are both calculated for the full data set, the averages are, as shown in Table 5, in most of the cases here quite close. But, in some of the investigated cases, the difference in the number of species represented at each trophic level leads to differences in average toxicity. One example is metribuzin (also shown in Figure 7) for which the GM-troph is about four times higher (2.9/0.73 = 3.9) than the GM-sp., as shown in Table 5. The main reason for this difference is that the substance is especially toxic to algae which are represented by six species whereas crustaceans only are represented by two species and fish only by three species. The effect is even more pronounced, as shown in Table 5 and Figure 7, when comparing the Median-troph with the Median-sp. giving rise to a ratio of 140 in difference (21/0.15 = 140). Also for 2-chloroaniline and terbutylazine the differences in species representation at each trophic level leads to differences between GM-troph and GM-sp., in these cases about a factor of 2, see Table 5, Figure 10 and Figure 11.

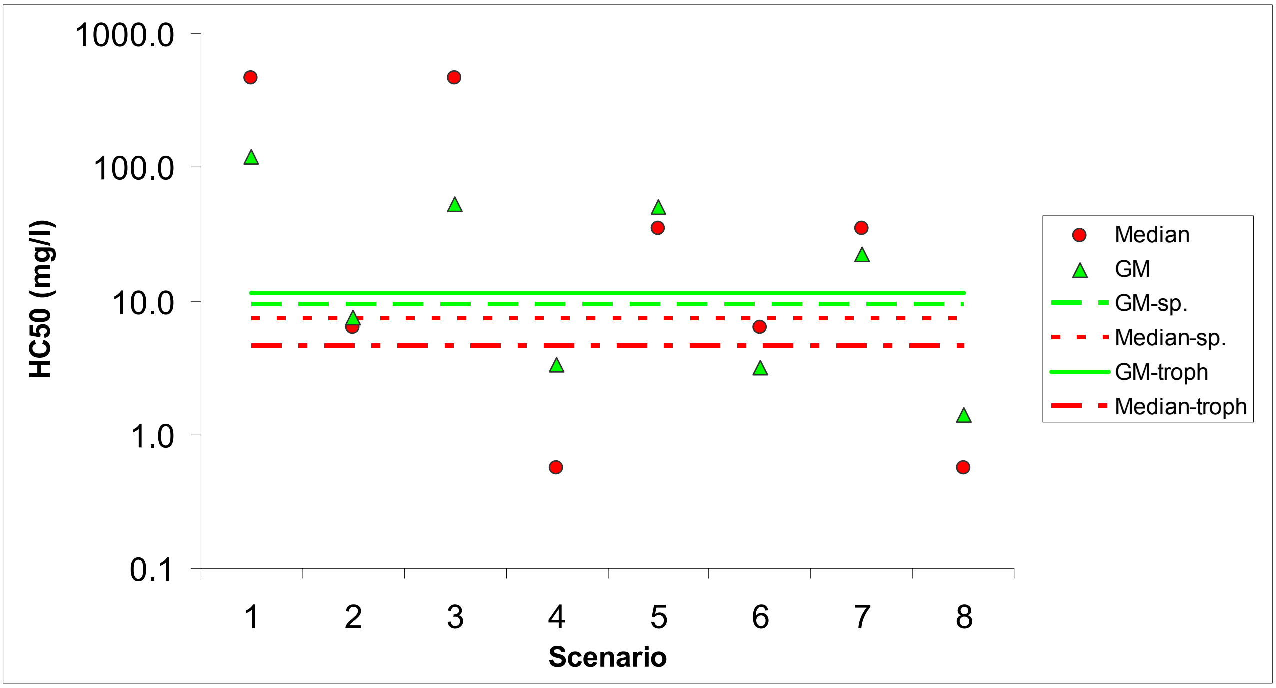

Figure 9. Average estimates of HC50$_{EC50}$ for the substance dimethoate. See Figure 7 for legend explanation.

These examples illustrate that there in some cases may be a problem with using the individual species data as basis for calculating the average rather than basing it on the geometric mean for each of the organism groups or taxa representing trophic levels. As pointed out by Aldenberg et al. (2002), a biased species selection leads to biased estimated parameters in SSDs including HC50. So, estimating the HC50 on the species level in cases with for example many data on fish and only a few on algae and invertebrates, and with a high difference in sensitivity between these three taxa, may lead to bias putting a weight on fish which may be disproportionate to the ecological relevance of this trophic level and instead reflect the fact that through regulation, it has been given a high priority in ecotoxicity testing. Furthermore, “it is generally assumed that members of the same taxonomic group are more similar to each other in sensitivity than to members of other taxonomic groups” (Forbes and Calow 2002b). The distribution of the GMs in Figure 7, Figure 10 and Figure 11 seems to confirm this assumption as the GMs for these three substances are distributed more evenly around GM-troph than around GM-sp. For the rest of the tested substances the difference between GM-troph and GM-sp. is too small as compared to the variation in GM to show any differences (except for 4-methyl-2-pentanone, not shown here) as illustrated by dimethoate in Figure 9. Combining these arguments with the fact that for most chemicals we only have three acute EC$_{50}$s, typically one from each of the taxa algae, invertebrates (crustacean) and fish, it seems most reasonable to put equal weight on each trophic level, represented by these three taxa, and therefore estimate the HC50 as the geometric mean of the geometric means for each trophic level, viz. GM-troph.

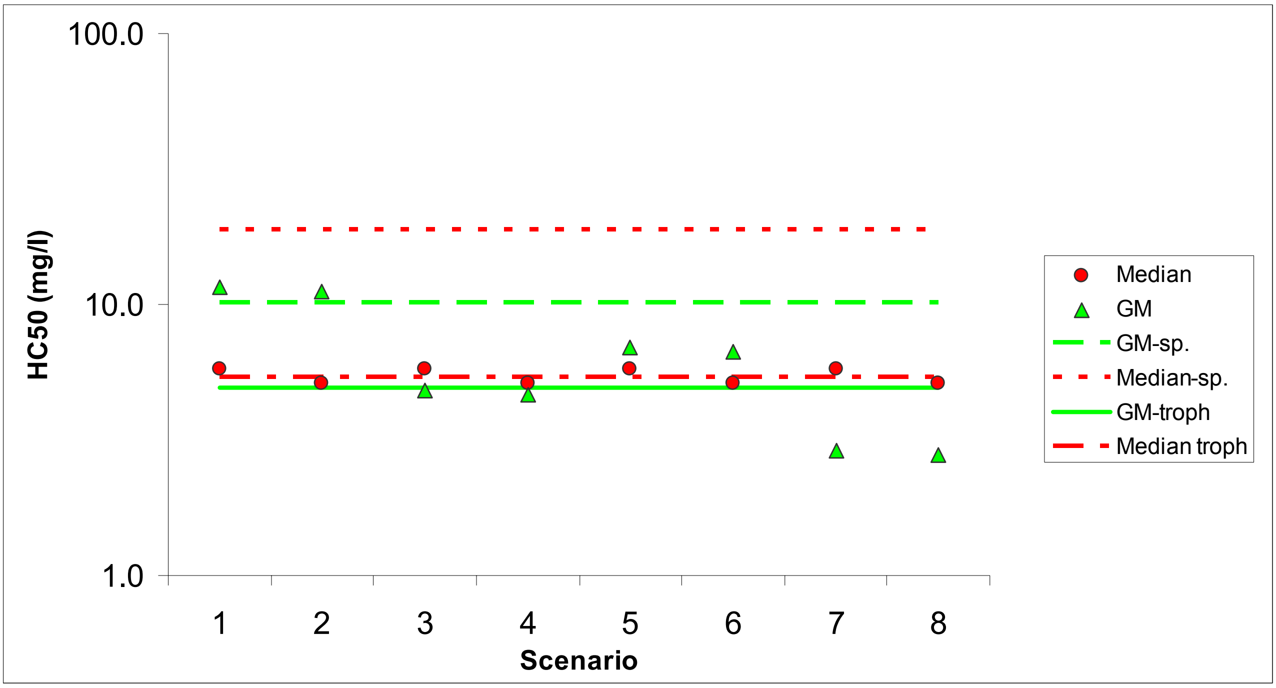

Figure 10. Average estimates of $HC50_{EC50}$ for the substance 2-chloroaniline. See Figure 7 for legend explanation.

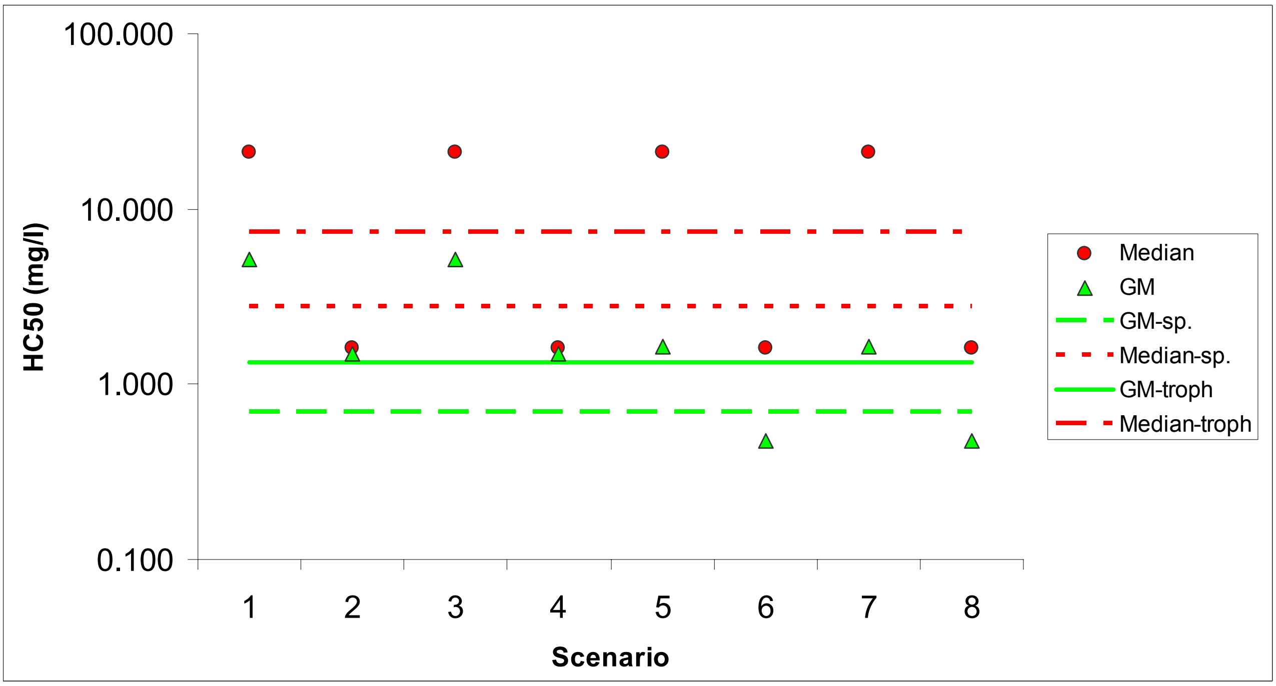

Figure 11. Average estimates of $HC50_{EC50}$ for the substance terbutylazine. See Figure 7 for legend explanation.

If we look at the results of the different approaches used to calculate confidence limits around the geometric mean for all 11 substances (not shown but look for examples in Chapter 6), it can generally be concluded that:

- 95% confidence limits around GM-troph are in most cases very wide making the statistically significant differentiation between the average toxicity among chemicals impossible
- Even the 80% confidence limits around the GM-troph are a bit wider or as narrow as limits based on the min-max values of the three data GM-troph data set
- The limits based on min-max values are relatively narrow for the substances tested here and in all but one case (i.e. 4-nitrophenol, not shown here), all GMs for the eight fictive scenarios overlap with the GM-troph calculated on the basis of the full data set (see example in Figure 8)
- In the case of 4-nitrophenol not even the 95% confidence limits around the GM (i.e. scenario 1 and scenario 8, not shown here) overlap with the GM-troph and for these two extreme scenarios the estimated GMs are 45 mg/l and 4.4 mg/l. With a GM-troph value of 13 mg/l this gives rise to an 'error' of a factor 3-4 for these two scenarios. If the min-max limits are used instead, i.e. the min value for scenario 1 (32 mg/l) or the max value for scenario 8 (4.9 mg/l), the 'error' equals a factor of 2-3.

As described in Section 1.6.2 the general expression for a PAF-based ecotoxicity characterisation factor (CF) may be given by:

$$CF = \frac{k}{HC50} \cdot dC \qquad (2)$$

Even though the value of 'k' in practice doesn't matter, 0.5 is chosen, meaning that the working point on the PAF curve is 0.5, and a linear gradient is used. This is done because in theory the determination of PAF = 0.5 is the least uncertain and least data demanding point on the PAF curve. Furthermore, the link to damage (i.e. reduction in species diversity) seems stronger for this 50% effect-based approach (PAF = 0.5) than for example the 5% effect-based approach (HC5, PAF = 0.05) or a no-effect (PNEC) based approach (Payet & Larsen 2004). The ecotoxicity characterisation factor (CF) estimated on basis of GM-troph may therefore be expressed as:

$$CF = \frac{0.5}{HC50_{EC50(GM-troph)}} \cdot dC \qquad (3)$$

This linear average gradient with working point at PAF = 0.5 is illustrated in Figure 12.

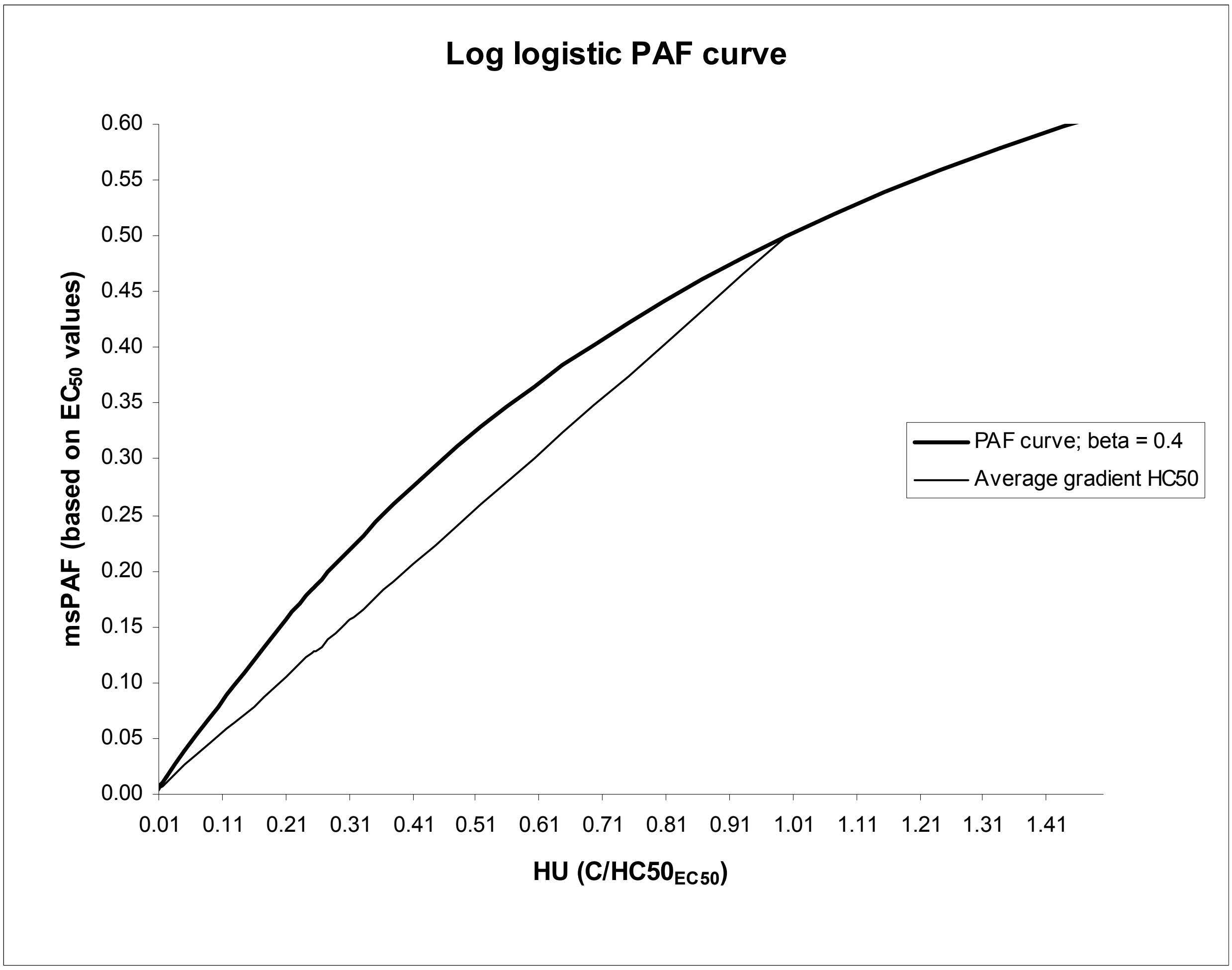

Figure 12. The average gradient with working point at PAF = 0.5 ($HC50_{EC50}$ = 1 HU) has a slope of 0.50 as illustrated here together with a log-logistic PAF curve with concentration (C) shown on a linear scale as Hazard Units, HU ($C/HC50_{EC50}$). The msPAF curve shown is defined by a β (beta) value of 0.4.

1.7.2 Conclusions on the development of GM-troph

Based on the real data scenario testing, the theoretical considerations of different average approaches for estimating HC50, the test of (confidence) limits on basis of three data points, and further including the discussions about data availability, weighting of trophic levels/taxa etc., the following recommendations are formulated for the EEI:

- The indicator should be based on the GM-troph calculated as the geometric mean of three EC_{50} values, one from each trophic level represented by algae, invertebrates (crustaceans) and fish.
- If more than one EC_{50} value is available for a trophic level then the GM-troph should be calculated as the geometric mean of the geometric means for each trophic level, i.e. GM-algae, GM-crustacean and GM-fish. These GMs are calculated as the geometric means of the genuses belonging to each of the trophic levels which again are calculated as the geometric means of the species belonging to each of the genuses. On the species level the geometric means are calculated, as normally done within ecotoxicology, as the geometric means of the single EC_{50} values for each species. See example of this calculation procedure in Chapter 6, Table 3.

- As limits around the GM-troph the lowest EC_{50} value should be used as the lower limit and the highest EC_{50} value as the upper limit in data sets with only three EC_{50} values, i.e. one from each trophic level.
- If more than one EC_{50} value from each trophic level is available then the max-min limits around the GM-troph should be based on the three geometric means on which the GM-troph is calculated, i.e. GM-algae, GM-crustacean and GM-fish, meaning that the lowest one of these three values is used as the lower limit and the highest one as the upper limit.

By choosing the GM-troph it is suggested to put equal weight on each of the three trophic levels instead of relying on an arbitrary species representation with weights indirectly determined by for example regulatory priority and therefore doubtful ecological relevance. So, by making a conscious choice of equal weights to each of the trophic levels, the possible bias from data sets with highly unequal number of tested species among the three trophic levels is avoided, which would occur if GM-sp. were used instead. As suggested by Forbes & Calow (2002b), a way to increase the ecological relevance when dealing with the species sensitivity distribution approach might be to assign weights to the input values from each taxa (or trophic level) reflecting the relative abundance of different taxa in the community/ecosystem in question. Combining this approach with theories of functional redundancy of species (Pratt and Cairns 1996) could be a very interesting research area for the further development of the EEI.

An EEI that equals $0.5/HC50_{EC50(GM\text{-}troph)}$ is chosen because the working point 0.5 is the least uncertain and least data demanding point on the PAF curve, see equation 3 and Figure 12.

It is not proposed to determine a statistically estimated uncertainty as basis for the limits around the GM-troph even though the number of input data is higher than three in some cases. Rather, it is preferred to use the same approach for all substances, and it is considered that the max-min approach is simple and seems to work fine (at least for the 11 substances tested). In most cases only three relevant data values are available anyway. The results obtained here indicate that the max-min range of the three data GM-troph (no matter the database) in practice overlap with the 'true' GM-troph (based on the full data set), just as well as confidence limits. So, even though the max-min limits cannot be used for statistical testing of the significance of differences between EEIs, these may be used for giving reasonable certainty that the 'true' GM-troph lies within the boundaries.

It is recommended to use EC_{50}(chronic) values when possible, but as only acute data will be available in most cases, the use of best estimate assessment factors are recommended to extrapolate from acute to chronic values. Even though there is a clear need for research in this area, an acute to chronic ratio of 10 between HC50(acute) and HC50(chronic) is recommended as a starting point.

Due to the comparative nature of LCIA seeking best estimates, it is recommended only to use test results from laboratory tests, fulfilling certain standard conditions, e.g. standard organism and restrictions on test duration and endpoints as described in Chapter 6, when estimating the HC50 value. These standard conditions for acute tests are described in details in Larsen et al. (2004b), but detailed criteria for choice of chronic data still need to be developed.

The ability of a geometric mean to represent the toxicity (including chronic toxicity) of very toxic substances and very sensitive species has not been dealt with yet, and further research is needed here. However, it may be anticipated, on the basis of the results from the tests done here of different average approaches on 11 substances (including very toxic pesticides, e.g. terbutylazine), that the GM-troph with its max-min limits at least to some degree accounts for very toxic substances if representative toxicity data are available.

For further research it is recommended that test on a wider range of substances should be performed to further verify the GM-troph approach and its ability to represent substances that are very toxic to specific species. Furthermore, detailed criteria for choice of chronic test data should be included together with studies on best estimate assessment factors for acute to chronic extrapolation.

1.8 Discussion and conclusion

The goal of this thesis has been defined by two questions as described in Section 1.1. The first question deals with the importance of the chemical- or toxicity-related impact categories:

1. Can the outcome of an LCA (e.g. the impact profile) be significantly dependent on whether or not toxicity related-impact categories are included?

The answer to this question may be evident to some LCA researchers because it seems to be a more or less general opinion in the LCA community that the chemical-related impact categories maybe important in LCA and that they are often excluded (e.g. Bunke et al. 2003, Landsiedel & Saling 2002). However, this has never been systematically documented until now. The case study included in this thesis (see Section 1.3 and Chapter 2) documents that for LCAs on printed matter the inclusion of chemical-related impact categories can be decisive for the outcome and that chemical-related impact categories are poorly or not at all included in previous studies. The importance for the total impact in the case study of for example the printing process is reduced from 41% to 10% if the chemical-related impact categories are excluded. So, the basis for defining for example ecolabelling criteria (typically based on life cycle thinking) on printed matter is substantially different depending on whether or not the chemical-related impact categories are (properly) included.

The case study also shows that even in this particular case, where special focus and effort on chemical emissions are included, it has only been possible to characterize 25% - 37% of the total number of known emissions, mainly due to lack of sufficient data. On top of this comes a general problem with lack of knowledge on upstream emissions (chemical emissions occurring at the materiel stage, i.e. extraction and production of raw materials) and in many cases lack of knowledge about chemical emissions from waste treatment. In the case study a newly developed tool for estimating upstream emission (Andersen & Nikolajsen 2003) are used, but only for estimating emissions in connection with pigment production (component in printing ink). Lack of emission data from the raw material producing industry is a severe and general problem in LCA. If this problem should be solved, preferably through access to industry data or less optimally from further development of estimation tools, the reliability of LCA case studies including chemical-related impact categories would improve significantly. Inclusion of improved knowledge about emissions from waste treatment would further strengthen this reliability.

Anyhow, in this case study the main part of the known chemical emissions that were not characterized is known to be of low concern if not emitted in very high quantities and could therefore be excluded as important. This is a special case and due to extensive research of chemicals within the printing industry (e.g. Larsen et al. 1995, 1998, 2002a) and will most probably not be the case for the major part of other product groups. So, the result of this case study also points out the need for a screening method which, on a very low database, is able to select those chemical emissions that are expected to contribute significantly to the chemical-related impact categories, viz. a selection method.

The second question defining the goal of this thesis deals with data availability:

2. How is the problem with low data availability solved the most optimal way?

This question is addressed on two levels, viz. the choice at the classification step of the LCIA procedure of chemical emissions to be assigned to the chemical-related impact categories in the characterisation step, and the estimation of the ecotoxicity effect indicator as part of the characterisation step. Together with the ecotoxicity fate indicator (not included in this thesis) these two issues represent some of the key areas where LCIA suffers from low data availability (as compared to demand), and they are the key obstacles for a more comprehensive inclusion of potential impacts from chemical emissions.

On the level of choosing the chemical emissions to be included in the characterisation step, question 2 is answered through the introduction of selection methods, as described in Section 1.4, Section 1.5, Chapter 3 and Chapter 4. A selection method is a chemical screening method, that, on a low to very low (e.g. QSAR-based) data base, is able to select those chemical emissions, among possibly several hundreds mapped in the inventory of an LCA case study, that contribute most significantly to the chemical-related impact categories of the of the associated characterisation method. The results of this thesis shows that only three chemical screening methods, associated with a characterisation method, and therefore here defined as selection methods, actually exist to day. These selection methods include the EDIP-selection method (Wenzel et al. 1997) and the Priofactor (Larsen et al. 1999a, 1999b), which both are associated with the characterisation method EDIP97 (Wenzel et al. 1997), and the CPM-selection method (Eriksson 1999) associated with the characterisation method CPM (Eriksson 1999). Selection method performance criteria developed as part of this thesis include demands on consistency in prioritisation with associated characterisation method, applicability to different chemical groups, high data availability combined with low data demand, data useable in characterisation, user friendliness and transparency. A mainly qualitative evaluation of the existing selection methods against these performance criteria shows that none scores high on all criteria. This indicates the need for development of new selection methods. Recommendations on which components to include, which issues to address and general principles for developing selections methods are therefore given.

A quantitative evaluation of the existing selection methods, and the risk ranking method EURAM (Hansen et al. 1999) tested as a ‘generic’ selection method, is performed. Based on the key performance criteria, i.e. consistency with associated characterisation method in ranking, these methods are tested against the two included characterisation methods EDIP97 and CPM, which are also tested against each other (see Section 1.5 and Chapter 4). The results of these tests show a good correlation between the ranking of all the tested methods, but strongest between the EDIP97 method and its two associated selection methods EDIP-selection (revised version) and Priofactor. For those methods where statistical test of correlation in ranking is possible (EDIP97, Priofactor, CPM and EURAM) the result shows significant correlation in all cases, but strongest between EDIP97 and CPM, and EDIP97 and Priofactor ($\alpha < 0.001$) and weakest between CPM and EURAM ($\alpha < 0.05$). The main reason for this result is that a common perception of what makes a substance ecotoxicologically problematic underlies all four methods, which is reflected in the fact that the expressions for all the methods include similar combinations of biodegradability (or persistence), bioaccumulation potential and toxicity (PBT). Nevertheless, some outliers as compared to the EDIP97 ranking, are identified. These outliers are due to specific characteristics of each of the methods which for certain combinations of substance properties may result in false negatives or false positives as compared to EDIP97. These characteristics include the influence of data availability on the size of assessment factors for conversion of acute effect data to chronic values, and whether or not mode of entry is taken into account in the fate modelling. Further, the reversing of the effect of toxicity on ranking by negative logKow values is observed when logKow is a direct factor in the expression, and there is a significant influence of the way in which the BCF is estimated and included.

These tests on selection methods were done on dissociating and amphiphilic substances and emitted amount was not included because a case study was not involved. An earlier test (see Chapter 3, Table 5), on different substance groups and including emitted amount (case study on a detergent for manual dishwashing), of the consistency performance of the Priofactor as compared to the associated characterisation method EDIP97, shows very high consistency (> 96%, both ecotoxicity and human toxicity) in the prioritisation of significant chemical emissions. So, even though there certainly is a need for development of new selection methods and improvement of existing ones the characterisation method EDIP97 is associated with relatively well functioning selection methods.

On the level of low data availability in the estimation of the ecotoxicity effect indicator, question 2 is answered by an identification of the most reasonable indicator approach and its key parameter (i.e. HC50), taking data constraints and the framework of LCA into account, and on that basis a low data demanding ecotoxicity effect indicator, viz. GM-troph, is developed.

An inventory of the different existing approaches for ecotoxicity effect indicators including damage approaches is done, and these approaches are evaluated against a developed set of performance criteria, see Section 1.6 and Chapter 5. The performance criteria include scientific validity, environmental relevance, reproducibility, transparency, data demand and availability, possibilities of spatial differentiation, and inclusion of quantification of uncertainty.

Two main approaches exist, viz. the assessment factor-based PNEC approach and the PAF-based approach (making use of species sensitivity distribution). The PNEC-approach (e.g. Hauschild et al. 1998) is only used for midpoint indicators (1/PNEC) whereas for the PAF-approach in some cases (e.g. Goedkoop & Spriensma 2001a, 2001b) attempts have been made to model all the way along the environmental mechanism to endpoint or damage (e.g. change in biodiversity). For identified approaches to damage modelling, only the ‘media recovery’ approach has been implemented (e.g. Goedkoop & Spriensma 2001a, 2001b) and that in a very simple way. For the ‘mean extinction time’, another damage approach, only one attempt has been made to include this population biology tool in LCA (Itsubo et al. 2003), and for the ‘genetic diversity approach’ no attempts have yet been made. All these damage approaches, especially the last one, are at an early state of development. This fact is reflected in the result of the evaluation of the damage approaches scoring high on environmental relevance but low on all other criteria.

The evaluation against the performance criteria of the assessment factor-based PNEC approach and the PAF-based approach shows pros and cons for both. The PNEC-approach has for example a lower data demand and is more transparent than the PAF-based approaches whereas the PAF-approaches have a potentially higher environmental relevance. Further, besides the tiered risk assessment-based conservative assessment factors, the PNEC approach suffers from the uncertainty of the NOEC value, which is dependent on the design of the test from which it is determined. The problem with the NOEC values is also relevant for the NOEC-based PAF-approaches.

The result of the analysis of the different approaches shows, that if we include the fact that in LCIA the ecotoxicity effect indicator is used for comparison between substances, all the different PAF-based ecotoxicity effect indicator may be expressed as k/HC50. The 'k' value may be somewhere between 0.2 and 43 depending on the actual method used but the key element in the ecotoxicity effect indicator is HC50. The crucial point in the determination of a PAF-based ecotoxicity effect indicator is therefore the data used and the principles applied for determining the HC50 value of each toxicant.

Taking the comparative nature of LCA and its aim for best estimate into account, and combining this with the possibilities for reducing the data demand of an EC_{50}-based PAF approach, and further including the (at least theoretical) connection to damage approaches, leads to the choice of an effect-based (not PNEC-based) PAF average ecotoxicity effect indicator expressed by $k/HC50_{EC50}$ for further development. Even though the value of 'k' doesn't matter in this comparative context, 0.5 is chosen because the working point 0.5 is the least uncertain and least data demanding point on the PAF curve.

In this development of the low data demanding ecotoxicity effect indicator GM-troph for the freshwater pelagic compartment (see Section 1.7 and Chapter 6) different ways of estimating the average toxicity (HC50), i.e. median, geometric mean and arithmetic mean, are tested in theory and on real data. The results show that the geometric mean is the most robust estimator. Seeking the coverage of many chemicals in LCA and considering the fact that the main part of the useable single species laboratory test data (EC_{50}) is on algae, crustacean and fish (so-called 'base set'), the choice of a minimum of three acute EC_{50} values from each of the three main taxa plants, invertebrates and vertebrates, is made. The so-called 'base set' is for example implemented in the EU regulation on dangerous substances (EEC 1967, and its amendments), in the American 'Chemical Right-to-Know Initiative' on high production volume chemicals (US EPA 2000), and in the OECD work on investigations of high production volume chemicals (OECD 2003). The three mentioned main taxa cover the trophic levels primary producers, primary consumers and secondary (and tertiary) consumers and are in practice represented by algae, invertebrates (crustacean) and fish. Due to the comparative nature of LCA, the possible bias from severe unequal species representation and inclusion of erroneous data, due to bad non-standardised test conditions, should be avoided by only including test on standard organism fulfilling certain defined test criteria on durations and endpoints.

Test on the difference between estimating the average toxicity (HC50) on the level of species (using averages of EC_{50} values within species as input data) and on the level of taxa or trophic levels (using averages of EC_{50} values within taxa or trophic levels as input data) indicate that in some cases of unequal representation between taxa or trophic levels, estimations based on the species level may be biased. For example, estimating the HC50 on the species level in cases with many data on algae and only a few on fish and invertebrates, and high difference in sensitivity between these three taxa, may lead to bias putting a weight on algae or primary producers which may be disproportionate to the ecological relevance of this trophic level and instead reflect the fact that through regulation, it has been given a high priority in ecotoxicity testing. These observed differences may be due to a higher similarity in sensitivity among members of the same taxonomic group than among members of different taxonomic groups (Forbes & Calow 2002b). So, in order to avoid the effect of possible haphazard or regulatory determined species representations in the data set used, which may be decisive for the weighting of each trophic level in the estimation, the geometric mean based on the average of the averages within each trophic level, i.e. GM-algae, GM-crustacean and GM-fish, is chosen for the ecotoxicity effect indicator GM-troph. Hereby, it is consciously chosen to put equal weight on each throphic level.

The use of trophic levels based on algae, invertebrates and fish is disputable due e.g. to the fact that many invertebrates are not herbivores (primary consumers) but carnivores (secondary consumers) or both (omnivores) and not all fish are carnivores. Furthermore, the trophic level of the organism varies with the life stage in many cases. However, for the main part of the existing standard organisms, the invertebrates (mainly crustaceans) are herbivores and the fish are carnivores (Larsen et al. 2004b). It may also be argued that not just the trophic level or taxa is important for the sensitivity but also factors like life stages including ways of reproduction. Taking these factors into account has not been within the scope of this thesis because these in most cases are not directly relevant for the main part of the available test data, i.e. acute toxicity test results. In the further research on trophic level-based HC50 estimation including chronic data these issues may become relevant, even though the number of standardised laboratory tests and available effect-based (i.e. EC_{50} chronic) data is restricted. Even if this issue might be disputable, as pointed out above, the main argument for introducing the use of trophic levels within the estimation of an HC50 for species sensitivity distribution or PAF use in LCIA, is to make a conscious choice with basis in ecology, while taking the available data into account, and not just relying on haphazard collection of species.

In order to secure a broader coverage of biological sensitivity, inclusion of other taxa like insects, mollusca and amphibians may be relevant. However, no standard tests (freshwater, pelagic) currently exist for these taxa (Larsen et al. 2004b), and the availability of test results is highly variable among chemicals. So, what has been done here is a trade off between on the one side seeking a broad coverage of biological sensitivities with the risk of introducing a bias in the weighting of chemical ecotoxicity effect indicators as compared to one another, and on the other side seeking a robust standardised basis for comparison but then running the risk of excluding very sensitive species. Taking into account the comparative context of LCA seeking best estimate and equal treatment of a high number of chemicals, and further considering the fact that non-standardised test data are most variable in quality and availability among chemicals, as compared to acute tests on standard organism, the choice of exclusively using results from tests on standard organisms, following certain restrictions on end point and time duration, seems most reasonable. However, the importance of excluding very sensitive species should be investigated and is therefore part of the recommended further research on ecotoxicity effect indicators.

Confidence limits around the GM-troph value have also been investigated. In most cases these are too wide, because the average is based on only three data values, which makes a statistically significant differentiation between the different toxicants nearly impossible. In cases with data sets well above three species EC_{50}s, narrower confidence limits may be achieved by using an average (i.e. HC50) on species level. However, then we still have the above mentioned possible problem with haphazard species representation in each taxa introducing bias and possible ‘false’ low uncertainty due only to a higher number of data. Test on fictive three data value test sets based on combinations of max and min values from the larger ‘mother’ data set indicate that the use of the min and max value among the three data value GM-troph data set (i.e. GM-algae, GM-crustacean and GM-fish) as max-min limits around GM-troph gives a reasonable (and as good as confidence limits) certainty that the ‘true’ GM-troph value (based on the full ‘mother’ data set) lies within the interval.

The inclusion of the toxicity-related impact categories in LCA at a similar level as the better established impact categories, like global warming, is far from achieved yet. However, relatively well functioning selection methods, e.g. the EDIP-selection (revised version) and Priofactor, for the key property based characterisation method EDIP97 are described in this thesis and an extended use by LCA practitioners of these screening methods would probably facilitate a more proper representation of toxicity-related impact categories in future LCA studies. Furthermore, this thesis describes and defines the framework including performance criteria and recommendations on how to improve existing selection methods and how to develop new ones. The way for further improvement of the involvement of toxicity-related impact categories is hereby facilitated.

Low availability and high uncertainty of characterisation factors on ecotoxicity combined with low robustness and/or low data availability (as compared to data demand) in estimation of new ones are dominating today. By introducing the GM-troph this thesis contributes with a robust, low data demanding effect part (EEI) of the ecotoxicity characterisation factor, which seems most reasonable among the many alternatives taking the framework of LCA and the data constraints into account. The GM-troph has the potential of facilitating a high number of characterisation factors which are robust with relatively low uncertainty if combined with a 'fate part' of equal strength.

It is the hope of the author that the potential improvements, on the inclusion of impacts from chemical emissions in LCA, which have been created during this Ph.D. study and reported in this thesis, will in practice lead to more complete LCA studies in the future.

1.9 References

Aldenberg T, Jaworska J, Traas T P (2002). Normal Species Sensitivity Distributions and Probabilistic Ecological Risk Assessment. Chapter 5 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L., Suter II G.W. and Traas T.P. (eds.), pp. 49-102. Lewis, Boca Raton, FL, USA.

Andersen LK, Nikolajsen MH. (2003). Life Cycle Assessment of chemicals at the Brdr. Hartmann A/S. Thesis elaborated at the Danish engineering education at The Technical University of Denmark. Supervisor. Michael Hauschild. IPL-048-03. http://ipt.dtu.dk/~mic/Master thesis reports/KraghAndersen&HolmNikolajsenMasterThesis.zip

Axelsson U, Dalhielm R, Marcus O (1997). Miljöprofilering – livscykelanalyser av grafiske produkter, del 2. TEKNIKRAPPORT nr. 3/97. IMT, Stockholm, Sweden.

Bennett D H, McKone T E, Kastenberg W (2000). Evaluating multimedia persistence: Classification and regression tree analysis. Environ Toxicol Chem 19, 810-819.

Bliss C I (1935). The calculation of the dosage-mortality curve. Ann. Appl. Biol. 22, pp 134-167.

Brüggemann R, Halfon E, Welzl G, Voigt K, Steinberg C E W (2001). Applying the concept of partial ordered sets on the ranking of near-shore sediments by a battery of tests. J Chem Inf Comp Sci 41 (4), 918-925.

Bunke D, Gensch C-O, Möller M, Rüdenauer I, Ebinger F, Graulich K (2003). Assessment of Toxicological Risk due to Hazardous Substances: Scoring of Risk Phrases. Int J LCA 8 (1), 6-7.

Chapman, P F, Crane M, Wiles J A, Noppert F, McIndoe E C (1996). Asking the Right Questions: Ecotoxicology and Statistics. SETAC, Belgium. The report of a workshop held in Royal Holloway University of London, Egham, Surrey, United Kingdom, 26-27 April 1995.

Chapman P M, Fairbrother A, Brown, D (1998). A critical evaluation of safety (uncertainty) factors for ecological risk assessment. Environ. Toxicol. Chem. 17 (1), 99-108.

Dalhielm R, Axelsson U (1995). Miljöprofilering – livscykelanalyser av grafiske produkter. TEKNIKRAPPORT nr. 4/95. IMT, Stockholm, Sweden.

Davis G, Fort D, Hansen B G, Irwin F, Jones B, Jones S, Socha A, Wilson R, Haaf B, Gray G, Hoffman B (1997). Framework for Chemical Ranking and Scoring Systems. Chapter 1 in: Chemical ranking and scoring: Guidelines for relative assessment of chemicals, Swanson M B and Socha A C (eds.), pp. 1-29. SETAC-US. Proceedings from the Pellston workshop on Chemical ranking and scoring, 12-16 February, 1995. Sandestin, Florida, USA.

de Koning A, Guinée J B (2002). Selection of metals and inorganics for the test set of substances. Contribution to Work-package 7 of the OMNIITOX Project. EC Project contract G1RD-CT-2001-00501. Institute of Environmental Science, Leiden University (internal report).

de Koning A, Guinée J, Pennington D W, Sleeswijk A, Hauschild M, Molander S, Nyström B, Pant R, Schowanek D (2002). Methods and typology report Part A: Inventory and classification of LCA characterisation methods for assessing toxic releases. Contribution to Work-package 7 of the OMNIITOX Project as part A of appropriate deliverable D11. http://www.omniitox.net/

EU (2001) White Paper. Strategy for a future Chemicals Policy (presented by the Commission). Commission of the European Communities. Brussels, 27.2.2001. COM(2001) 88 final.

Drivsholm T, Maag J, Christensen SV, Hansen E (1996). Ressourceforbrug og miljøbelastning for tre grafiske produkter i et livscyklusperspektiv. Work Report No. 63 (book in Danish). Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/1996/87-7810-747-4/pdf/87-7810-747-4.pdf

Drivsholm T, Maag J, Christensen SV, Hansen E (1997). Miljøeffekter og ressourceforbrug for tre grafiske produkter i et livscyklusperspektiv. (book in Danish with English summary). Environmental Project No. 341. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/1997/87-7810-682-6/pdf/87-7810-682-6.pdf

EEC (1967). Approximation of laws, regulations and administrative provision relating to the classification, packaging and labelling of dangerous substances (Council Directive 1967/548/EEC, June 27).

EC (2003a): Environmental Risk Assessment. Chapter 3 (Part II) in: Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances, Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European

Parliament and the Council concerning the placing of biocidal products on the market. Institute for Health and Consumer Protection. European Commission. ECB, JRC, Ispra, Italy.

EC (2003b) Proposal for a Regulation of the European Parliament and of the Council concerning the Registration, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency and amending Directive 1999/45/EC and Regulation (EC) {on Persistent Organic Pollutants}. COM (2003) 644, Brussels, 29 October 2003.

ECOTOX (2003). ECOTOXicology Database system. US EPA: http://www.epa.gov/ecotox/

Eriksson Å (1999). A comparative study of four models for ecotoxicological impact assessment in LCA – a case study of tyre emissions. Honour thesis in environmental science. Tutor Sverker Molander. June 1999. Göteborgs Universitet, Sweden.

Forbes , V. E., Calow, P. (2002a). Extrapolating in Ecological Risk Assessment: Balancing Pragmatism and Precaution in Chemical Controls Legislation. BioScience, 52(3), 249-257.

Forbes , V. E., Calow, P. (2002b). Species Sensitivity Distribution Revisited: A Critical Appraisal. Human and Ecological Risk Assessment 8(3), 473-492.

Goedkoop M, Spriensma R (2001a). The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Report. Third edition. Pré Consultants, Amersfoort, The Netherlands. http://www.pre.nl

Goedkoop M, Spriensma R (2001b). The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Annex. Third edition. Pré Consultants, Amersfoort, The Netherlands. http://www.pre.nl

Hansen B G, Van Haelst A G, Van Leeuwen K, Van der Zandt P (1999). Priority setting for existing chemicals: European Union risk ranking method. Environ Toxicol Chem 18, 772-779.

Hauschild M, Wenzel H, Damborg A, Tørsløv J (1998). Ecotoxicity as a criterion in the environmental assessment of products. In: Hauschild M, Wenzel H (eds) Environmental Assessment of Products: Volume 2: Scientific background, pp. 203-314. Chapman & Hall, London, Great Britain.

Hauschild M, Wenzel H (eds) (1998). Environmental Assessment of Products: Volume 2: Scientific background. Chapman & Hall, London, Great Britain.

Hauschild M, Pennington D (2002). Indicators for Ecotoxicity in Life Cycle Impact Assessment. Chapter 6 in: Life-cycle Impact Assessment: Striving Towards Best Practice, Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds.), pp. 149-176. SETAC-Europe, Brussels, Belgium.

Hauschild MZ (2004). Assessing environmental impacts in a life cycle perspective. *Environ. Sci. Technol. (accepted).*

Huijbregts M, Thissen U, Guinée JB, Jager T, Kalf D,Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000). Priority assessment of toxic substances in life cycle assessment. Part I: Calculation of toxicity potentials for 181 substances with the nested multi-media fate, exposure and effects model USES-LCA. *Chemosphere, 41 (2000), 541-573.*

Hakoyama H, Iwasa Y (2000). Extinction risk of a density-dependent population estimated from a time series of population size. J. Theor. Biol. 204: 337-359.

ISO (1997). ISO 14040: Environmental management – Life cycle assessment – Principles and framework. International Organisation for Standardisation, Geneva, Switzerland.

ISO (1998). ISO 14041: Environmental management – Life cycle assessment – Goal and scope definition and inventory analysis. International Organisation for Standardisation, Geneva, Switzerland.

ISO (2000a). ISO 14042: Environmental management – Life cycle assessment – Life cycle impact assessment. International Organisation for Standardisation, Geneva, Switzerland.

ISO (2000b). ISO 14043: Environmental management – Life cycle assessment – Life cycle interpretation. International Organisation for Standardisation, Geneva, Switzerland.

Itsubo N., Ii,R., Abe,K., Nakagawa,A., Hayashi,K., Inaba,A. (2003). Biodiversity Damage Assessment – Applying the Theory of Biology in LCIA. Slides from platform presentation (WE2/8) at the SETAC Europe 13th Annual Meeting at Hamburg, Germany April 27 – May 1, 2003.

IUCLID (2000). European Chemical Bureau: IUCLID CD-ROM Year 2000 edition. Public data on high volume chemicals. ISBN 92-828-8641-7.

Johansson M (2002). Livscykelanalys av arkoffsettrykning. Jämförande analys av vatenfri och konventionell offsettrykning samt computer-to-plate och konventionell prepress. Rapport nr. 2002:09. Framkom, Stockholm, Sweden.

Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer G, Rosenbaum R (2003). Impact 2002+: A New Life Cycle Impact Assessment Methodology. Int J LCA 8 (6) 324-330.

Lande R (1998). Anthropogenic, ecological and genetic factors in extinction and conservation. Researches on population ecology 40(3): 259-269.

Landsiedel R, Saling P (2002). Assessment of Toxicological Risk for Life Cycle Assessment and Eco-efficiency Analysis. Int J LCA 7 (5), 261-268.

Larsen HF, Tørsløv J, Damborg A (1995). Areas of intervention for cleaner technology in the printing industry - assessment of waste water (book in Danish with English summary). Environmental Project No. 284. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/1995/87-7810-330-4/pdf/87-7810-330-4.pdf

Larsen HF, Pedersen AR, Birch H, Rasmussen D, Hansen LE (1998). Evaluation of Best Available Technology (BAT) in screen cleaning (book in Danish with English summary).

Environmental Project No. 381. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/1998/87-7810-975-2/pdf/87-7810-975-2.pdf

Larsen H F, Christensen F M, Rasmussen J O, Helweg C, Olsen S I (1999a): CETOX-LCA-Handbook, LCA on ‘chemical-heavy’ products (book in Danish). CETOX, Hørsholm, Denmark.

Larsen H F, Christensen F M, Rasmussen J O, Helweg C, Olsen S I (1999b). Screening tool for prioritization of chemicals to be included in a LCA study. Presented at the 9th Annual Meeting of SETAC-Europe, 25-29 May 1999 in Leipzig, Germany. Abstract No. 4c/001.

Larsen HF, Helweg C, Pedersen AR, Boyd HB, Laursen SE, Hansen J (2000). Chemicals in textiles (book in Danish with English summary). Environmental Project No. 534. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/2000/87-7909-800-2/pdf/87-7909-801-0.pdf

Larsen HF, Helweg C, Pedersen AR, Andersen M, Wallström E, Hoffmann L (2002a). Evaluation of Best Available Technology (BAT) in washing off water-based flexographic inks in the packaging printing industry (book in Danish with English summary). Environmental Project No. 730. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/2002/87-7972-320-9/pdf/87-7972-321-7.pdf

Larsen HF, Birkved M, Hauschild M, Pennington D, Guinée J (2002b). Inventory of LCIA selection methods for assessing toxic releases. Methods and typology report part B. Contribution to Work-package 7 of the OMNIITOX Project as part B of appropriate deliverable D11. EC Project contract G1RD-CT-2001-00501. http://www.omniitox.net/

Larsen HF, Hansen MS, Hauschild M (2004a). Ecolabelling of printed matter. Part II: Life cycle assessment of model sheet fed offset printed matter. Environmental Project No. XXX. (final draft April 2004). Danish Environmental Protection Agency. Final draft preliminary available at: http://ipltest.kpd.ipt.dtu.dk/ipl/upload/lcv/127_2.pdf

Larsen HF, Payet J, Molander S, Hauschild M (2004b). Implementation of the OMNIITOX Base Model. Contribution to work package 8 of the OMNIITOX project as part A of appropriate deliverable D41. Part VIII – Implementation of the ecotoxicological effects module. EC Project contract G1RD-CT-2001-00501. http://www.omniitox.net/

Länge R, Hutchinson T, Scholz N, Solbe J (1998). Analysis of the ECETOC Aquatic Toxicity (EAT) database. II – Comparison of acute to chronic ratios for various aquatic organisms and chemical substances. Chemosphere 36 (1), 115-127.

Margni M, Pennington D, Birkved M, Larsen H F, Hauschild M (2002). Test set of organic chemicals for LCIA characterisation method comparison. Contribution to Work-package 7 of the OMNIITOX Project. DRAFT September 2002. EC Project contract G1RD-CT-2001-00501 (internal report).

N-CLASS (2003). N-CLASS Database. Physical/chemical, health and environmental effect classification for substances placed on Annex I of Council Directive 67/548/EEC (on the classification, packaging and labelling of dangerous substances). Database administrator: J. Falck, KemI. The present database is a web version of the N-CLASS Database that earlier were issued in TemaNord 1999:538. The Nordic Council of Ministers. www.kemi.se/nclass

Newman, M C, Dixon P M (1996). Ecologically Meaningful Estimates of Lethal Effect in Individuals. Chapter 8 in: Ecotoxicology - A Hierarchical Treatment, Newman, MC, Jagoe, CH (eds.), pp. 225-253. Lewis, Boca Raton, FL, USA.

Newman MC, Ownby DR, Mézin LCA, Powell DC, Christensen TRL, Lerberg SB, Anderson B-A, Padma TV (2002). Species Sensitivity Distributiions in Ecological Risk Assessment: Distributional Assumptions, Alternate Bootstrap Techniques, and Estimation of Adequate Number of Species. Chapter 7 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II G.W. and Traas TP (eds), pp. 119-132. Lewis, Boca Raton, FL, USA.

Nielsen U, Pedersen BM, Larsen HF, Knudsen HH (2000). Car washing facilities, status and strategies (book in Danish with English summary). Environmental Project No. 537. Danish Environmental Protection Agency. http://www.mst.dk/udgiv/publikationer/2000/87-7944-124-6/pdf/87-7944-125-4.pdf

Norberg J, Swaney D P, Dushoff J, Lin J, Casagrandi R, Levin S A (2001). Phenotypic diversity and ecosystem functioning in changing environments: A theoretical framework." PNAS 98(20): 11376-11381.

OECD (1998). Detailed Review Paper on Aquatic Testing Methods for Pesticides and Industrial Chemicals. Part 1: Report and Part 2: Annexes. Series on Testing and Assessment No. 11. OECD, Paris, France.

OECD (2003). Manual for investigations of HPV chemicals. Chapter 2: SIDS, the SIDS plan and the SIDSA dossier. OECD Existing Chemicals Programme. http://www.oecd.org

Payet J, Jolliet O (2003). Comparative assessment of the toxic impact of metals on aquatic ecosystems: The AMI method. In "Life-Cycle Assessment of Metals: Issues and research directions", Alain Dubreuil, editor. SETAC, Pensacola, FL, USA.

Payet J, Pennington D, Hauschild M, Jolliet O (2003). Comparative Assessment of toxic Impact on Aquatic Ecosystems: The AMI method (Assessment of the Mean Impact). Submitted to Environ. Toxicol. Chem.

Payet J, Larsen H F (2004). Endpoint Modelling for the Life Cycle Impact Assessment on Ecosystems. *In prep.*

Pennington D, Payet J, Hauschild M (2004). Aquatic ecotoxicological indicators in life-cycle assessment. Environ. Toxicol. Chem. 23 (7), 1796-1807.

Pratt J R, Cairns J Jr (1996). Ecotoxicology and the Redundancy Problem: Understanding Effects on Community Structure and Function. Chapter 12 in: Ecotoxicology - A Hierarchical Treatment. Newman MC, Jagoe CH (eds.), pp. 347-370. Lewis, Boca Raton, FL, USA.

RIVM (1999). Appendix A in: Environmental Risk Limits in The Netherlands. Part III Data. Könemann H. (ed.). Report No. 601640 001. RIVM, Bilthoven, The Netherlands.

Solbe J, Mark U, Buyle B, Guhl W, Hutchinson T, Kloepper-Sams P, Länge R, Munk R, Scholz N, Bontinck, Niessen H (1998). Analysis of the ECETOC Aquatic Toxicity (EAT) database. I – General introduction. Chemosphere 36(1), 99-113.

Steen B (1999). A systematic approach to environmental priority strategies in product development (EPS). Version 2000 - General system characteristics. Chalmers University of Technology, Technical Environmental Planning. Göteborg, Sweden.

Stephens M A (1986). Tests based on EDF statistics. In: Goodness-of-Fit Techniques. D'Agostino, R.B., Stephens, M.A. (eds.), pp. 97-193. Marcel Dekker, New York, USA.

Udo de Haes HA, Lindeijer E (2002). The conceptual Structure of Life-Cycle Impact Assessment. Chapter 8 in: Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds): Life-cycle Impact Assessment: Striving Towards Best Practice, pp. 209-225. SETAC-Europe, Brussels.

US EPA (1997). Notice of availability of waste minimization software and documents. EPA530-C-97-003, Federal Register, 62:33868.

US EPA (1998). Notice of availability of draft RCRA waste minimization PBT chemical list. 530-Z-98-009, Federal Register, 63:216.

US EPA (2000). Data collection and development on high production volume (HPV) chemicals. Federal Register 65 (248) 81686-81698. http://www.epa.gov/chemrtk/

Wenzel H, Hauschild M, Alting L (1997). Environmental Assessment of Products, Vol. 1. First edn. Chapman & Hall, London, Great Britain.

2 Importance of chemical-related impact categories - a case study

This Chapter is a verbatim version of the following paper submitted to Journal of Cleaner Production:

Larsen HF, Hansen MS, Hauschild M (2004). Including chemical-related impact categories in LCA on printed matter – does it matter? *Submitted to Journal of Cleaner Production.*

Including chemical-related impact categories in LCA on printed matter – does it matter?

Henrik Fred Larsen[1*], Morten Søes Hansen[2], Michael Hauschild[1]

[1]Department of Manufacturing Engineering and Management, Technical University of Denmark (DTU) Building 424, DK-2800, Lyngby, Denmark. Tel: +45 45 25 48 00. Fax: +45 45 93 55 56

[2] Sustainable Initiatives Department, Steelcase S.A., 54-56 Rue Jean Giraudoux, FR-67035 Strasbourg Cedex 2, France. Tel: +33 388 13 30 30. Fax: +33 388 13 31 43

* **Corresponding author** (hfl@ipl.dtu.dk)

Abstract

Existing product Life Cycle Assessments (LCAs) on offset printed matter all point at paper as the overall dominating cause of environmental impacts from the life-cycle of this category of products. The studies focus on energy consumption including the emissions and impact categories related to energy, and the dominating role of paper is primarily founded in the energy-related impact categories global warming, acidification and nutrient enrichment. The chemical-related impact categories ecotoxicity and human toxicity are only included to a limited degree or not at all. In this paper we include the impacts from chemicals in the life cycle by making use of some of the newest knowledge about emissions from the production at the printing industry combined with knowledge about the composition of the printing materials used during the production of offset printed matter. In cases with available data also upstream emissions from the production of printing materials are included. The results shows that inclusion of the chemical-related impact categories makes the LCA-profile of sheet fed offset products much more varied. Especially the ecotoxicity impact category indicator may contribute significantly, and paper no longer becomes the overall dominating factor.

Keywords: Chemicals; Chemical-related impact categories; Ecolabelling; LCA; Printed matter

1. Background

Studies covering the life cycle from cradle to grave of printed matter products have been carried out over the last ten years. Though the number of studies is limited [1,2,3,4,5,6], four to five of them include offset printed matter. All these life cycle assessments (LCAs) focus on energy consumption and energy-related impact categories, whereas chemical-related impact categories covering ecotoxicity and human toxicity are only included to a limited degree or not at all. Results of these existing LCAs all point to paper as the dominating contributor to the potential environmental impact from the life-cycle of offset printed matter. In only one of the existing studies is *sheet fed* offset produced printed matter included as a separate entity, and in that particular case the chemical-related impact categories are not included at all.

In this study we include the chemicals and their potential impacts to a higher degree and focus on an LCA of generic sheet fed offset printed matter produced at a model sheet fed printing company.

The LCA methodology chosen in this study is the EDIP97 method [7]. This methodology with its relatively simple key property based impact assessment part seems feasible for the LCA approach relevant for use in ecolabelling of products associated with many chemical emissions.

This paper is based on the peer reviewed report “Ecolabelling of printed matter, Part II – Life Cycle Assessment of model sheet fed offset printed matter” by Larsen et al. [8]. The report which is done in accordance with ISO 14040-series is part of the project “Ecolabelling of printed matter” financed by The Danish EPA and with the aim of creating a product life cycle basis for the development of ecolabelling criteria on printed matter. The results are used as input to the on-going revision of the existing Nordic Swan ecolabelling criteria and the development of the European Flower ecolabelling criteria for printed matter.

2. Goal and scope definition

The goal of the study is to identify the distribution of potential environmental impacts and consumption of resources over the life cycle of generic printed matter produced on a model sheet fed offset printing company in Europe. The results are to be used for developing ecolabelling criteria.

The main activities have been covered for all stages of the life cycle to the degree that readily available data has made possible. To meet the goal of the study, average or typical data have been used. In the stage of use only transport may be important. Transport is not included in the main scenarios but its importance is assessed on basis of existing studies in the sensitivity analysis. The product system is shown in Fig. 1.

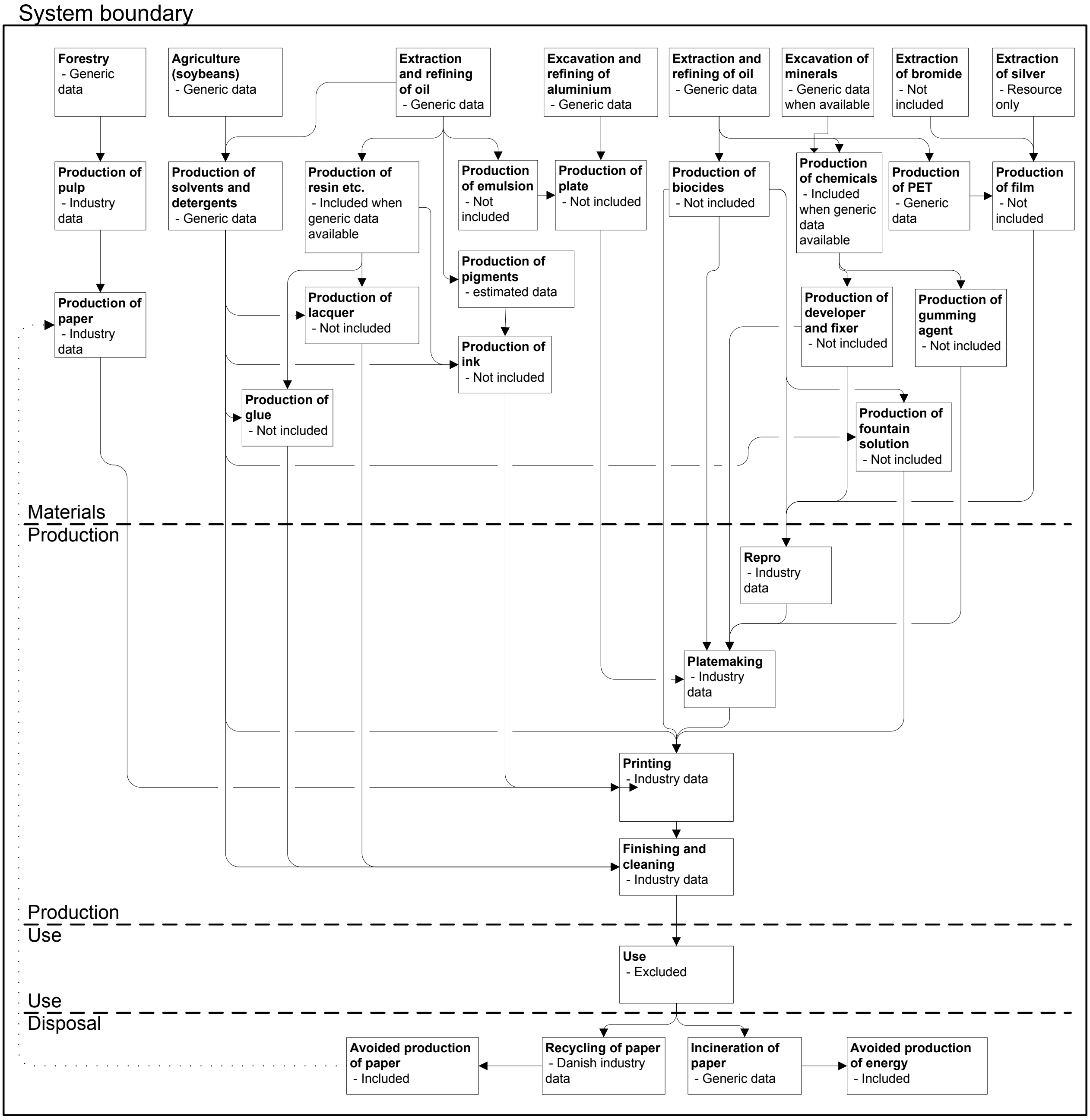

Fig. 1. Product system for generic sheet fed offset printed matter.

There is a special focus on the production stage but upstream emissions assessed to be of possible significance are included (e.g. estimated emissions from pigment production) or dealt with in the sensitivity analysis.

The functional unit is 1 ton of sheet fed offset produced printed matter, i.e. printed communication covering books, pamphlets etc.

The impact categories considered in the study include global warming, ozone depletion, acidification, nutrient enrichment, photochemical ozone formation, chronic human toxicity via water and soil, chronic ecotoxicity in water and soil, acute human toxicity via air, acute ecotoxicity in water, hazardous waste, nuclear waste, slag and ashes, and bulk waste. Resource consumption is also included.

As the time scope for the production stage 1990 – 2002 has been chosen and the technological scope is mainly modern technology (not state-of-the-art) used at least in Northern Europe.

Marginal data are used for production of electricity (natural gas) and paper production (virgin fibres) as the main approach in the reference scenario. In all other cases average data are used.

Waste water treatment is not included in the reference scenario, making this scenario also relevant for Southern and Eastern Europe. However, a special scenario with waste water treatment is included and can be considered as being relevant for Northern Europe, especially Sweden and Denmark.

The reference scenario has two sub scenarios, one where the avoided energy consumption and avoided emissions from incineration and recycling of paper are not credited to the paper production (designated paper gross) and one where they are credited to the paper production (designated paper net). For consumption of aluminium, it is assumed that recycled aluminium is used and the extra energy used to produce virgin aluminium to replace the loss during the recycling process is allocated to the functional unit. For both paper and aluminium the effect of changing the allocation used is discussed or investigated by the use of sensitivity analysis.

As this study is going to be used for ecolabelling, the main focus is on the production stage, i.e. page production (repro), plate making, printing, finishing and cleaning. The raw materials included in the production stage cover the dominant types typically used in ‘traditional’ sheet fed offset, i.e. film, film developer, fixer, biocides, plates, plate developer, gumming solution, paper, alcohol (isopropyl alcohol, IPA), printing ink, fountain solution, lacquer (varnishes), glue and cleaning agents. The composition of these raw materials is as far as possible based on known typical recipes from product data sheets and Danish, Swedish and German investigations, e.g. [11,34,35,36,37]. However, due to lack of data and relevance, some simplifications and assumptions about the components have been made.

Due to the focus on the production stage and lack of data on consumptions and emissions, the material and disposal stages are only fully taken into account as far as they are covered by the unit process data which has been used in the models. This means that emissions of specific substances are typically not included. Ink, paper and energy production are exceptions for which emissions of specific substances are included at least to some extent. Other known possible significant emissions at the material and the disposal stage are discussed by use of sensitivity analysis.

The consumption of raw materials and emissions to water and air at the model printing company are mainly based on average values for 10 – 70 Swedish and Danish offset printing companies [10,11,12].

Besides the reference scenario for which the conditions are described above, seven special scenarios have been examined. These scenarios are based on the reference scenario but vary from this in a few parameters. Scenario 1 makes use of an average scenario for electricity production, in order to be able to compare with the results of an earlier LCA study. Scenario 2 assumes a saturated paper market to see the consequences on the use of recycled paper at the model printing company. Scenarios 3 and 4 investigate the sensitivity to variations within the observed ranges in the paper and ink consumption respectively. In scenario 5 waste water treatment is included for the production stage, and in scenario 6 the effect of substitution among biocides applied in the production stage is shown. Finally scenario 7 deals with the situation where all production water is recycled and no waste water at all is emitted from the model printing company, which is actually the case at some modern printing companies. All these special scenarios are only included in this paper to the degree that they shed light on the robustness of the reference scenario. Detailed description of the special scenarios and results of applying them can be found in Larsen et al. [8].

3. Methodology

The impact assessment is performed using the EDIP97 method [7] which is a midpoint life cycle impact assessment (LCIA) method including characterisation, normalisation against the impact from an average person (the ‘person equivalent’, PE) and weighting based on distance to political reduction targets (expressing the impact scores in ‘targeted person equivalents’, PET). Resource consumption is also normalised as person equivalents and weighted using the scarcity as expressed in the supply horizon for the resources (expressing the weighted resource use in units of person-reserves, PR).

For the chemical-related impact categories (i.e. chronic human toxicity, chronic ecotoxicity, acute human toxicity, acute ecotoxicity) the chronic ones are aggregated into one category called ‘persistent toxicity’ during the normalisation step leading to only three chemical-related impact categories after normalisation. No aggregation has been done for the other impact categories during normalisation. After weighting it is possible to sum all impact scores per functional unit into one aggregated value expressed in PET. In the same way the total resource consumption can be aggregated into one value expressed in PR per functional unit.

Four separate waste impact categories (i.e. bulk waste, slag and ashes, hazardous waste, radioactive waste) are included in EDIP97 to represent the potential impacts from (solid) waste streams not modelled to for example emissions from land fillings.

Further description of the methodology used here can be found in Larsen et al. [8] and of the EDIP97 methodology in general in Wenzel et al. [7] and Hauschild & Wenzel. [9].

4. Results

4.1 Inventory

The starting point for the inventory is the production stage of generic printed matter produced at a model sheet fed offset printing company. Each raw material used in the production stage is divided into its components and the input and output of their production processes (i.e. material stage) are mapped and included whenever readily available and relevant, see Fig. 1. For many of the composite raw materials no data exists on production (i.e. typically a mixing process). However for their components generic data on input and output are available and used in many cases. In any case data on emission of specific substances at the material stage are typically not available and this kind of data are almost exclusively used in the production stage for which they have been available and focused upon in this study. Omissions that are assessed to be of possible significance are discussed in the sensitivity analysis.

An overview of the consumptions and emissions at the model sheet fed offset printing company is given in Appendix B. The range in the consumption of the most important raw materials typically lies within a factor of about 10, but with some exceptions (e.g. cleaning agents). For the non-volatile substances (e.g. biocides) appearing in rinse water and fountain solutions, emissions are assumed to be 100% emitted to water. 70 – 95% of volatile solvents are assumed to be emitted to air and in this case only 0.1% or 1% (depending on the type) is emitted to water with IPA as an exception (14% emitted to water). The rest of the used solvents are disposed of as chemical waste.

Detailed information on composition of raw materials, and a full compilation of all emissions and resource consumptions for the reference scenario can be found in Larsen et al. [8].

4.2 Impact assessment

Substances contributing to the energy-related impact categories (e.g. global warming, nutrient enrichment and acidification) are limited in number and well-defined, and characterisation factors are already available. However, for the chemical-related impact categories, the number of contributing substances is much larger and characterisation factors are available only for a fraction of them.

33% of the substances emitted to air and mapped as contributing to human toxicity are covered by characterisation factors, and for ecotoxicity the figure is 26%. Expressed in quantities (kg), 48% is covered by characterisation factors for human toxicity and 64% for ecotoxicity if the known main non-contributing emissions for ecotoxicity (such as SO_2 and calcium) are excluded. For the waterborne emissions, 25% and 37% of the substances are covered by characterisation factors for human toxicity and ecotoxicity respectively, and if expressed as quantities, the figures are 48% for human toxicity and 53% for ecotoxicity when main non-substance specific (e.g. suspended solids and COD) and most probably non-contributing emissions are excluded. However, the major part of the specific substances emitted to water for which no characterisation factors exist, comprises inorganic salts, polymers and acids/bases of the type that are generally assessed to be low in toxicity [11,13,14,15,16]. In addition, there are a few known substances belonging to groups such as siccatives and softeners, which might contribute significantly to the chemical-related impact categories, but which have not been possible to cover. New characterisation factors for ecotoxicity of 11 substances covering pigments, biocides and others have been calculated as part of this study, and are shown in Appendix C.

4.2.1 Category indicator results

The total category indicator results for one functional unit in the reference scenario are shown in Table 1. The energy-related impact categories are dominated by contributions from energy production (material stage) especially for paper production but also for the processes at the model printing company. For the chemical-related impact categories the main contributions come from emissions of solvents (e.g. hexane and tetradecane) used during cleaning and printing at the model printing company (production stage) but there are also significant contributions from emission during pigment production (e.g. dichlorobenzidine) and from emissions from energy production (e.g. metals), which both belong to the material stage. For resources the major consumptions are water (used mainly for paper production), energy carriers comprising natural gas, oil and wood, and kaolin used in the production of paper.

Table 1
Category indicator results per fu for the reference scenario

Name	Amount	Unit
Global warming	1,350,000	g CO_2-equiv.
Ozone depletion	0.0000106	g CFC11-equiv.
Acidification	4,000	g SO_2- equiv.
Photochemical ozone formation	1,560	g C_2H_4- equiv.
Nutrient enrichment	5,390	g NO_3^- - equiv.
Human TOX, water	1,540	m^3 water
Human TOX, air	38,800,000	m^3 air
Human TOX, soil	20.4	m^3 soil
EcoTOX, water, chronic	133,000	m^3 water
EcoTOX, water, acute	17,700	m^3 water
EcoTOX, soil	4,940	m^3 soil
Bulk waste	50,800	g
Hazardous waste	1,830	g
Radioactive waste	1.99	g
Slags and ashes	7,270	g
Primary energy, material	7,360	MJ
Primary energy, process	29,600	MJ
Al (aluminium)	317	g
Lignite	4,390	g
Chalk ($CaCO_3$)	64,600	g
Cr (chromium)	20.3	g
Cu (copper)	9.42	g
Fe (iron)	216	g
Ground water	1,470,000	g
Quartz	196	g
Clay	0.931	g
Mn (manganese)	3.74	g
Sodium chloride (NaCl)	15,600	g
Natural gas	30,6000	g
Ni (nickel)	8.68	g
Dammed water	14,300,000	g
Surface water	30,100	g
Crude oil	125,000	g
Anthracite	7,240	g
Wood (soft) DS	94,1000	g
Wood (hard) DS	0.183	g
U (Uranium)	1.57	g
Unspec. fuel	-1,340	MJ
Unspec. water	46,000,000	g
Zn (zinc)	0.151	g
Hydrogen	3.69	g
Unspec. biomass	425	g
Kaolin	258,000	g
Bentonite	23.4	g
Ag (silver)	56.3	g

4.2.2 Normalized category indicator results

By normalising the category indicator results a normalised LCA profile appears, see Fig. 2. The dominant impact categories are ecotoxicity (i.e. acute ecotoxicity) and global warming followed by hazardous waste and persistent toxicity. Ecotoxicity accounts for about 400 mPE (milli-person-equivalents) and the main contributing activities are printing (240 mPE) and paper production (80 mPE). For global warming the value is about 240 mPE dominated by contributions from paper production (170 mPE) and energy consumption at the model printing company (60 mPE). Hazardous waste accounts for about 160 mPE and is almost fully dominated by paper production (150 mPE). Persistent toxicity accounts for 140 mPE dominated by cleaning (66 mPE), printing (43 mPE) and paper production (24 mPE). If negative contributions from paper incineration and paper recycling (recovery) are allocated to paper in the profile (i.e. paper net is used) the contribution from paper to, for example, global warming is reduced from 71% to 43%.

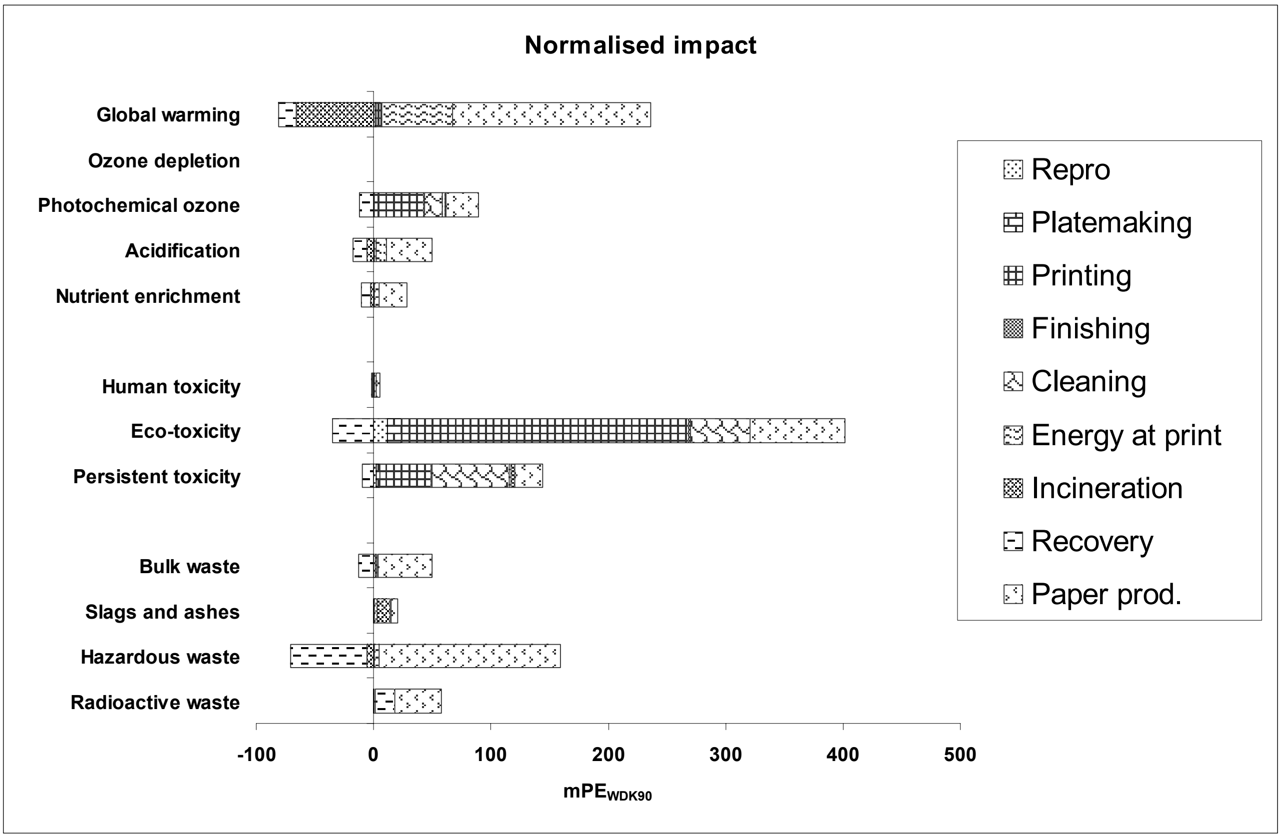

Fig. 2. Normalized LCA profile for the reference scenario.

The normalised profile for the consumption of non-renewable resources is shown in Fig. 3. This profile is heavily dominated by consumption of kaolin (110000 mPE) during paper production (used as filler). However kaolin can easily be substituted by talc and/or chalk leading to a reduction by several orders of magnitude in importance of the filler. The second highest normalised resource consumption is consumption of natural gas, accounting for 1600 mPE dominated by consumption during paper production (970 mPE) and consumption at the model printing company (450 mPE).

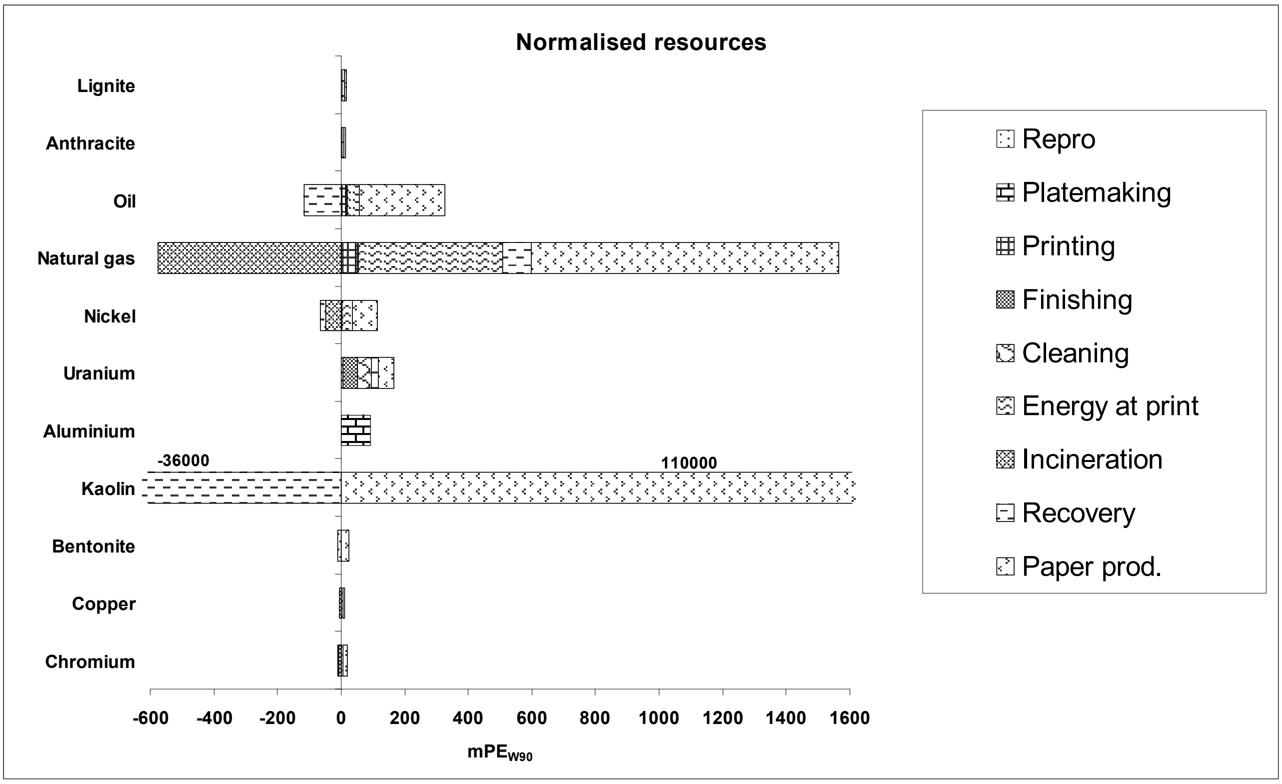

Fig. 3. Normalized profile for resource consumption (reference scenario).

4.2.3 Weighted category indicator results

The weighting factors for environmental impacts in EDIP97 vary between 1 and 3 but most of them lie between 1 and 1.5. Weighting hence only has minor effects on the normalised impact profile, the most prominent effect being that the ecotoxicity category becomes even more dominant than after normalisation and that persistent toxicity becomes the second most important and global warming only the third most important, see Fig. 4. Following weighting, all the environmental impact scores can be aggregated into one impact score, i.e. the total aggregated weighted potential impact score (hereafter called 'aggregated impact' score), which makes it easier to show and analyse the relative contribution from the different activities in the life cycle. This is illustrated in Fig. 5 (paper as gross value) and in Fig. 6 (paper as net value). The result as shown in Fig. 6 is that the highest contribution to this aggregated impact comes from printing (41%) followed by paper net (31%), cleaning (17%), energy consumption at the model printing company (6%), plate making (2%), repro (2%) and finally finishing (0.4%).

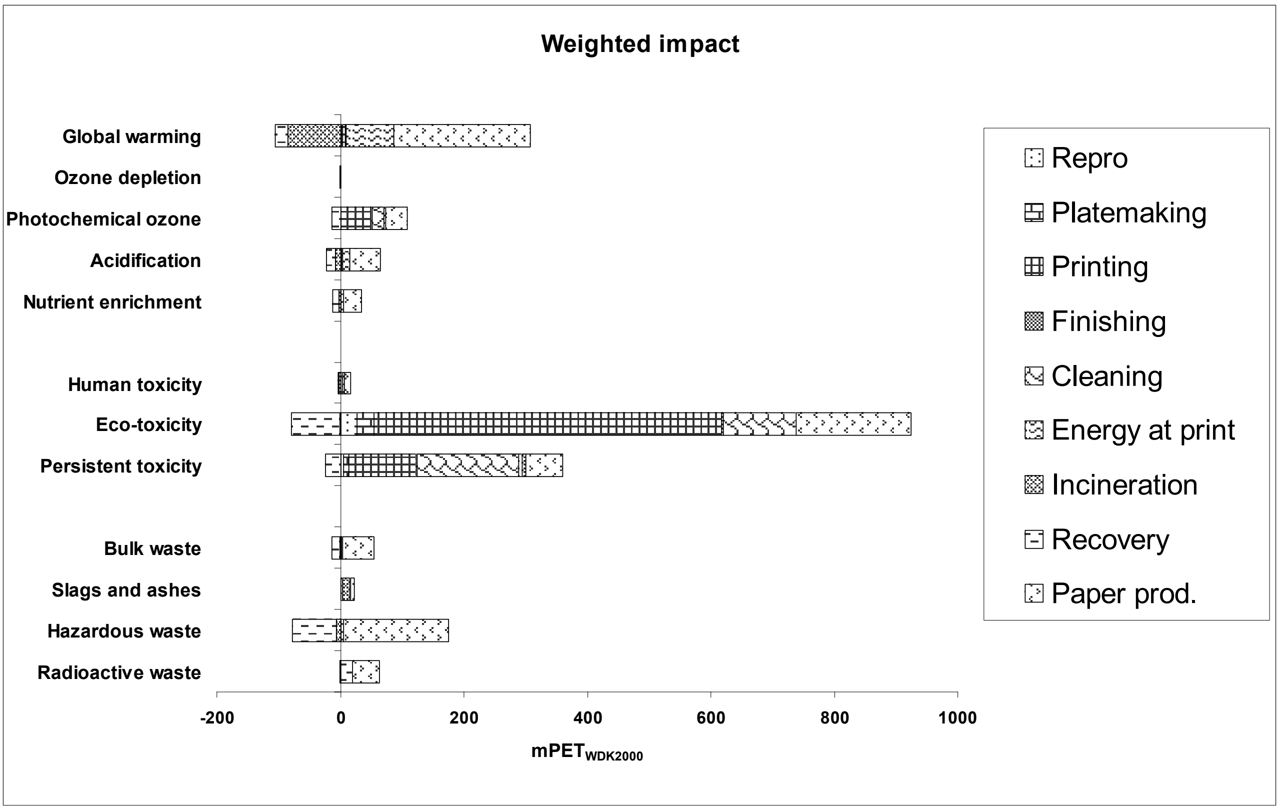

Fig. 4. Weighted profile for reference scenario.

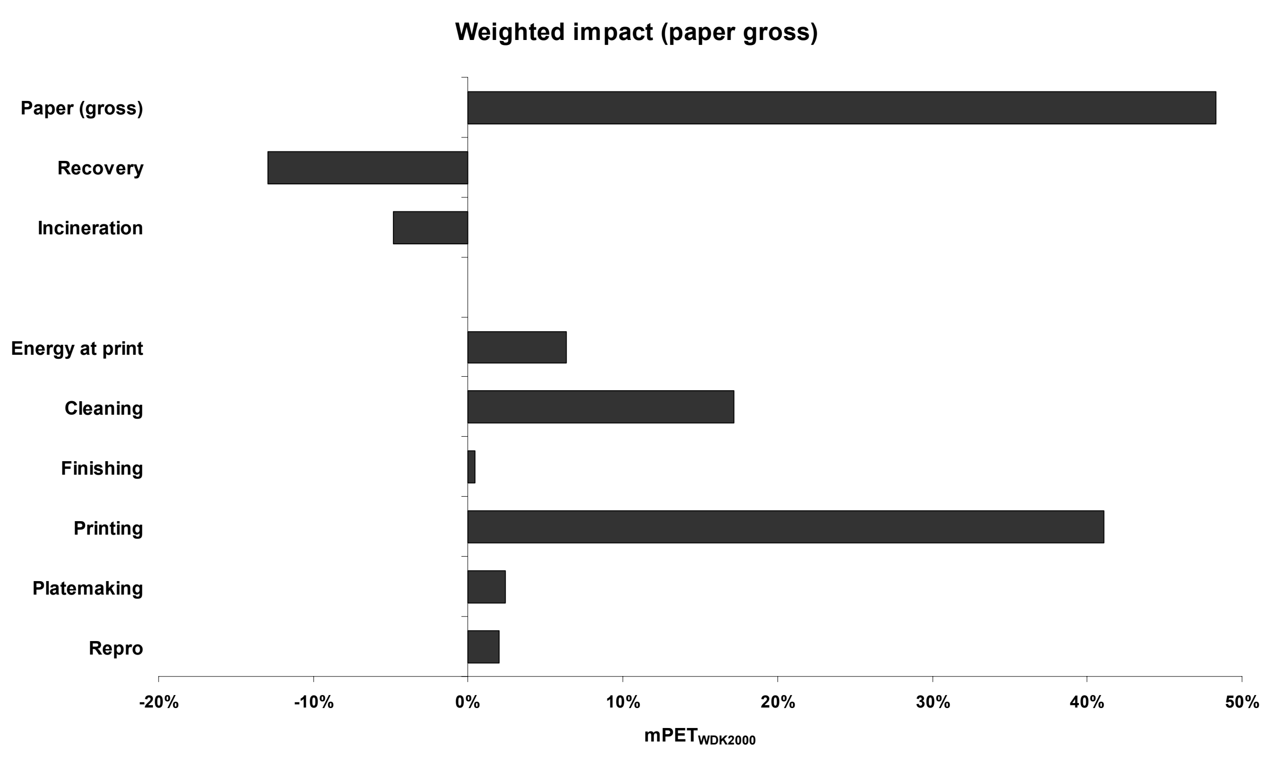

Fig. 5. Aggregated weighted LCA profile for the reference scenario in relative figures and with paper as gross value.

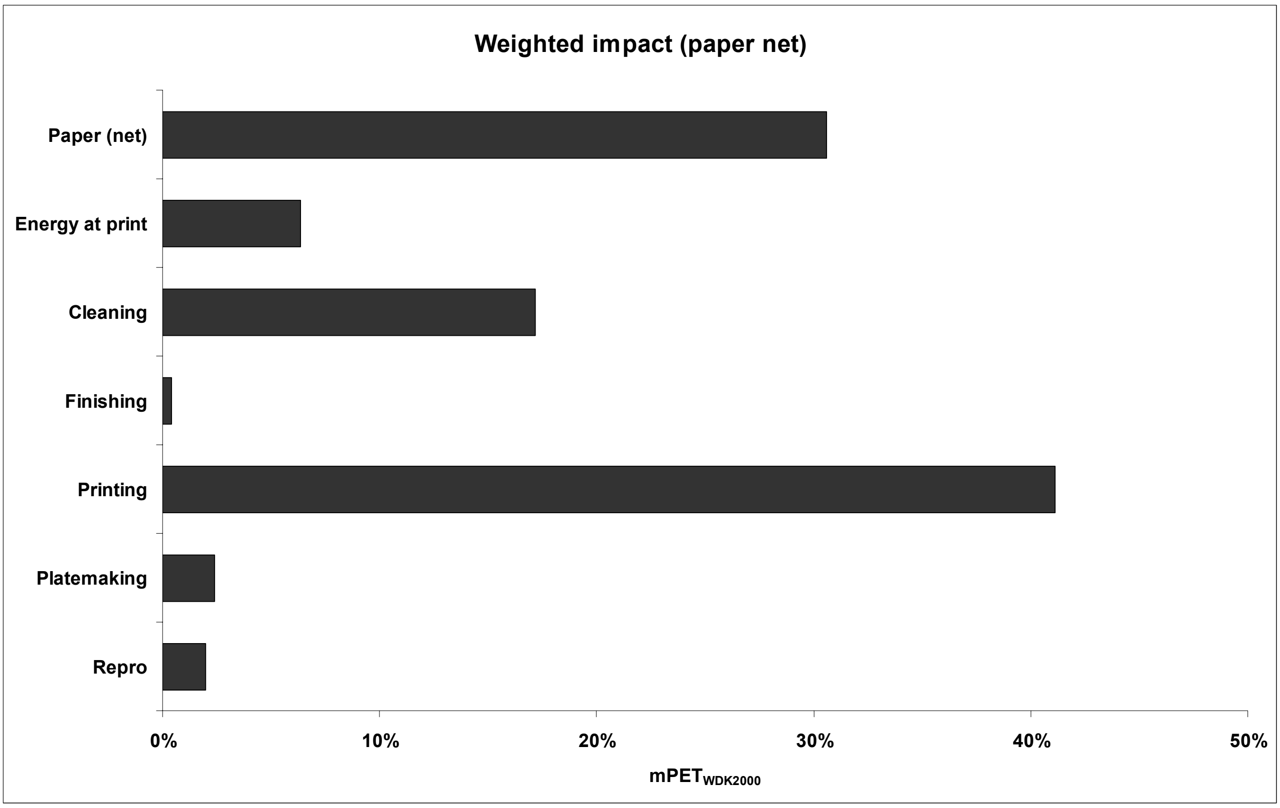

Fig. 6. Aggregated weighted LCA profile for the reference scenario in relative figures and with paper as net value.

After weighting of the resource profile kaolin is still dominant but especially natural gas, oil and uranium have increased importance due to their higher scarcity, see Fig. 7. If we exclude kaolin, following the substitution argument given in Section 4.2.2, and use the net value for paper, and further aggregate all weighted resource consumptions and express the result in percentage of the total, we arrive at the profile shown in Fig. 8. In this case the highest share of resource consumption comes from paper net (48%) followed by energy consumption at the model printing company (33%), repro (6%), finishing (4%), printing (4%), cleaning (3%) and plate making (2%).

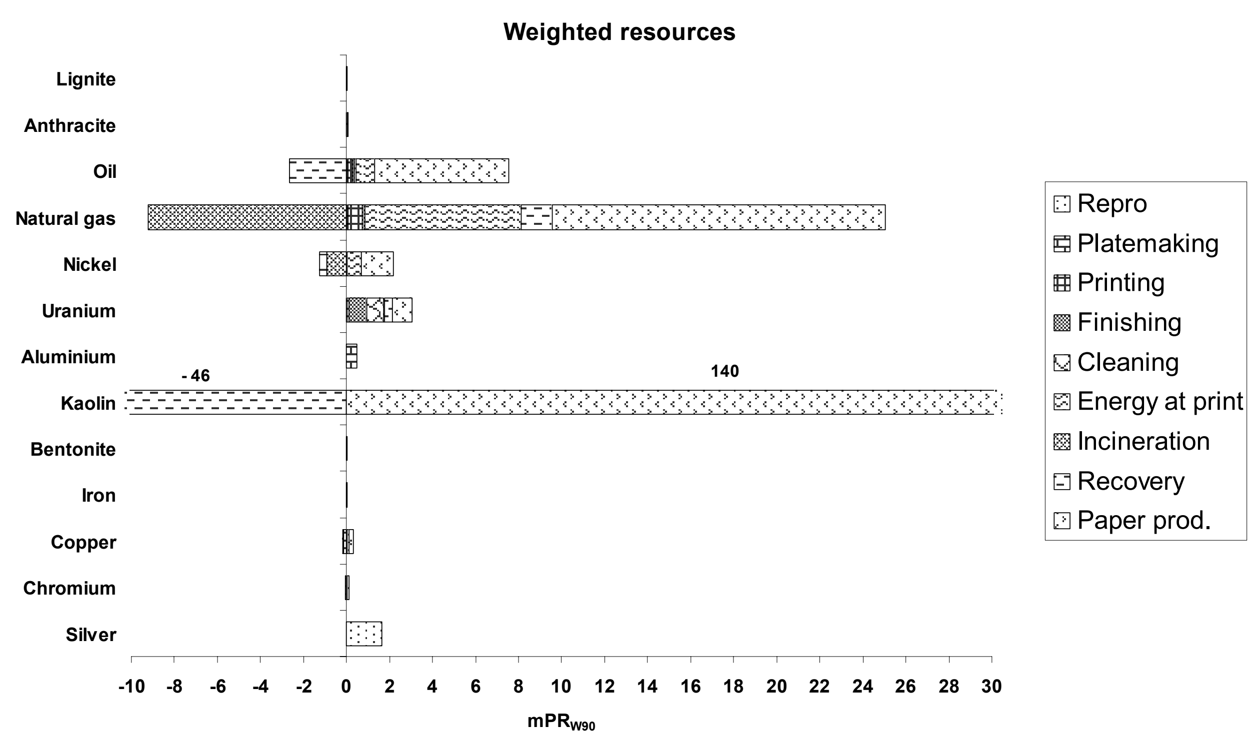

Fig. 7. Weighted profile for resource consumption (reference scenario).

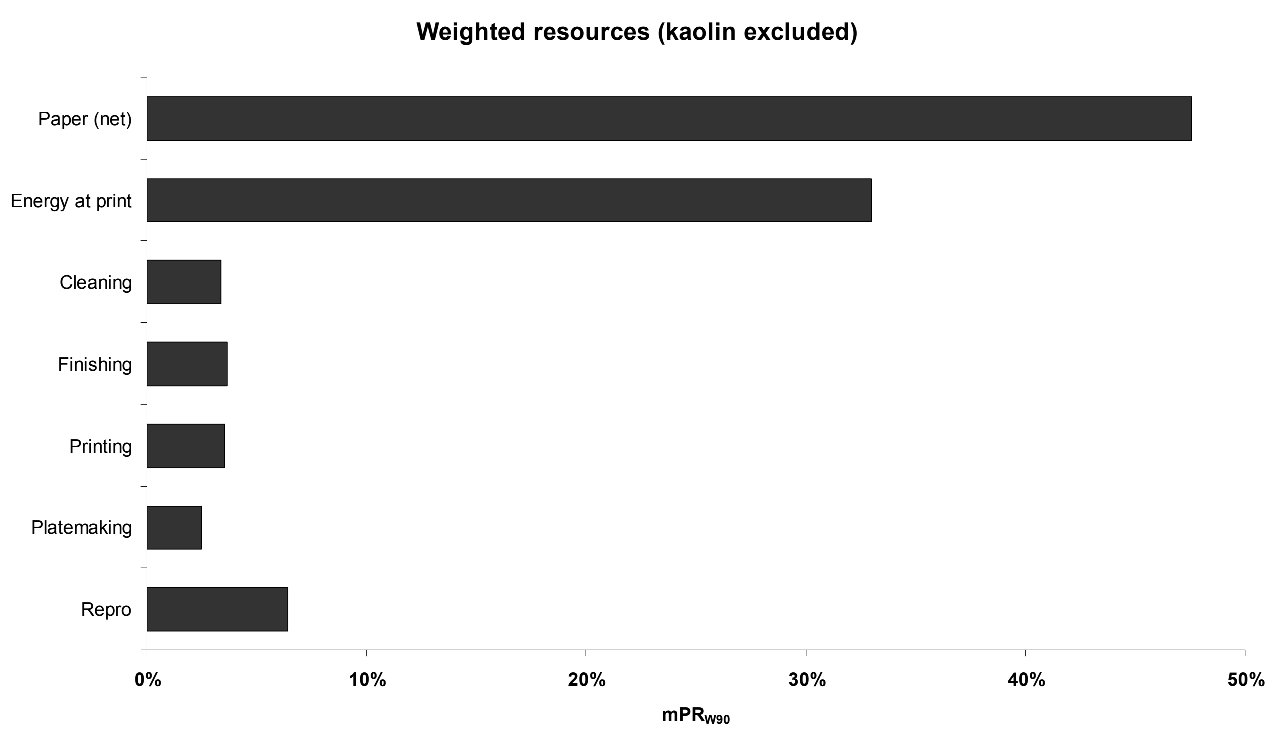

Fig. 8. Aggregated weighted resource profile for the reference scenario in relative figures and with total paper as net value and kaolin excluded.

4.3. Interpretation

In order to investigate the robustness of the reference scenario and examine the effect on the impact and resource profiles of varying the consumption and emissions at the model printing company within observed ranges (relevant for ecolabelling), several sensitivity analyses have been carried out.

4.3.1. European normalisation references and weighting factors

The effect is investigated of using drafted new updated normalisation references and weighting factors covering the 15 current EU member states [17] instead of the Danish ones [7] as used in the reference scenario. The results shows, that there is no significant change to the overall LCA-profiles for the reference scenario. In this regard the weighted reference scenario used in this study is thus considered robust and valid on a European scale. The effect on the balance between the energy-related and the chemical-related impact categories is shown in Table 2, see Larsen et al. [8] for further details.

Table 2
Comparison of the result of using different normalisation references and weighting factors for calculating the total potential impact within energy-related and chemical-related impact categories. Percent change as compared to NR-1990 and to WF-1990 [7] shown in brackets

Normalisation references used	**Total potential impact**	
	Energy-related impact categories [a]	**Chemical-related impact categories** [b]
NR-1990 [7]	284 mPE	508 mPE
NR-1994EU-15 [17]	317 mPE (+12%)	764 mPE (+50%)
Weighting factor used		
WF-1990 [7]	359 mPET	1200 mPET
WF-1994EU-15 [17]	330 mPET(-8%)	576 mPET (-52%)

[a] Global warming, photochemical ozone formation, acidification and nutrient enrichment
[b] Acute human toxicity, acute ecotoxicity and persistent toxicity

Even though the weighted potential impact from the chemical-related impact categories is reduced to about one half (see Table 2) if the updated weighting factors are used (i.e. WF-1994EU-15 [17]) it is still about twice as big as the one for the energy-related impact categories. Furthermore, as stated by Busch [32] the updated weighting factors for the chemical-related impact categories are most probably underestimated. If photochemical ozone formation is excluded from the energy-related impact categories in Table 2 (in our case the main contribution is emission of process solvents from printing and cleaning), the dominating role of the chemical-related impact categories becomes even more pronounced.

4.3.2. Alternative allocation principles for paper

For paper the use of other allocation principles, than the paper gross and paper net used in this study, i.e. ‘cut-off’ and quasi-co-product as described in the INFRAS study [6], is discussed. The ‘cut off’ allocation principle means that all potential environmental impacts are allocated to the virgin paper production (primary production) and the ‘waste’ paper (including the printed matter) for recycling is considered as raw material for a new production process not carrying any burdens from the primary process. Using this principles in our case will imply that only the negative contribution from incineration (and not recycling, i.e. recovery) is allocated to the paper used in our functional unit. This would result in a contribution of 43% (48% - 5%) from paper to the aggregated impact, see Fig. 5. On the other hand, according to the quasi-co-product allocation principle the total burden and benefits, including all paper cycles, are allocated evenly to each cycle (one cycle equals one quasi-co-product) the paper (i.e. fibre) goes through. The result of using this principle in our case would be a significant reduction in the contribution from paper per functional unit. This is because we would assume 2-3 cycles for the paper (i.e. chemical pulp reused once or twice) leading to a production of 2-3 co-products equally sharing the extra potential environmental impact from production of the primary product (based on virgin fibres). However, this allocation principle demands that the same functional unit can be used for all co-products and this is not true in our case because sheet fed offset to a very high degree uses virgin paper, which is reflected in an utilisation rate (share of recycled paper in total production) of only 8.6% for production of printing and writing paper, CEPI [33]. The recycled high grade paper from sheet fed offset is therefore used after repulping for other product types such as packaging to a high degree. It is concluded that due to the dominant use of virgin paper within sheet fed offset the choice of paper net, meaning that avoided energy consumption and avoided emissions from incineration and recycling of paper is allocated to paper, is most relevant for the reference scenario in our case.

4.3.3. AOX emission from paper production

One of the known emissions of toxic substances from paper production that it has not been possible to include in this study is AOX (halogenated organic substances emitted to water). The AOX emission mapped in the inventory (107 g Cl/fu) correspond to an average toxicity substitute of 222 g dichlorobenzene per fu if estimated in accordance with the principles in the INFRAS study [6]. This very rough estimate indicates that this emission accounts for about 3% of the aggregated impact and therefore might be important in the life cycle of sheet fed offset printed matter. However, it is assessed that taking other emissions from other activities into account that have also not been possible to include (e.g. emission of siccatives at the printing process) the AOX emission will probably not change the overall LCA profile decisively. But, this assessment is of course based on existing available knowledge within the scope of this study.

4.3.4. European paper disposal scenario

The inclusion of a European paper disposal scenario is investigated. In the reference scenario 53% of the paper is recycled (actually recovered) and the rest is incinerated with energy utilisation. This scenario covers paper in general and is valid for Denmark [38], but in other European countries it may be different. According to the newest recycling statistics from the Confederation of European Paper Industries (CEPI) [33] covering 2002 the average recycling rate in the EU countries is about 53% which is identical to the rate used in the reference scenario. However differences exist between the different EU member countries which are reflected in the paper collection rate (average 56%) with a range of about 45% (e.g. Portugal and Italy) to about 70% (e.g. Finland and Germany) according to CEPI [33].

On a European scale, paper not recovered is mainly disposed of as waste for either land filling or incineration. If we assume that at least the main part of this paper is disposed of as municipal waste and use the data from EUROSTAT [39] on disposal of municipal waste to estimate the average European partition between incineration and land filling for the paper waste the result is about 70% paper waste land filled and about 30% paper waste incinerated in EU. By using these figures we end up with 53% paper for recycling, 33% for land filling and 14% for incineration. In the INFRAS study [6] based on a disposal scenario for Germany a split of 60% for recycling, 26% for land filling and 14% for incineration is used. Due to anaerobic conditions in the land fillings the paper deposited will during decomposition emit methane to air. Methane emissions contribute to global warning and if we assume that the methane generation accounts for 0.3 kg methane/kg paper [1] which is a theoretical maximum, we end up with a significant extra contribution to global warming of 2960 kg CO_2-equiv./fu in this alternative scenario. The LCA profile based on aggregated impacts for this alternative scenario (i.e. 33% paper for land filling) as compared to the reference scenario is shown in Fig. 9.

As shown in Fig. 9, the effect of including land filling is an increase in the relative importance of paper from 31% to 46% and a reduction in the importance of printing from 41% to 32%. Also the importance of the other activities is reduced, e.g. cleaning is reduced from 17% to 13% and energy at print (consumption at the printing company) is reduced from 6% to 5%.

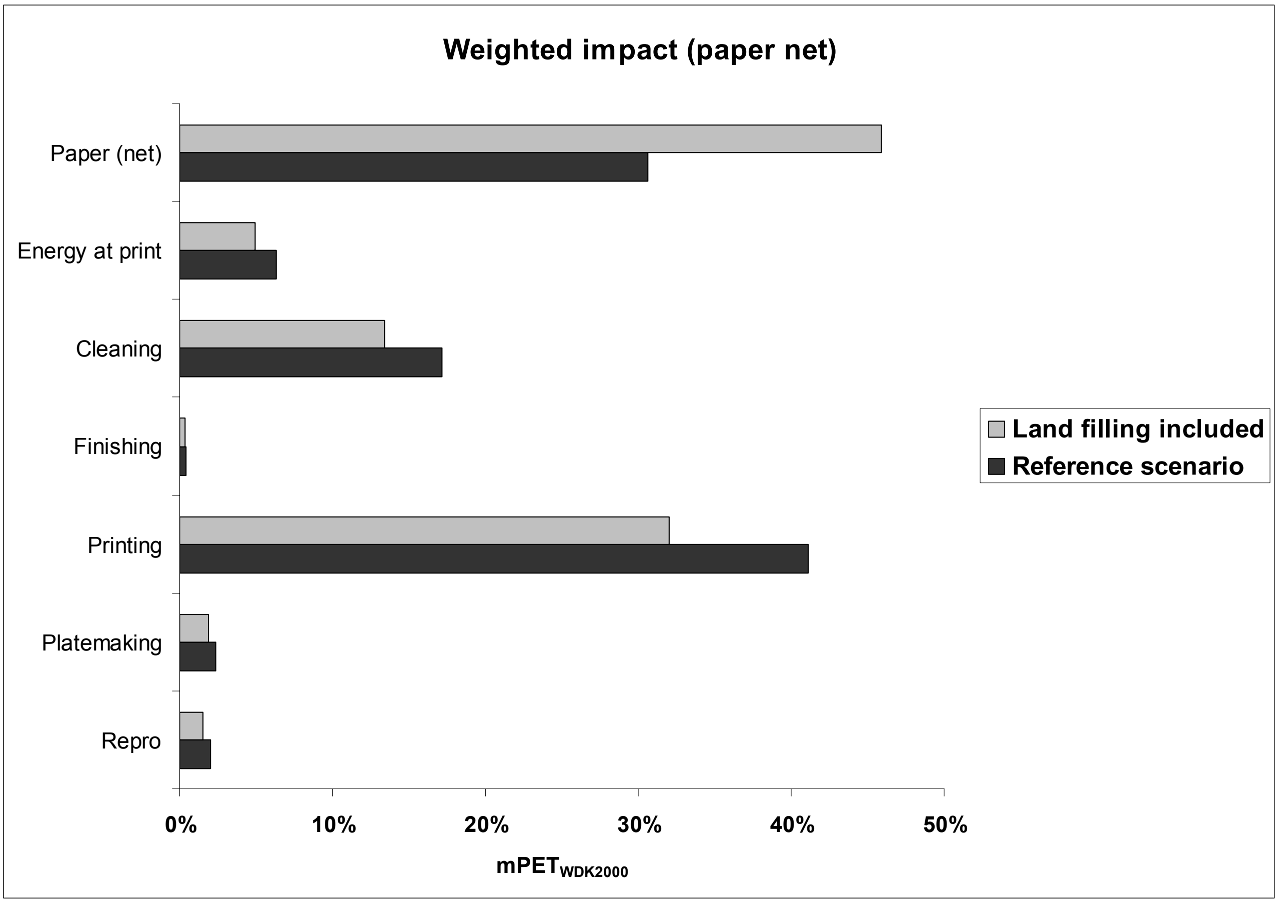

Fig. 9. Comparison between the weighted LCA profile for the alternative scenario including land filling of paper waste (based on conservative assumptions) and the reference scenario. Contributions from recycling, incineration and land filling are allocated to paper, i.e. paper shown as paper net.

The recycling rates used here are based on a European average for paper in general. However, about 19% of the paper on the market is not recyclable, comprising hygiene paper, cigarette paper, papers used for construction materials a.m. [33] leading to a recycling rate for recyclable paper (such as sheet fed offset printed matter) of 65%. If we use this rate we end up with 65% paper for recycling, 25% for land filling and 10% for incineration, and the resulting importance of paper net becomes 42% and that of printing 34%.

These two scenarios including land filling of paper are both based on the assumption that methane emission from land filling can be included as a worst case. However, the following points all point in the direction of a reduced importance of methane emissions:

- The recycling rate for sheet fed offset printed matter (including paper waste from the printing company, average 16% of consumption) is probably substantially higher than 65% due to the fact that high grade paper quality is used.
- The methane generation rate of 0.3 kg methane/kg paper is worst case assuming that all carbon (part of cellulose) in the paper is converted to methane and nothing to CO_2 (e.g. due to oxidation in the upper layer of the land fill)

- Collection and utilisation of methane from land fills for energy production actually occur in Europe but the extent is unknown.

Unfortunately only a few quantitative data has been readily available and only for the two last mentioned points. In a comprehensive study to the European Commission on "Waste Management Options and Climate Change" by Smith et al. [18], it is assumed that only 50% of the carbon content in paper is degraded to methane (the rest is emitted as CO_2) and only 35% of this amount is actually released as methane during the first 100 years in a land fill. Furthermore, on the basis of data for Austria, Spain and the United Kingdom for the year 2000, Smith et al. [41] estimates an EU average of 37% methane collected of the total amount released, and this fraction has most probably increased due to EU legislation on the issue. If we in our case assume that only 65% of the paper used for sheet fed offset is recycled and 50% of the generated methane (based on the conservative value, i.e. 0.3 kg methane/kg paper) is utilised for energy production (avoided burning of fossil fuel not allocated to the functional unit) or otherwise oxidised to CO_2, the impact profile for this alternative reference scenario will be identical to that of the reference scenario, i.e. importance of printing 41%, importance of paper 31% etc.

These estimations are based on few data and assumptions but are most probably closer to the truth than the rather conservative estimation shown in Fig. 9. It is therefore assessed that the inclusion of land filling of paper waste probably will not change the LCA profile for sheet fed offset printed matter substantially, and the reference scenario is therefore assessed to be sufficiently robust to represent the average European situation for paper disposal.

4.3.5. Comparison with previous studies

In the previous LCA studies of offset printed matter [1,2,3,4,5,6] which exclude the chemical-related impact categories or include them to a very limited degree, the importance of paper in the LCA profiles is at the level of 70 – 80%. In this study paper net accounts for only 31% but if the chemical-related impact categories are excluded this figure is raised to 67% which is at the same level as in the previous studies.

The printing process accounts for 41% (production of printing ink included) of the aggregated impact in the reference scenario, see Fig. 6. Such a high importance is not shown at all in previous LCA studies of offset printed matter which is most likely due to the very limited inclusion of the chemical-related impact categories.

4.3.6. Production and emission of printing ink

The production of printing ink (part of 'Printing' in Fig. 6) accounts for 17% of the aggregated impact in the reference scenario, mainly due to estimated emissions during pigment production (data not shown). Even though these estimations done by Andersen & Nikolajsen [22] are based on risk assessment tools they are assessed to be non-conservative, see Appendix C. A short critical review of the estimations has revealed errors that after corrections lead to an increase in the importance of production of printing ink from 17% to 20%. This may point to a higher importance of pigment production.

On basis of the observed range of printing ink consumption at printing companies (1.8 kg/fu – 26.5 kg/fu), it is found that this one parameter counts for 23% of the aggregated impact at the lower range value up to 74% for the upper range value. If it is assumed that emissions of printing ink residues at the model printing company are not proportional to the consumption but constant (probably most realistic) the corresponding importance becomes 34% and 63% respectively.

Looking at the potential impact from the emissions of printing ink (part of 'Printing' in Fig. 6) at the model printing company separately (excluding the printing ink production) it accounts for 18%

of the aggregated impact in the reference scenario. If we assume a variation of a factor 10 (0.3% - 3%) for the 1% ink emission used in the reference scenario it leads to a variation in the importance of the ink emission of 6% to 39% of the aggregated impact. Again this shows the high importance of printing ink and high sensitivity in the reference scenario to variation in this parameter. Anyway, it is assessed that an emission of 1% of the consumption represents emission of ink residues for a generic sheet fed offset LCA fairly accurately.

4.3.7. Emission of IPA at the printing process

The contribution from emission of IPA (part of 'Printing' in Fig. 6) to the aggregated impact in the reference scenario is 6%. Variation in the emitted amount according to the observed range of consumption at the printing companies (0.0785 kg/fu – 10.4 kg/fu) leads to 0.1% contribution for the lower range value and 7% for the upper range value.

4.3.8. Emissions at the cleaning process

In the reference scenario, cleaning is the third most important activity, accounting for 17% of the aggregated impact, see Fig. 6. Full substitution of aliphatic based cleaning agents with vegetable oil based ones may reduce the contribution to about 0.8% whereas full substitution of cleaning agents (except surfactants) with light aliphatic types may increase the contribution to 27%.

4.3.9. Emissions at the repro process

The 2% contribution in Fig. 6 to the aggregated impact from the repro process at the model printing company is mainly due to emission of hydroquinone (1.4%) and to lesser degree biocides (0.25%). Emissions not covered are assessed as being insignificant.

4.3.10. Emissions at plate making

For plate making the 2.4% contribution to the aggregated impact in Fig. 6 is especially due to biocide emissions (1.7%) whereas the use of aluminium plates only contributes 0.24%. If it assumed that the model printing company uses aluminium plates based on virgin aluminium exclusively, the importance of plate making increases to 3.7% and that of aluminium to 1.5% (full allocation of the potential impact to the functional unit).

4.3.11. Emissions at finishing

The finishing activity at the model printing company only contributes 0.43% to the aggregated impact, see Fig. 6. Processes like laminating which are included in the existing Swan ecolabelling criteria are excluded here because they normally do not take place at the printing company but at special companies (e.g. book binders). Even though inclusion of these processes might increase the importance of finishing it is assessed that the overall LCA profile for sheet fed offset printed matter will not change substantially.

4.3.12. Transport

As described earlier, transport has not been included as a separate activity in this generic LCA study. However, based on relevant existing studies [1,2,6,19,20] it is assessed that transport accounts for around 5% of the aggregated impact covering the whole life cycle of the generic sheet fed offset printed matter.

4.3.12. Waste

Especially due to lack of data, waste, i.e. nuclear waste, chemical waste, bulk waste, and slag and ashes are only treated as total amounts (kg, not differentiated by characterisation factors) in this study. However, for example chemical waste from the printing company and de-inking sludge from recycling of paper might contribute significantly to the aggregated impact of the functional unit. Furthermore, the waste treatment processes should be included in an LCA study.

5. Conclusion

The goal of this study is to identify the distribution of potential environmental impacts and consumption of resources during the life cycle of generic printed matter produced on a model sheet fed offset printing company. This distribution is represented by LCA-profiles on overall results in Fig. 8 and in Fig. 10 below. These results are based on average consumptions and emissions from primarily Scandinavian sheet fed offset printing companies but are assessed as being fairly representative for average modern technology in Europe. The functional unit is one ton of printed matter.

The contributions in Fig. 8 and Fig. 10 are divided into the activities at the model printing company. However paper is isolated because all previous studies focusing on energy-related impact categories point to paper as the overall dominating factor.

For the potential environmental impacts printing is dominant with a contribution of 41% to the aggregated impact, thereof 18% from ink emission at the model printing company, and 17% from emissions of synthesis chemicals at upstream pigment production. Paper contributes 31% mainly due to emissions related to energy consumption, see Fig. 10 (grey bars). If the chemical-related impact categories are excluded the picture is turned upside down, i.e. now paper becomes dominating, see Fig. 10 (black bars). In other words, the effect of including the chemical-related impact categories in the LCA profile on sheet fed offset printed matter is substantial. In our case the importance of paper is reduced from 67% to 31% and the importance of printing increased from 10% to 41%.

Based on experience from this study it therefore seems likely that including the chemical-related impact categories to a higher degree in LCA studies on other product groups, and at least those involving a lot of chemical emission (e.g. other types of printed matter and textiles), may change an otherwise energy-related impact profile significantly.

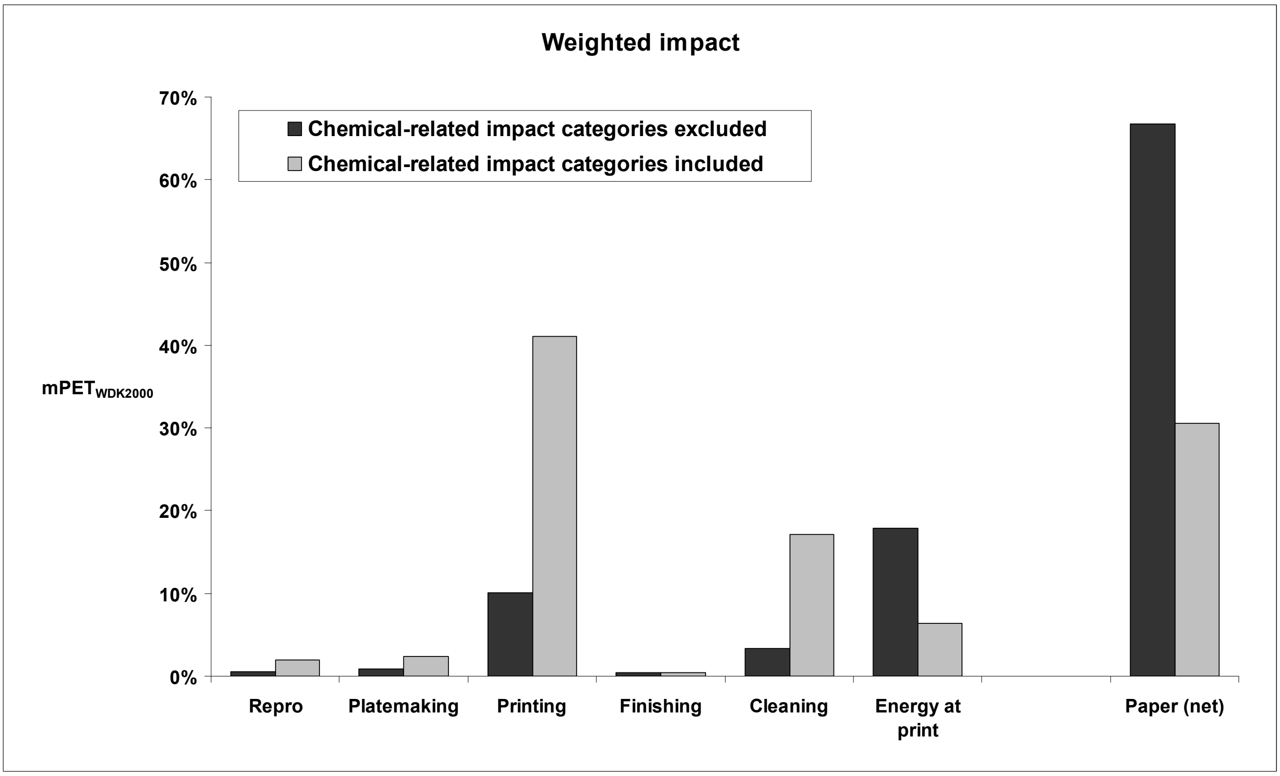

Fig. 10. Comparison of weighted profiles with or without chemical-related impact categories included.

For the aggregated weighted resource profile paper (48%) and energy consumption at the model printing company (33%) are dominant mainly due to consumption of energy carriers (natural gas and oil), see Fig. 8.

On the basis of a sensitivity analysis including European normalisation references, weighting factors and disposal scenarios, it is concluded that the results of this LCA study are valuable for both ecolabelling of offset printed matter (especially sheet fed) on a Nordic scale (Swan labelling) and a European scale (Flower labelling).

The strength of this LCA approach for use in ecolabelling of printed matter is not only the exact LCA profile of the reference scenario based upon average values but also the possibilities to use sensitivity analysis based upon known or theoretical ranges within values on consumption, emissions or other parameters. The sensitivity analysis provides guidance on how much weight to put on the individual parameters in the development of ecolabelling criteria based on a life cycle approach. The LCA approach is also valuable when dealing with substitution, i.e. substituting one chemical with another technically suitable type and observing the change in the distribution of the potential impacts within the life cycle.

Further research

The main issues that it has not been possible to include fully in this study and that might change the outcome include upstream emissions (e.g. production of ink components), methane emission from land filling of paper, and fate of chemical waste (e.g. from the printing industry). Research in these areas is needed if the liability of the LCA on printed matter is to be further strengthened and thereby improving the foundation for life cycle based ecolabelling criteria on printed matter.

Acknowledgement

The work is a joint activity between the project “Ecolabelling of printed matter” and KEMI (Centre for chemicals in industrial production) sponsored by the Danish EPA and the Danish Ministry of Science Technology and Innovation respectively.

Appendix A: Glossary

Abbreviations:

Danish EPA	The Danish Environmental Protection Agency
EDIP	Environmental Design of Industrial Products
EPA	(US.) Environmental Protection Agency
fu	functional unit
IPA	Isopropyl alcohol
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
mPE	milli-person-equivalents
$\text{mPE}_{\text{WDK90}}$	mPE based on World and Danish NRs for the year 1990
mPET	milli-person-equivalents-targeted
$\text{mPET}_{\text{WDK2000}}$	mPET based on World and Danish WFs with target year 2000
NR	Normalisation Reference

PE	Person Equivalents
PET	Person Equivalents Targeted
PR	Person-Reserves
WF	Weighting Factor
WWTP	Waste Water Treatment Plant

Definitions

Chemical-related impact categories	Impact categories on ecotoxicity and human toxicity
Energy-related impact categories	Global warming, acidification and nutrient enrichment, and in many cases photochemical ozone formation
Paper gross	Avoided energy consumption and avoided emissions from incineration and recycling of paper are not allocated to the paper production but shown as separate processes
Paper net	Avoided energy consumption and avoided emissions from incineration and recycling of paper are allocated to the paper production

Appendix B: Consumptions and emissions at the model sheet fed offset printing company

Table B1
Consumption at the model sheet fed offset printing company; kg or m^2 per functional unit (fu). Values used in reference scenario in bold

Material/chemical	**Phase**	**Amount per fu** (range in brackets) [10]	**Amount per fu** (range in brackets) [a]
Film (m^2/fu)	Repro	-	**5.63** (1.9 – 9.76)
Film developer (kg/fu)	Repro	**2.85** (1.19 – 6.00)	1.77 (0.1 – 3.63)
Fixer (kg/fu)	Repro	**3.17** (1.25 – 9.66)	3.58 (0.66 – 9.4)
Biocide agent (kg/fu)	Repro	-	**0.00019** (0.000008 – 0.00039) [b]
Water for rinsing (kg/fu)	Repro	-	**5.77** (0.24 – 11.6)
Plate (Al) (m^2/fu)	Plate making	-	**4.16** (1.0 – 8.45)
Plate emulsion (kg/fu)	Plate making	-	**0.015** (0.0037 – 0.031)
Plate developer (kg/fu)	Plate making	**0.90** (0.50 – 1.4)	1.22 (0.094 – 3.5)
Gumming agent (kg/fu)	Plate making	-	**0.030** (0.0052 – 0.055)
Biocide agent (kg/fu)	Plate making	-	**0.0012** (0.00056 – 0.0018) [b]
Water for rinsing (kg/fu)	Plate making	-	**37.4** (16.7 – 54.0)
Paper (kg/fu)	Printing	1100 [e] (1030 – 1190)	**1200** [c] (1030 – 1470)
Printing ink (kg/fu)	Printing	**5.8** (1.8 – 14)	12.1 (4.5 – 26.5)
IPA (kg/fu)	Printing	**3.93** (0.0785 – 5.18)	4.85 (2.84 – 10.4)
Fountain solution (kg/fu)	Printing	-	**1.00** (0.474 – 1.90)
Water for dilution (kg/fu)	Printing	-	**29** (11 – 46)
Cleaning agents total (kg/fu)	Cleaning	-	**2.50** (0.30 – 10.6)
- veg. oil based (kg/fu)	Cleaning	-	**0.61** (0.05 – 2.56)
- organic solv. based (kg/fu)	Cleaning	-	1.10 (0.56 – 2.33)
- aliphatic based (kg/fu)	Cleaning	-	**0.61**
- 'ekstraktionsbenzin' (kg/fu)	Cleaning	-	**0.61**
- alcohol based (kg/fu)	Cleaning	-	**0.61**
- detergent based (kg/fu)	Cleaning	-	**0.05**
Water for rinsing (kg/fu)	Cleaning	-	**22** (0.26 – 65)
Water based lacquer (kg/fu)	Finishing	[d]	**4.98** (0.51 – 6.97)
Offset lacquer (oil based) (kg/fu)	Finishing	[d]	**0.22** (0.006 – 0.38)
Hotmelt glue (kg/fu)	Finishing	-	**0.75** (0.067 – 1.44)
Energy consumption (kWh/fu)	Total general	-	1210 (768 – 1620)
- electricity (kWh/fu)	General	-	**705** (629 – 858)
- district heating (kWh/fu)	General	-	**176** (0 – 765)
- fuel oil (kWh/fu)	General	-	**243** (0 – 486)
- natural gas (kWh/fu)	General	-	**83.9** (0 – 304)
Water (kg/fu)	Total general	-	**1160** (385 – 2690)

[a] Based on inventory data from eleven offset printing companies: One sheet fed, one heatset and one cold-set-newspaper [11], six sheet fed [12] and two cold-set-newspaper [2].
[b] Kathon (active ingredient). Estimated on basis of content in rinsing water and rinsing water consumption.
[c] Spillage of paper for recycling 16% (4.5% - 32%).
[d] Total lacquer consumption 5.6 (3.2 – 8).
[e] Spillage of paper for recycling 9.6% (3.3% - 19%).

Table B2
Emitted fractions of different materials and substances for the model sheet fed offset printing company (percentage of consumption). Values used in reference scenario in bold

Material/chemical	% to air	% to waste water	% to chemical waste	% waste for incineration	% to recycling	% with product
Film [10]						
PET (89% w/w)	0	0	0	100	0	0
Ag (6% w/w)	0	**0.43** (0.020 -0.72)	0	0	**99.6**	0
Br (5% w/w) [a]	-	-	-	-	-	-
Film developer [10]	0	**4.2**	0	0	95.8	0
Fixer [10]	0	**19**	0	0	81	0
Biocide agent (repro)	0	**100**	0	0	0	0
Plate (Al)	0	0	0	0	**100**	0
Plate emulsion [11]	0	**24**	**36**		(40) [b]	0
Plate developer [11]	0	**40**	**60**	0	0	0
Gumming agent [11]	0	**100**	0	0	0	0
Biocide agent (plate making)	0	**100**	0	0	0	0
Paper [11,12,2]	0	0	0	0	**16** [c]	**84**
Printing ink [11,12]	0	**1**	**20**	0	0	80
IPA [11]	**86**	**14**	0	0	0	0
Fountain solution agent [11]						
IPA	**86**	**14**	0	0	0	0
Glycol + biocides	0	**100**	0	0	0	0
Cleaning agents [11]						
- veg. oil based	0	**1**	**99**	0	0	0
- organic solv. based						
- aliphatic based	**70**	**1**	**29**	0	0	0
- extractionsbenzine	**95**	**0.1**	**4.9**	0	0	0
- alcohol based	**95**	**1**	**4**	0	0	0
- detergent based	0	**50**	**50**	0	0	0
Water based lacquer [12]	0	**5**	0	0	0	95
Offset lacquer (oil based) [11]	0	**0.1**	**20**	0	0	79.9
Hotmelt glue [d]	-	-	-	-	-	-

[a] Excluded due to lack of data.

[b] Assumed to be incinerated during recycling process of aluminium.

[c] Actually this is the paper spillage/waste at the printing company gathered with the purpose of recycling. However as for the paper that is part of the product it is assumed that 53% is recycled and 47% is incinerated according to the Danish situation in 2000 on general recycling of paper [38].

[d] Quantitative useful data on emission of Hotmelt during use is not readily available. But based on the qualitative description in MiljøNet [40] Hotmelt probably primarily contributes to potential occupational health and safety problems in the workers' environment which is not included in this LCA. However, air emission of organic solvent components and other organic substances created during the heating process may contribute to LCA impact categories like photochemical ozone formation and human toxicity via air.

Appendix C: New EDIP97 characterisation factors

Table C1
Characterisation factors estimated in this study and accumulated characterisation factors for pigments upstream

CAS No.	Substance name	Characterisation factors (equivalency factors) (m^3/g)						
		Emissions to water			Emissions to soil		Emissions to air	
		$EF_{(etwa)w}$	$EF_{(etwc)w}$	$EF_{(etsc)w}$	$EF_{(etwc)s}$	$EF_{(etsc)s}$	$EF_{(etwc)a}$	$EF_{(etsc)a}$
147-14-8	Pigment Blue 15 [a]	1	1	0	0	0.000000033	0	0
2682-20-4	2-Methyl-4-isothiazolin-3-one (MI) [a]	200	1000	0	0	2070	0	0
26172-55-4	5-Chloro-2-Methyl-4-isothiazolin-3-one (CMI) [a]	455	4480	0	0	2560	0	0
123-31-9	Hydroquinone [a]	227	728	0	0	54.3	0	0
141-43-5	2-Aminoethanol [a]	0.667	1.33	0	0	3.16	0	0
56-81-5	Glycerol [a]	0.000185	0.00037	0	0	0.00086	0	0
28519-02-0	Benzenesulfonic acid, dodecyl(sulfophenoxy)-, disodium salt [a]	62.5	1160	0	0	0.0203	0	0
52-51-7	2-Bromo-2-nitropropane-1,3-diol (Bronopol) [a]	27	135	0	0	314	27	251
79-07-2	2-Chloroacetamide [a]	179	357	0	0	500	71.4	400
5468-75-7	Pigment Yellow 14 (u.s.) [b]	5.03	9.26	2.76	-	-	-	-
147-14-8	Pigment Blue 15 (u.s.) [b]	5.31	10.4	1.29	-	-	-	-

[a] Calculation of characterisation factors based on data from PhysProp [23], ECOTOX [24], ChemFate [25], IUCLID [26], Madsen et al. [27], CERI [28], Mackay et al. [29], US-EPA [30] and in some cases also including QSAR estimations on basis of EPIwin [31].
[b] Accumulated upstream characterisation factors, i.e. summing up all potential impact from water, air and soil emission from the production process (synthesis) of the pigments [22].
u.s.: Upstream

The accumulated upstream characterisation factors for Pigment Blue 15 and Yellow 14 in Table C1 are not related directly to emissions, i.e. they are not to be multiplied by an emitted amount as is the case for the other characterisation factors. Instead these accumulated characterisation factors are expressed per gram produced of the two pigments. The factors must therefore be multiplied by the consumption of the relevant pigments at the production stage (model printing company). The result represents the potential impact from the emissions during the production of the pigments (material stage). These upstream characterisation factors are based on a novel estimation technique making use of knowledge about chemical synthesis combined with generic emission scenarios [22]. The emissions scenarios on which these upstream characterisation factors are based are taken from the EC Technical Guidance Document (TGD) on risk assessment [21]. This kind of scenario is used for first tier risk assessment/screening and may therefore be conservative. However, Andersen & Nikolajsen [22] have consistently used the lowest among the proposed values for emitted fraction in every case (produced amount > 2000 ton, assuming WWTP at the production facilities). The size of the characterisation factor for Pigment Yellow 14 upstream is mainly determined by emission of 3,3-dichlorobenzidine and 2-chloroaniline during the synthesis of the pigment. For Pigment Blue 15 upstream, the main contributing emission is cuprous chloride [22].

References

[1] Dalhielm R, Axelsson U. Miljöprofilering – livscykelanalyser av grafiske produkter. TEKNIKRAPPORT nr. 4/95, IMT, 1995.

[2] Axelsson U, Dalhielm R, Marcus O. Miljöprofilering – livscykelanalyser av grafiske produkter, del 2. TEKNIKRAPPORT nr. 3/97, IMT, 1997.

[3] Johansson M. Livscykelanalys av arkoffsettrykning. Jämförande analys av vatenfri och konventionell offsettrykning samt computer-to-plate och konventionell prepress. Rapport nr. 2002:09. Framkom/December 2002.

[4] Drivsholm T, Maag J, Christensen SV, Hansen E. Ressourceforbrug og miljøbelastning for tre grafiske produkter i et livscyklusperspektiv. Work Report No. 63 (book in Danish). Danish Environmental Protection Agency, 1996. http://www.mst.dk/udgiv/publikationer/1996/87-7810-747-4/pdf/87-7810-747-4.pdf

[5] Drivsholm T, Maag J, Christensen SV, Hansen E. Miljøeffekter og ressourceforbrug for tre grafiske produkter i et livscyklusperspektiv. (book in Danish with English summary). Environmental Project No. 341. Danish Environmental Protection Agency, 1997. http://www.mst.dk/udgiv/publikationer/1997/87-7810-682-6/pdf/87-7810-682-6.pdf

[6] INFRAS. LCA Graphic Paper and Print Products (Part 2: Report on the industrial processes assessment). An environmental project of: Axel Springer Verlag, STORA and CANFOR. Scientific consultant: INFRAS, Zürich, Switzerland, 1998.

[7] Wenzel H, Hauschild M, Alting L. Environmental Assessment of Products, Vol. 1. First edn. Chapman & Hall, London, Great Britain, 1997.

[8] Larsen HF, Hansen MS, Hauschild M. Ecolabelling of printed matter. Part II: Life cycle assessment of model sheet fed offset printed matter. Environmental Project No. XXX. (final draft April 2004). Danish Environmental Protection Agency. Final draft preliminary available at: http://ipltest.kpd.ipt.dtu.dk/ipl/upload/lcv/127_2.pdf

[9] Hauschild M., Wenzel H. Environmental Assessment of Products. Vol. 2. First edn. Chapman & Hall, London, Great Britain, 1998.

[10] Brodin L, Korostenski J. Miljøbelastningar från grafisk industri i Sverige. Grafiska Miljögruppen. Report version 2 (15-04-1995). Report to SFS, 1995.

[11] Larsen HF, Tørsløv J, Damborg A. Areas of intervention for cleaner technology in the printing industry - assessment of waste water (book in Danish with English summary). Environmental Project No. 284. Danish Environmental Protection Agency, 1995. http://www.mst.dk/udgiv/publikationer/1995/87-7810-330-4/pdf/87-7810-330-4.pdf

[12] Anonymous. Data from six Danish sheet fed offset printing companies. Based on inventories from 1999-2002.

[13] Larsen HF, Pedersen AR, Birch H, Rasmussen D, Hansen LE. Evaluation of Best Available Technology (BAT) in screen cleaning (book in Danish with English summary). Environmental Project No. 381. Danish Environmental Protection Agency, 1998. http://www.mst.dk/udgiv/publikationer/1998/87-7810-975-2/pdf/87-7810-975-2.pdf

[14] Larsen HF, Helweg C, Pedersen AR, Boyd HB, Laursen SE, Hansen J. Chemicals in textiles (book in Danish with English summary). Environmental Project No. 534. Danish

Environmental Protection Agency, 2000. http://www.mst.dk/udgiv/publikationer/2000/87-7909-800-2/pdf/87-7909-801-0.pdf

[15] Larsen HF, Helweg C, Pedersen AR, Andersen M, Wallström E, Hoffmann L. Evaluation of Best Available Technology (BAT) in washing off water-based flexographic inks in the packaging printing industry (book in Danish with English summary). Environmental Project No. 730. Danish Environmental Protection Agency, 2002. http://www.mst.dk/udgiv/publikationer/2002/87-7972-320-9/pdf/87-7972-321-7.pdf

[16] Nielsen U, Pedersen BM, Larsen HF, Knudsen HH. Car washing facilities, status and strategies (book in Danish with English summary). Environmental Project No. 537. Danish Environmental Protection Agency, 2000. http://www.mst.dk/udgiv/publikationer/2000/87-7944-124-6/pdf/87-7944-125-4.pdf

[17] Stranddorf HK, Hoffmann L, Schmidt A. LCA Guideline: Update on impact categories, normalisation and weighting in LCA. Selected EDIP97-data. Final draft February 2004. To be published as an Environmental Project by the Danish Environmental Protection Agency. http://www.mst.dk/

[18] Smith A, Brown K, Bates J, Ogilvie S, Rushton K. Waste Management Options and Climate Change. Final report to the European Commission, DG Environment. AEA Technology, 2001.

[19] Frees N, Hansen MS, Ottosen LM, Tønning K, Wenzel H. Opdatering af vidensgrundlaget for de miljømæssige forhold ved genanvendelse af papir og pap. (book in Danish with English summary). Draft report (No. 13) to the Danish Environmental Protection Agency. January 2004. To be published as an Environmental Project by the Danish Environmental Protection Agency. http://www.mst.dk/

[20] Villanueva A, Wenzel H, Strömberg K, Viisimaa M. Review of LCA studies on the recycling and disposal of paper and cardboard. DRAFT-Final-Report, 10 February, 2004. European Topic Centre on Waste and Material Flows.

[21] EC. Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances, Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Institute for Health and Consumer Protection. European Commission. ECB, JRC, Ispra, Italy, 2003.

[22] Andersen LK, Nikolajsen MH. Life Cycle Assessment of chemicals at the Brdr. Hartmann A/S. Thesis elaborated at the Danish engineering education at The Technical University of Denmark. Supervisor. Michael Hauschild. IPL-048-03, 2003. Link: Life cycle assessment of chemicals at Brdr. Hartmann A/S

[23] PhysProp. PhysProp Database. First published 1993. Syracuse Research Corporation 301 Plainfield Road, Suite 350 Syracuse, New York 13212-2510. 2004. http://www.syrres.com/esc/physdemo.htm

[24] ECOTOX. ECOTOXicology Database system. US EPA. 2004. http://www.epa.gov/ecotox/

[25] ChemFate. ChemFate Database. First published 1983. Syracuse Research Corporation 301 Plainfield Road, Suite 350 Syracuse, New York 13212-2510. 2004. http://www.syrres.com/esc/chemfate.htm

[26] IUCLID. IUCLID CD-ROM Year 2000 edition. Public data on high volume chemicals. European Chemical Bureau. ISBN 92-828-8641-7. 2000.

[27] Madsen T, Boyd HB, Nylén D, Pedersen AR, Pedersen GI, Simonsen F. Environmental and Health Assessment of Substances in Household Detergents and Cosmetic Detergents Products. Environmental Project No. 615. Danish Environmental Protection Agency, 2001. http://www.mst.dk/udgiv/publications/2001/87-7944-596-9/pdf/87-7944-597-7.pdf

[28] CERI. Chemical Evaluation and Research Institute (CERI), Japan 1-4-25 Koraku Bunkyo-ku. Tokyo 112-0004. 2004. http://qsar.cerij.or.jp/cgi-bin/DEGACC/index.cgi?e

[29] Mackay D, Ma K-C, Shiu WY (2000). Physical-Chemical Properties and Environmental Fate Handbook . CRC press. ISBN: 0849321921. 2000.

[30] US-EPA. US-EPA High Production Volume (HPV) Challenge Program, 2004. http://www.epa.gov/chemrtk/smrestbl.htm

[31] EPIwin. EPIwin suite v3.10. United States Environmental Protection Agency Office of Pollution Prevention and Toxics (OPPTS) 1200 Pennsylvania Avenue, NW Mail Code 7401M Washington, DC 20460. 2001. http://www.epa.gov/opptintr/exposure/docs/episuite.htm

[32] Busch NJ. Calculation of weighting factors. Chapter 11 in: Stranddorf HK, Hoffmann L, Schmidt A (ed.). LCA technical report: Impact categories, normalisation and weighting in LCA. Update on selected EDIP97-data. Final draft February 2004. To be published as an Environmental Project by the Danish Environmental Protection Agency. http://www.mst.dk/

[33] CEPI. Special Recycling 2002 statistics. CEPI. October 2003. www.cepi.org.

[34] Ludwiszewska J. Grafiske branchen och dess kemikalieanvänding: Exempel från nogra företag inom Hälsingborgs kommun – Miljö- och Hälsoskyddskontoret Hälsingborg Kommun. Rapport 1/92 + Bilagsdel, 1992.

[35] Baumann W, Gräfen M. Emission Scenario Document. Photographic Industry. IC10. Institute for Environmental Research. University of Dortmund. 11/19/99, 1999.

[36] Baumann W, Gräfen M. Emission Scenario Document. Printing Industry. IC15 (‘others’). Institute for Environmental Research. University of Dortmund. 11/19/99, 1999.

[37] Baumann W, Rothardt T. Druckereichemikalien; Daten und Fakten zum Umweltschuts" 2. Uberarbeitete and ergänzte Auflage. Springer-Verlag. ISBN 3-540-66046-1. 1999.

[38] Tønning K. Statistik for returpapir og –pap 2000. (book in Danish). Environmental Project No. 683. Danish Environmental Protection Agency, 2002. http://www.mst.dk/udgiv/publikationer/2002/87-7972-076-5/pdf/87-7972-077-3.pdf

[39] EUROSTAT. Municipal waste collected. Municipal waste incinerated. Municipal waste land filled, 2002: http://europa.eu.int/comm/eurostat/newcronos/queen/display.do?screen=welcome&open=/stri

nd_copy_817397594099/enviro_copy_336220120048&language=en&product=YES&root=YES_copy_539019591709#/strind_copy_817397594099/enviro_copy_336220120048

[40] Miljønet. MiljøNet. Graphic Association Denmark. (database in Danish), 2004. http://www.miljonet.org/

3 Selection methods

This Chapter is a copy of the following paper published in the International Journal of LCA:

Larsen HF, Birkved M, Hauschild M, Pennington D, Guinée J (2004). Evaluation of Selection Methods for Toxicological Impacts in LCA. Recommendations for OMNIITOX. *Int J LCA 9(5), 307-319.*

OMNIITOX: LCA Methodology

Evaluation of Selection Methods for Toxicological Impacts in LCA

Recommendations for OMNIITOX

Henrik Fred Larsen[1]*, Morten Birkved[1], Michael Hauschild[1], David W. Pennington[2] and Jeroen B. Guinée[3]

[1] Department of Manufacturing Engineering and Management, Technical University of Denmark (DTU) Building 424, DK-2800, Lyngby, Denmark
[2] Industrial Ecology, Life Cycle Systems, GECOS, Swiss Federal Institute of Technology Lausanne (EPFL), 1015 Lausanne, Switzerland
[3] Centre of Environmental Science (CML), Leiden University, P.O. Box 9518, 2300 RA Leiden, The Netherlands

---

* **Corresponding author** (hfl@ipl.dtu.dk)

DOI: http://dx.doi.org/10.1065/lca2004.08.164

Abstract

Goal, Scope and Background. The aim of this study has been to come up with recommendations on how to develop a selection method (SM) within the method development research of the OMNIITOX project. An SM is a method for prioritization of chemical emissions to be included in a Life Cycle Impact Assessment (LCIA) characterisation, in particular for (eco)toxicological impacts. It is therefore designed for pre-screening to support a characterisation method. The main reason why SMs are needed in the context of LCIA is the high number of chemical emissions that potentially contribute to the impacts on ecosystems and human health. It will often not be feasible to cover all emissions with characterisation factors and, therefore, there exists a need to focus the effort on the most significant chemical emissions in the characterisation step. Until now not all LCA studies include toxicity-related impact categories, and when they do there are typically many gaps. This study covers the only existing methods explicitly designed as SMs (EDIP-selection, Priofactor and CPM-selection), the dominating Chemical Ranking and Scoring (CRS) method in Europe (EURAM) and in the USA (WMPT) that can be adapted for this purpose, as well as methods presenting novel approaches which could be valuable in the development of improved SMs (CART analysis and Hasse diagram technique).

Methods. The included methods are described. General guidance principles established for CRS systems are applied to SMs and a set of criteria for good performance of SMs is developed. The included methods are finally evaluated against these criteria.

Results and Discussion. Two of the most important performance criteria include providing consistent results relative to the more detailed, associated characterisation methods and the degree of data availability to ensure broader chemical coverage. Applicability to different chemical groups, user friendliness, and transparency are also listed amongst the important criteria. None of the evaluated methods currently fulfil all of the proposed criteria to a degree that excludes the need for development of improved selection methods.

Conclusion and Recommendations. For the development of SMs it is recommended that the general principles for CRS systems are taken into account. Furthermore, special attention should be paid to some specific issues, i.e. the emitted amount should be included, data availability should enable broad chemical coverage, and when identifying priority chemicals for the characterisation, the developed SM should generate few false positives (chemical emissions classified wrongly as being of high concern) and no (significant) false negatives (classified wrongly as being of low concern) as compared to the associated characterisation method. These recommendations are not only relevant for a stand alone SM, but also valuable when dealing with simple characterisation methods associated with a more detailed characterisation method.

Outlook. There are several questions that need to be answered before an optimal SM can be developed, inter alia: Is it optimal to just use simple measured data with high availability or are QSAR estimates of more complex, relevant data better? Which key parameters to include and how? Is a statistical approach, like linear regression of characterisation factors or CART analysis, the best solution?

Keywords: Chemical ranking and scoring (CRS); evaluation criteria; life cycle impact assessment (LCIA); OMNIITOX; selection methods; simple characterisation methods; toxicity-related impact categories

Introduction

Today very few Life Cycle Assessment (LCA) studies include human toxicity and ecotoxicity in the impact assessment, and those which do typically do it in an incomplete way. A reason for this is that in many cases a high number of chemical emissions (termed emissions) potentially contribute to these toxicity-related impact categories ('tox' impact categories), and for most of them there are no available characterisation factors. Applicable tools to deal with this problem do not exist. This calls for methods that are able to select/prioritize those emissions that contribute most significantly to the 'tox' impact categories, where the emissions of consideration are not otherwise limited in the scope of the LCA study. Such methods are here called selection methods (SMs) and their overall aim is to focus the characterisation effort on the most significant chemical emissions when Life Cycle Impact Assessment (LCIA) on toxic releases is performed.

The concept of a selection method has been created within OMNIITOX in order to differentiate from the wider and more ambiguous group of methods covered by the phrase 'LCA screening method'. The latter has been used for concepts with the same purpose as defined for an SM, but the phrase can also mean something quite different, e.g. simple screening level LCA methodology including other impact categories than those which are toxicity related.

The research dealt with here is described in further detail in the OMNIITOX report 'Inventory of LCIA selection methods for assessing toxic releases' (Larsen et al. 2002). The aim of this study has been to come up with preliminary recommendations on development of an SM for use in the classification step of LCIA to support characterisation, i.e. the Base Model (BM) as well as a Simple Base Model (SBM) (see Guinée et al. 2004). It was decided within the OMNIITOX research programme (Molander et al. 2004) to aim at performing the selection with a characterisation method (in this the SBM) which is based on a statistical derivation from the BM using QSAR data to some extent (Guinée et al. 2004). This approach supplements the different approaches to developing SMs which are exemplified in this paper. In addition to its function as a characterisation method, the SBM thus also serves as a selection method, and most of the results presented for the SM are equally applicable to simple characterisation methods like the SBM: the evaluation criteria developed, the recommendations on method development, the analysis of Chemical Ranking and Scoring (CRS) methods and general CRS principles in an LCIA framework. Regardless whether the selection is performed using a simple characterisation method like the SBM or an individual SM, the study described here is an indispensable part of the basis for the development of the selection approach.

In this paper we first describe the characteristics of an SM, followed by a description of existing SMs and other relevant CRS methods. General principles for CRS methods are applied to the special demands on an SM. Criteria for the evaluation of SMs are then presented, and afterwards the included methods are evaluated. Properties of the different methods in the context of the SM approach are then discussed.

1 Selection Methods

An SM can be considered as a CRS method with some special constraints, the most important being the requirement for consistency with the associated characterisation method for which it is supposed to identify the most important emissions (consistency between the lower and higher levels of complexity in the assessment). The aim of the SM is to select (prioritize) those emissions from an inventory of a specific LCA-study that are most likely to contribute – according to a specific characterisation method – significantly to the impact categories on ecotoxicity and human toxicity. In this way, the SM serves for the step of the Life Cycle Impact Assessment (LCIA) called classification or in ISO 14042 terminology: Assignment of emissions to impact categories.

Let's say that we were able to perform the characterisation (i.e. calculate impact potentials) for all the emissions of chemicals mapped in an inventory, which could be several hundred chemicals of interest in some studies, and then subsequently rank their impact potentials. The ideal SM would rank the emissions in the same way (or even better, give the same relative value to each emission) as the characterisation method, but based on a significantly lower data demand.

More pragmatically, the SM does not need to rank the emissions in exactly the same way as the characterisation method, as long as the significant contributing emissions are subsequently selected for inclusion in the characterisation step. Imperfection in ranking may occur as false positives, i.e. emissions that are identified for further assessment as high concerns, ultimately result in low concern through further evaluation. This is somewhat undesirable because it reduces the ability of the SM to limit the characterisation work. The opposite of false positives, false negatives, are even less desirable because emissions of high concern will not be prioritized for characterisation. As SMs must be based on limited information, a trade-off is often sought by evaluating how many false positives relative to how many false negatives are acceptable, i.e. where to draw cut-offs between high and low potential for concern.

Another important aspect of an SM is the data demand, and thereby the time demand, which preferably should be significantly less than for the full characterisation method – otherwise one could just as well skip the selection and go directly to characterisation. As is the case with characterisation methods, SMs should be applicable to all types of chemicals (in principle any chemical emitted and mapped in the inventory). Furthermore, for each chemical, the substance data required for the use of the SM should be available for all emissions encountered in the inventory. Exceptions may include, for example, metals or other elements for which simplistic SMs are not always applicable and where more detailed measures like characterisation factors may already exist.

2 Existing SMs and other CRS Methods

Since very few SMs actually exist with a direct link to more detailed/robust characterisation methods, it was decided to expand the scope of the analysis to comprise other CRS methods developed for a similar screening purpose within environmental risk or hazard assessment, i.e. prioritizing/ranking of emissions and/or chemicals. It was anticipated that these methods could be adapted, or could contribute with applicable elements and principles, to the development of an SM and the development of SBM in the OMNIITOX research programme.

The number of CRS methods used within hazard assessment and risk assessment is very high. According to Davis et al. (1997) hundreds of methods exist (or have existed) which can be based on different procedures: pre-screening (scientific judgement), hazard ranking approach (threshold effects, no exposure included), ordinal assignment of data (scores, algorithm that weights) and risk-based quotient (including both exposure and effects, and a margin of safety). The basic principles in most of the recent CRS methods include some kind of assessment of the persistence, bioaccumulation and (eco)toxicity of the chemicals in question (so-called PBT approaches).

Table 1 presents a list of chosen CRS methods, including all known SMs and one very simple characterisation method (CPM). The chosen CRS methods used outside LCIA are expected to represent the most important methods, or types of methods, representing the situation in the European Union (EURAM) and in the USA (WMPT). Two mathematical/statistical tools (Hasse and CART), until now only used

Table 1: List of existing SMs and chosen CRS- and mathematical/statistical methods

Method name	Includes	Typical use	Reference
EDIP-selection method	Ecotoxicity and human toxicity	LCIA	(Hauschild and Wenzel 1998, Wenzel et al. 1997)
Priofactor	Ecotoxicity and human toxicity	LCIA	(Larsen et al. 1999b and 1999a)
CPM-method; qualitative part	Ecotoxicity	LCIA	(Eriksson 1999)
CPM-method; quantitative part[a]	Ecotoxicity	LCIA	(Eriksson 1999)
EURAM	Ecotoxicity and human toxicity	Risk Assessment	(Hansen et al. 1999)
WMPT (adopted also in P2P)	Ecotoxicity and human toxicity	Hazard Assessment (and LCIA)	(US EPA 1997, Pennington et al. 2002)
Hasse diagram technique	Ecotoxicity and human toxicity[b]	(Risk Assessment)	(Halfon et al. 1996, Sørensen et al. 1998)
CART	Ecotoxicity and human toxicity[b]	(Risk assessment)	(Bennett et al. 1999, 2000 and 2001)

[a] Simple characterisation method
[b] Can be used for both

to a limited degree within risk assessment, are also included because they are considered to represent promising alternative approaches for the selection of chemicals. In the table, the typical use is given, and it is indicated whether the method includes the evaluation of ecotoxic effects, of human toxic effects, or both.

A method that is not shown in **Table 1** but which may become relevant for the development of an SM and/or the planned development of a SBM within the OMNIITOX project (Guinée et al. 2004) is the 'log linear regression equation' method based on a multivariate analysis of the associated characterisation method. A preliminary version of the method was presented by van de Meent et al. (2002), but sufficient documentation was not available in order to prioritize the method for further evaluation in this study. Furthermore, CRS methods based on risk phrases for human toxicity to be used in connection with LCIA have recently been published (Bunke et al. 2003). However, these methods are not included here because the use of risk phrases for ranking was already adopted in the EDIP-selection method, the Prio-factor, and EURAM.

Each method is shortly described below. A more detailed description of all the methods can be found in Larsen et al. (2002) or in the literature related to the method.

2.1 EDIP-selection method

The EDIP-selection method was developed during the creation of the EDIP method (Wenzel et al. 1997). This is a full LCA method including tools, for example, for calculating key property based characterisation factors for ecotoxicity and human toxicity. In the EDIP-documentation, this SM is described as a qualitative/semi-quantitative tool for screening chemical emissions and for prioritization of chemicals to be included in the quantitative characterisation step of the EDIP method.

Table 2: Exposure scores for the EDIP-selection method

Emission expected	Classified as R53 or R58	Score
Yes	Yes	8
Yes	No	4
No	Yes	4
No	No	1

R53: May cause long-term adverse effects in the aquatic environment
R58: May cause long-term adverse effects in the environment

The EDIP-selection method is based on risk phrases, i.e. the R-sentences used in EU labelling of chemicals based on hazard assessment (ECC 1967 and its amendments, e.g. EC 2001) and an assessment of whether the chemical is emitted or not. For each chemical, two impact scores are calculated, one for ecotoxicity and one for human toxicity, by multiplying an exposure score with an (eco)toxicity score.

The ecotox impact scores (**Table 4**) are calculated by multiplying an exposure score (**Table 2**) with an ecotoxity score (**Table 3**). The R53 and R58 used in the criteria for the exposure score are both based on the persistence and/or bioaccumulation potential of the substance in question. The ecotoxicity score is, in practice, only based on acute aquatic ecotoxicity (R50, R51, R52) because assignment of terrestrial risk phrases are typically missing.

Table 3: Ecotoxicity scores for the EDIP-selection method (final ecotoxicity score equals the sum of the two scores, i.e. 8, 6, 5, 4, 2, 1, 0)

Ecotoxicity	Aquatic ecotoxicity				Terrestrial ecotoxicity	
Criteria	R50 or R50/53	R51/53	R52 or R52/53	N.C.	R54 or R55 or R56 or R57	N.C.
Score	4	2	1	0	4	0

R50: Very toxic to aquatic organisms
R51: Toxic to aquatic organism
R52: Harmful to aquatic organisms
R53: See notes in Table 2
R54: Toxic to flora
R55: Toxic to fauna
R56: Toxic to soil organisms
R57: Toxic to bees
N.C.: No Classification

Table 4: Ecotox impact scores for the EDIP-selection method

Exposure score	Ecotoxicity score						
	0	1	2	4	5	6	8
1	0	1	2	4	5	6	8
4	0	4	8	16	20	24	32
8	0	8	16	32	40	48	64

For the calculation of the human impact scores the same exposure score as for ecotox is used (see Table 2). The human toxicity part is also based on risk phrases (e.g. R20-28, R40, R45, R46, and R49), but here several effect categories are included, e.g. acute toxicity, genotoxicity and carcinogenicity (Larsen et al. 2002).

As is evident from the description, the EDIP-selection method can be characterised as a PBT approach based on regulatory hazard assessment and only including emissions as yes or no (not the emitted amount).

The EDIP-selection method has only been evaluated against the EDIP characterisation method in one case study on a detergent for manual dishwashing (Larsen et al. 1999a). The study included 42 emissions. The ecotoxicity part of the EDIP-selection method was not able to discriminate amongst all emissions and resulted in 29 false positives. The main reason for this was the lack of data for terrestrial ecotoxicity, which has a conservative effect on the scoring, i.e. the highest score for terrestrial ecotoxicity (4) was given, see Table 3. For the human toxicity part of the EDIP-selection method, 33 emissions were prioritized resulting in 10 false positives and 5 false negatives.

2.2 Priofactor

The Priofactor is an SM developed for the EDIP method that was developed due to the poor ability of the EDIP-selection method to prioritize emissions, as described in section 2.1. Instead of optimising the risk phrase approach, as used in the EDIP-selection method, it was decided to use a key parameter approach much closer in principle to the EDIP method. The Priofactor is therefore an example of an SM that can be used as a characterisation method, but with a lower demand on data quality and the amount of data than the associated 'higher tier' characterisation method, i.e. the EDIP method. The development of the Priofactor is described in Larsen et al. (1999a) and Larsen et al. (1999b).

The Priofactor is divided in three impact potential categories and therefore involves three calculations per emission – one for potential ecotoxicological contribution and two for potential human-toxicological contribution (direct via air and indirect via water/soil). These calculations require readily available data on (bio)degradation, bioaccumulation, (eco)toxicity, and an estimate on the emitted amount to predict the relative contribution from each substance to the total toxicological impact potential for each category. The Priofactor makes it possible to select those emissions that contribute with more than, for example, 0.1% or 1% to the total impact potential for each category. In this way, the more time-consuming detailed impact assessment in the characterisation step can be restricted to those emissions.

The overall principles for calculating the Priofactor are:

$$\text{Priofactor} = Q \cdot \text{Subpriofactor} \qquad (1)$$

Q is the emitted amount and a subpriofactor is estimated for each of the three categories i.e. ecotoxicity, human toxicity air and human toxicity water/soil. The ecotox-subpriofactor (m^3/g) is calculated as:

$$\text{Ecotox} - \text{subpriofactor} = \frac{\text{BDF} \cdot \text{BCF}}{\text{EC}_{50}(\text{g}/\text{m}^3)} \qquad (2)$$

Where BDF is the BioDegradationFactor (values between 0.1 and 1 depending on persistence), BCF is the BioConcentrationFactor and EC_{50} is the concentration of the substance in question having an acute (lethal) effect on 50% of test organisms in an OECD standard acute laboratory test.

The human toxicity subpriofactors are calculated on almost the same principles, but instead of EC_{50}s, Toxfactors are used. The Toxfactors can have values between 2 and 2000 (air) or 200 and 2000 (soil/water) depending on the severity of the classification (i.e. assigned risk phrases) of the substance in question. For the human toxicity subpriofactor (air), a factor between 0.1 and 1.0 based on the half-life in air of the substance is used instead of BDF.

On the basis of the description, the Priofactor can be characterized as a PBT approach that takes the emitted amount into account in a quantitative way.

The Priofactor was evaluated against the EDIP method in the same case study as the EDIP-selection method (Larsen al 1999a). For the ecotoxicity part, the Priofactor selection resulted in four false positives and three false negatives, but importantly here is that the chemical emissions prioritized by the Ecotox-priofactor accounted for 99.63%, whereas the three false negatives only accounted for 0.31% of the total impact potential of the EDIP characterisation. For the human toxicity part the results of the evaluation was almost as good as for the Ecotox-priofactor (**Table 5**).

Table 5: Results of evaluation of the Priofactor against the EDIP method

	Ecotox-priofactor		Human-tox-priofactor (air)		Human-tox-priofactor (water/soil)	
	Number	Relative share of total EDIP impact potential (%)	Number	Relative share of total EDIP impact potential (%)	Number	Relative share of total EDIP impact potential (%)
False positive	4	0.00	1	0.00	6	0.00
False negative	3	0.31	13	3.15	3	1.23
Prioritized emissions	14	99.63	9	96.77	15	98.74
Total emissions	42	100	28	100	42	100

2.3 CPM

The CPM method is described in Eriksson (1999). It consists of a first screening part (i.e. the qualitative part) that could be regarded as an SM (hereafter called CPM-selection method). In the second part of the method (i.e. the quantitative part termed the CPM-characterisation method) characterisation factors for chronic ecotoxicity in water are calculated, but the method is not included in a full LCIA method.

The description of the CPM-characterisation method is only included here to illustrate how a close connection between the data needed for the selection and the characterisation can be achieved and to show a special approach on how to deal with inorganics. As the CPM-characterisation method is a characterisation method, it is not included in the evaluation of SMs in section 5.

Both the CPM-selection method and the CPM-characterisation method are divided into a decision tree/algorithm that handles organic substances and another decision tree/algorithm that handles inorganic substances (mainly metals). The individual methods are described in the following subsections.

2.3.1 CPM-selection method

The CPM-selection method on organic substances makes use of a decision tree based on the three intrinsic substance properties ecotoxicity, biodegradation and bioaccumulation (**Fig. 1**). The criteria for the thresholds (i.e. question marks in Fig. 1) are identical to the ones used in the EU labelling of chemicals based on hazard assessment (EEC 1967, and its amendments, e.g. EC 2001), see **Table 6** showing criteria for ecotoxicity. Only substances considered as not hazardous are not prioritized (see Fig. 1).

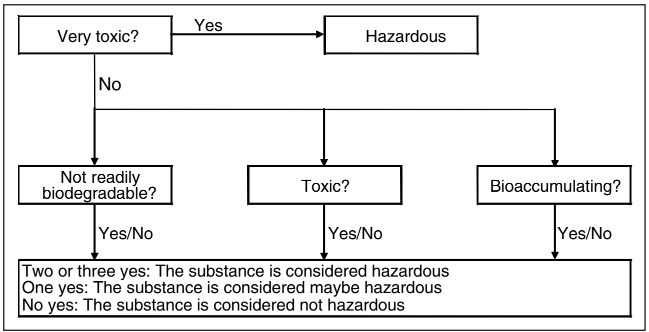

Fig. 1: Decision tree for the selection of organic substances by the CPM-selection method

The decision tree for inorganics is shown in **Fig. 2**. For this group of substances, biodegradability and bioaccumulation is excluded and substituted by covalent bonding properties, redox sensitivity and properties of partitioning between water and solid phase (K_d). For covalent bonding, soft acids (strong forming, i.e. covalent bounds with ligands) are given the score 3, whereas hard acids (weak forming, i.e. electrostatic bounds with ligands) are given the score 1. Substances in between, i.e. borderline acids, are given the score 2. For redox sensitivity, substances that can change their valence state is given the score 2, others are given the score 1. Substances with a K_d value below 50 are considered as contaminating (i.e. bio-available), otherwise not contaminating. Only substances considered as not hazardous are not prioritized (see Fig. 2).

The CPM-selection method can be characterised as a very simplistic PBT approach, not taking emitted amount into account, but paying attention to some of the special properties of inorganics. An evaluation of this SM against the CPM-characterisation method has, as far as known to the authors, never been published.

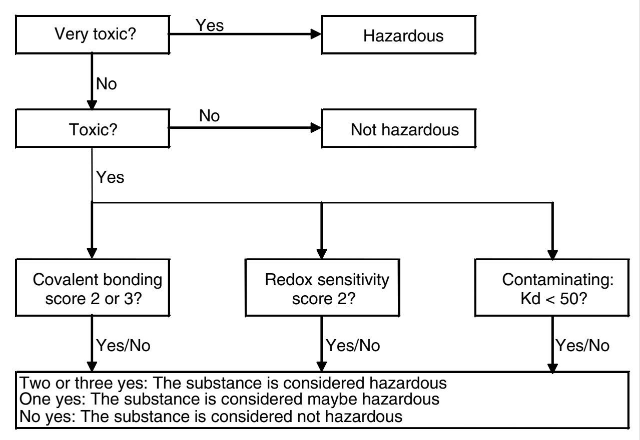

Fig. 2: Decision tree for the selection of inorganic substances by the CPM-selection method

Table 6: Ecotox criteria for the CPM-selection method

Test organism	Test result	CPM evaluation	Test result	CPM evaluation
Fish, LC50 (mg/l)	< 1.0	Very toxic	< 100	Toxic
Daphnia, EC50 (mg/l)	< 1.0	Very toxic	< 100	Toxic
Algae, EC50 (mg/l)	< 1.0	Very toxic	< 100	Toxic

2.3.2 CPM-characterisation method

The CPM-characterisation method is a quantitative method that calculates a characterisation factor (called impact factor) for each substance based on its intrinsic properties. It consists of two parts, one for organic substances and one for inorganic substances. For the organic part, the impact factor is calculated in the following way:

$$\text{Impact factor (organics)} = \frac{\text{Log}K_{ow} \cdot H}{\text{NOEC} \cdot \text{DEG}} \tag{3}$$

Where K_{ow} is the octanol/water partitioning coefficient, H is the Henry's law constant, NOEC is the chronic No Observed Effect Concentration and DEG is the percentage biodegraded in an OECD test for ready biodegradability. H is only included in the calculation if the atmospheric half-life of the substance is over 80 days. For the inorganic part, the calculation is performed in the following way:

$$\text{Impact factor (inorganics)} = \frac{\text{CB} \cdot \text{RS}}{\text{NOEC} \cdot \log K_d} \tag{4}$$

Here, CB is the covalent bonding score (1, 2 or 3), RS is the redox score (1 or 2) and K_d the partitioning coefficient, all three defined in the previous section.

2.4 EURAM

The EU Risk Ranking Method (EURAM) (Hansen et al. 1999) was developed within the EU as a part of the second of four steps, i.e. priority setting, in the evaluation of existing chemicals: Data collection, priority setting, risk assessment and risk reduction. It is used for screening chemicals for selection of the potentially most problematic ones for subsequent risk assessment. The target of the method has been the 2465 high production volume chemicals (HPVC's) for which data are compiled in the European Conform Chemical Information Database (IUCLID 2000). EURAM prioritizes chemicals on the basis of their potential risk to humans (human toxicity) and the environment (ecotoxicity). It is to a large extent consistent with the EU risk assessment methodology described in the Technical Guidance Document (TGD) (EC 1996).

The environmental fate or distribution part of EURAM includes a multimedia equilibrium partitioning model and calculates a score for the Predicted Environmental Concentration (PEC), whereas the environmental effect scoring is based on PNEC-values (Predicted No Effect Concentration).

The human effect scoring is based on R-phrases, and the fate part is simple and based on discrete exposure fraction values depending on the boiling point, vapour pressure and K_{ow} of the substance in question. Although EURAM includes methodologies for other protection goals than humans and the aquatic environment, i.e. soil, top predators, the atmosphere and microorganisms in sewage treatment plants, these are not included in this paper on SMs. This is because effect data for these protection goals are very limited and the EU therefore only uses these scores for prioritization in conjunction with expert judgement.

As far as the authors are aware, EURAM has not been used directly as an SM in LCIA. Though more advanced in some parts, it is, however, based on some of the same basic principles as the previously described SMs and may therefore be relevant as a potential basis for an LCIA selection tool. For aquatic ecotoxicity, an Aquatic Score (AS) is calculated in the following way:

$$\begin{aligned} \text{AS} = {} & [1.37(\log(\text{Emission} \cdot \text{Dist}_{env} \cdot \text{Deg}) + 1.301)] \\ & \cdot [0.7(-2 \cdot \log \text{PNEC}) + \text{AP}] \end{aligned} \tag{5}$$

Where Emission is the emitted amount (here truncated at min 50 ton and max 1,000,000 ton), Dist_{env} is the fraction distributed to the aquatic environment (here truncated at min 0.01 in an EURAM unit world), Deg is a score for biodegradation (0.1; 0.5 or 1.0 depending on biodegradation in OECD tests on readily and inherent biodegradability), PNEC is the Predicted No Observed Effect Concentration and AP is the Accumulation Potential (values of 0; 1; 2 or 3 depending on the BCF value of the substance). The constants within formular 5 are included to ensure that AS gets values between 0 and 100.

The EURAM aquatic score can be characterized as a PBT approach taking both emitted amount and distribution, i.e. the amount ending up in the aquatic environment, into account.

For human health, a Human Health score (HS) is calculated in the following way:

$$\text{HS} = [1.785(\log(\text{Emission} \cdot \text{Dist}_{HH}) + 0.398] \cdot \text{HEF} \tag{6}$$

Where Dist_{HH} is a fraction between 0.05 and 1 based on threshold values for the boiling point, vapour pressure and $\log K_{ow}$ of the substance and HEF is the Human health EFfect score assigned values between 0 and 10 depending mainly on the risk phrases assigned in combination with results from some specific laboratory tests, for example, genotoxicity and reproductive toxicity. The constants included in formular 6 are there to truncate the HS between 0 and 100.

The EURAM human health score can be characterised as a BT approach (persistency (P) not included) based on regulatory hazard assessment for human health, but including emitted amount and a threshold based factor for the fraction contributing to human exposure.

2.5 Waste minimization prioritization tool (WMPT)

In 1997, the US EPA's Office of Solid Waste (OSW) and EPA's Office of Pollution Prevention and Toxics (OPPT) issued a beta test version (1.0) of the WMPT (US EPA 1997, 1998). This methodology provides a screening-level assessment of the potential chronic hazard of chemicals in the context of human health and the aquatic environment. This is typical of the approaches adopted by many other national and international organisations. Previous tools also accounted for emission quantity, but this was not explicitly retained in the 1997 WMPT.

The main purpose of the WMPT system was to screen across the thousands of chemicals that may potentially appear in hazardous waste streams in terms of their Persistence (P), Bioaccumulation (B), and Toxicity (T). To conduct this broad-based PBT screening, the WMPT makes use of data from a variety of EPA and outside sources following data source preference hierarchies. For example, Reference Dose (RfD) and Reference Concentration (RfC) data from the Agency's Integrated Risk Information System (IRIS) were considered to be highest preference for toxicity (T) scoring for human non-cancer effects. If these data were unavailable, the tool uses data from lower-preference sources, such as acute toxicity LC_{50} (lethal concentration killing 50%) data for rodents from non-peer reviewed databases.

Data from various sources are placed on similar scales by comparing data values with established fencelines (or cutoffs) to place the values into low, medium, and high concern bins (or categories) for each of P, B, and T. For example, if a chemical has a bioconcentration factor (BCF) greater than, or equal to, 1000 then it is placed in the high-potential bin and assigned a bioaccumulation (B) score of 3. Similarly, values from 250 to 999 were placed in the medium bin (a medium score of 2 indicating a possibility for both high or low concern), and values below 250 were placed in the low concern bin (score of 1).

As far as possible, the data fencelines between categories were made consistent with the EPA's protocols at the time for screening new and existing chemicals under the Toxic Substances Control Act (TSCA). Where Agency precedents were unavailable for establishing fencelines, they were set so that 25% of the values would be considered high potential for concern, 50% medium, and 25% low (1:2:1). We note that there are a number of pros and cons to this type of simple binning approach, but, on balance, the EPA felt that a three-bin system was the best approach to place disparate types of data on comparable scales and that this was generally consistent with the degree of uncertainty associated with the data.

Comparisons with mechanistic-model based characterisation approaches were presented in Pennington and Bare (2001) and, in the context of selection/classification in LCA, in Pennington and Bare (2003). The WMPT method can be characterized as a PBT approach not taking the emitted amount into account. However, a way to account for the emitted amount at each level of PBT concern was demonstrated (Pennington and Bare 2001). This enabled chemicals of similar concern to be grouped and only those emitted in higher quantities in each group which are to be considered further. Some low concern groups could additionally be eliminated, depending on the scope of the LCA study.

2.6 Hasse diagram technique

In contrast to most other screening methods used, the Hasse diagram technique (HDT) is a purely objective screening method based on a mathematical method called partial order. The HDT has been used in several ways to screen and select chemicals of concern (Sørensen et al. 1998, Fomsgaard and Sørensen 1999, Lerche et al. 2002) and for ranking of sediments (Brüggemann et al. 2001). The use of the method was tremendously facilitated by the development of the WHASSE programme (Brüggemann 1999).

As an example, two chemicals (1 and 2) can be compared in relation to potential environmental risk using the parameters K_{ow}, DT50 (half-life) and $1/(EC_{50})$. If chemical 1 posses a potentially higher danger to the environment than chemical 2, then all three evaluation parameters of chemical 1 can be higher than those of chemical 2. However, it is rare to have a large group of chemicals where all included parameters make it possible to make a linear ranking purely based on the 'unweighted' parameters, since one chemical could, for example, be more toxic but less persistent than its counterpart. This problem is traditionally solved by weighting toxicity in relation to persistence; otherwise it would not be possible to compare indistinguishable chemicals.

The HDT deals with indistinguishable chemicals in larger sets by dividing the set of chemicals to be compared into groups or branches (**Fig. 3**) of distinguishable chemicals. In these groups/branches, all evaluation parameters of one chemical are lower than the same parameters of the chemical ranking higher within the same group/branch. This typically results in more than one group/branch, and the determination of the absolute order of the individual chemicals between groups/branches is not possible directly, which is why HDT is a partial ordering method.

To determine the absolute order, it is necessary to compare the individual groups of indistinguishable chemicals using methods like linear extension. By linear extensions the order theoretical probability can be derived, so that a chemical gets a certain rank as presented in Lerche et al. (2003). Please refer to Brüggemann et al. (2001) for further details on the HDT theoretical frame.

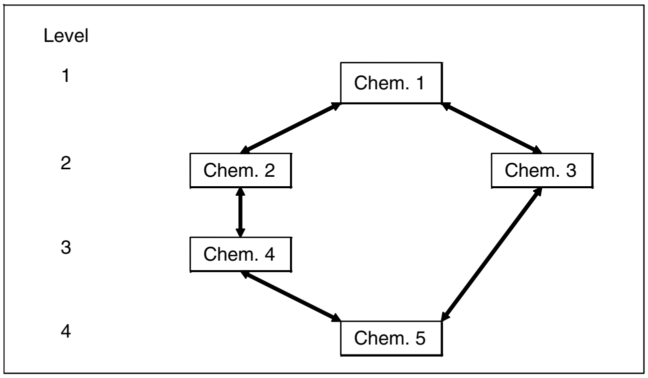

Fig. 3: Comparison of 5 chemicals. From the Hasse diagram (HD), it is seen that chemicals 3 and 4 rank above chemical 5. This means that all evaluation parameters on 3 and 4 are higher or lower than those of chemical 5. However, the absolute relation of the rank of chemical 3 in relation to chemical 4 is not possible to determine from the HD, since these are indistinguishable. Arrows indicate comparisons (distinguishable compounds)

2.7 CART

Existing examples of Classification And Regression Tree analysis (CART analysis) build on the assumption that the variation of properties follow a certain statistical distribution (as demonstrated in Bennet et al. 2000, Bennet et al. 2001, Eisenberg and McKone 1998). Using this assumption and Monte Carlo simulation, for example, it is possible to create a large set of hypothetical chemical compounds with properties varying according to a specified distribution and limits. As an alternative, large data sets for heterogenous chemicals could be analysed similarly.

The individual chemicals can be grouped according, for instance, to persistence or hazard. Using the set of properties and persistence, as one example, the CART analysis results in an evaluation tree created according to desired preferences (**Fig. 4**). The preferences can include minimizing false positives and virtually eliminating false negatives, or ensuring classification into a certain number of categories. As illustrated by the tree presented in Fig. 4, the persistence of a given chemical can be readily estimated with a well-defined certainty and in a structured manner from a subset of its properties.

3 Application of general principles for CRS to SMs

Davis et al. (1997) presented general principles, or a framework, of how to develop and select (for a specific purpose) chemical ranking and scoring systems. As far as we know, while other types of evaluation have been conducted, the only CRS system that has been evaluated against the general principles is EURAM and this was done by the method developers themselves. They concluded that the EURAM method fulfils all the basic criteria, i.e. the 17 general principles (Hansen et al. 1999). These principles are reviewed below and applied to the SM framework) and, as relevant, to the SMs and the other CRS methods included in this paper. More specific principles on exposure, human toxicity and ecotoxicity are dealt with in the background report (Larsen et al. 2002).

1) There should be a clearly defined purpose. For an SM, the purpose is to identify those emissions that are likely to contribute significantly to the impact category indicators for ecotoxicity and human toxicity prior to using an associated characterisation method with more data requirements.

2) There should be compatibility with the risk assessment paradigm. For an SM, it is relevant that it is compatible with the methods used and principles of LCIA for ecotoxicity and human toxicity indicators. Apart from the conceptual background and the purpose, these methods and principles are, to a large degree, currently inspired by, and to some degree compatible with, the risk assessment paradigm (e.g. Olsen et al. 2001).

3) Uncertainty should be acknowledged and assessed. Like dedicated CRS systems, SM results are highly uncertain, but the crucial point is not the absolute results, or scores, but the consistency with the associated characterisation method.

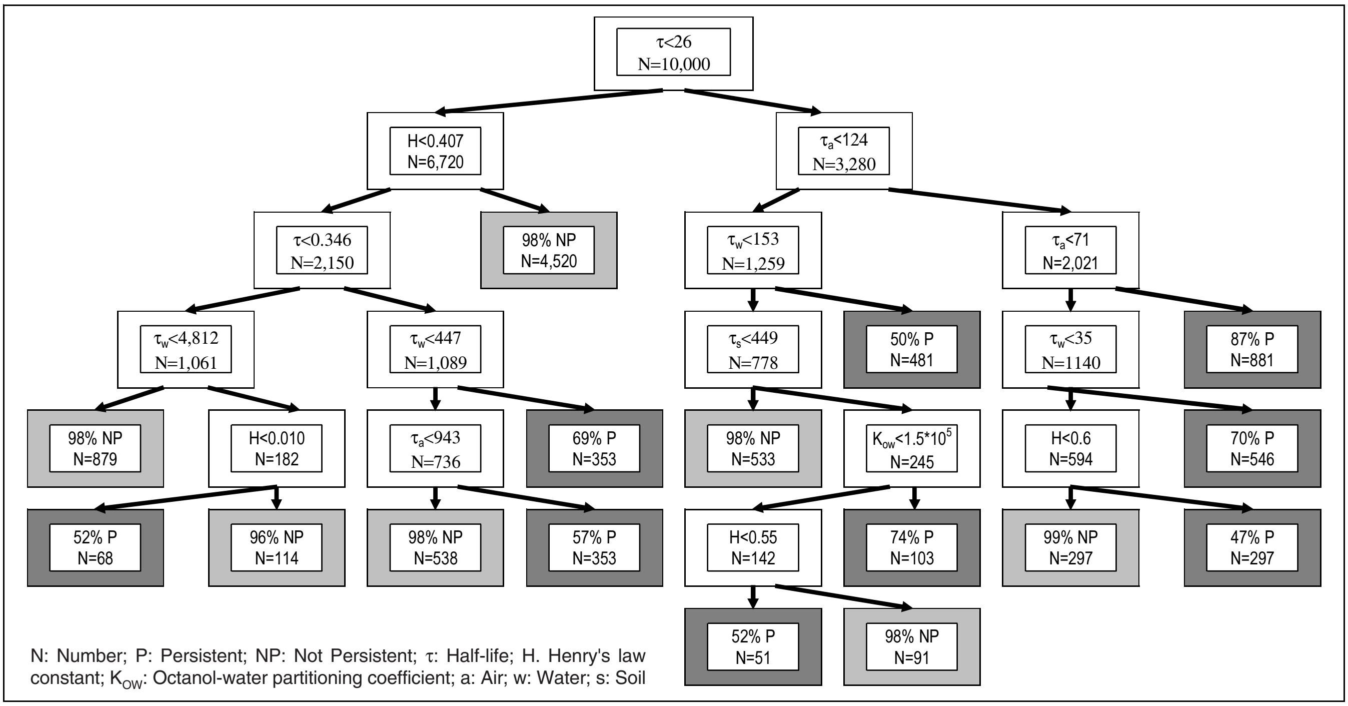

Fig. 4: Example of CART tree for emissions to air, from the mode of entry approach (from Bennett et al. 2001). The tree should be interpreted in that way that classification starts at the top, proceeding by evaluating the first inequality. If the inequality is true (i.e. answer is yes) the evaluation proceeds along the left branch. If the inequality is false (i.e. answer is no) the evaluation then proceeds along the right branch until reaching a terminal node (classification). Associated with each terminal node, dark grey for classification as persistent or light grey for classification as non-persistent, is a percentage indicating the confidence limit of the classification of the terminal node in question

4) The role of professional judgement should be acknowledged. Theoretically, the aim must be that professional judgement is only involved in the creation and evaluation of the SM (and possible updating) and that the user should be able to use the method without the need for specific scientific judgement. In practice, this is a rarely achievable objective in a pure sense.

5) There should be a broad consideration of effects. While LCIA addresses a very wide range of potential environmental impacts, the SMs are only supposed to cover the toxicity-related impact categories. Even for these, characterisation methods can operate with several subcategories, e.g. acute aquatic toxicity, chronic terrestrial toxicity and chronic aquatic toxicity, see de Koning et al. (2002), for more examples. It may therefore be necessary for an associated SM to deal with more than one 'scoring group' for each of the issues of ecotoxicity and human toxicity to be consistent with the characterisation method. But, it should be stressed that the aim is to keep the SM as simple as possible, i.e. not more sophisticated than just sufficient to be consistent with the characterisation method. Of the SMs dealt with in this paper, the EDIP-selection method deals with one 'scoring group' for each of the issues of ecotoxicity and human toxicity, whereas the Priofactor divides the human toxicity part in two 'sub-scoring groups', i.e. tox-priofactor (air) and tox-priofactor (soil/water). This sub-categorising is not directly based on effect type, but on exposure way. In the CPM-selection method, which only deals with ecotoxicity, two 'scoring groups' exist. Here, the differentiation is based on different behaviour in the environment (fate) for two different substance groups, i.e. organic and inorganic substances.

6) The role of valuation in aggregation and weighting should be recognised. Here, Davis et al. (1997) states that 'it generally is preferable that a chemical ranking system does not aggregate across major effect types', but in case that it should be done, the procedure should be transparent. The main argument is that aggregation and weighting require value judgement (political assessment) and when dealing with risk assessment, this judgement is dependent on the risk management context. For an SM, we assess that aggregation across ecotoxicity and human toxicity may not be a good idea, unless the results are correlated, because characterisation methods typically distinguish at least between these two and the selection would therefore most probably become inconsistent with the characterisation. The only CRS method included in this paper that includes the option to aggregate across ecotoxicity and human toxicity is the WMPT method. Here, it was done in a transparent way, although this was not retained in the context of the LCA-related publications, see section 2.5.

7) Methods and outputs should be transparent. It is preferable that an SM is based on transparent theoretical logic which is consistent with the characterisation method, transparent in mathematical formulations, and is well documented.

8) Method should be neutral to data availability. Davis et al. (1997) stated that a CRS method 'should not systematically 'punish' or 'reward' chemicals with extensive data versus chemicals with no data'. This principle is in line with the aspiration of LCIA to provide a best estimate of the impact, while it deviates from the common procedure of risk screening where an approach is generally adopted that penalises substances with poor data availability. Generally, and including SMs, there are some mostly unsolved problems on how to deal with a lack of data, especially a lack of measured data. We assess that for SMs, one way to approach a solution to this problem is further use of the available state of the art QSARs to fill gaps, following hierarchy procedures (such as in the WMPT). In addition, as long as the number of false positives does not become unacceptably high, conservative handling of chemicals with no data is acceptable for an SM because it does to some degree help 'catch' possible false negatives.

9) Method should accommodate extreme variability in data availability across chemicals. Davis et al. (1997) pointed out that CRS 'systems must distinguish high-threat chemicals from chemicals with missing data'. This is also important for an SM to avoid bias in the ranking of emissions, as described above in principle 8. However, it should be noted that chemicals with a relatively low toxicity may contribute significantly to the toxicity-related impact potentials in an LCA, because the emitted amounts and the actual context (e.g. no highly toxic chemicals involved) can have a large influence on the outcome. Additionally, the impact potentials of the other impact categories included in the assessment may be low in an actual case study.

10) A tiered approach is practical and desirable. One could state that introducing an SM in an LCIA creates a two tiered approach, i.e. tier 1 comprises selection and tier 2 comprises characterisation. In cases where a lot of chemical emissions have to be ranked it may be practical, time saving and desirable to use a two tiered SM approach with increasing demand on e.g. data amount and quality. In cases where the number of emissions to be ranked is low, tier 1 might be skipped. Another possibility is to include a pre-selection in tier 1, e.g. that emissions of metals are pre-selected for characterisation based on the pre-existence of characterisation factors or high quality data sufficient to carry out a higher tier assessment. None of the existing SMs and the other CRS systems described in this paper are explicitly tiered (excluding CPM as a joint method).

11) Similar effects/exposure categories should be assessed across tiers. To avoid too many false positives and false negatives, the same main effects and exposure categories should be assessed in the SM (including eventually tiers) as in the associated characterisation method. To what degree this needs to be done for an SM depends on the complexity of the associated characterisation method and especially on the consistency, i.e. degree of agreement in prioritization of emissions between the SM and the characterisation method. All three SMs dealt with in this paper (EDIP-selection, Priofactor and CPM-selection) include effect and partly exposure (biodegradation and bioaccumulation), but only the Priofactor includes the emitted amount.

12) Critical information should be preserved. Critical information, e.g. indicators of data quality in scoring for each emission and decisive data for each scoring, may become important when reviewing an LCA study.

13) Data selection guidelines should be specified. Data selection guidelines pointing out acceptable data sources, establishing a hierarchy of data sources, rules for manipulation, etc. are very important in order to avoid bias and errors in the ranking of the emissions. For SMs, at least some degree of consistency with the data sources used for the associated characterisation method is desirable, although the data demand of the SM should be lower in quantity and arguably also in quality. The SMs and the other CRS methods described in this paper include data selection guidelines to varying degrees. The EDIP-selection method points to a single source (i.e. the EU list of dangerous substances) as the main basis. The Priofactor method is not that specific (especially not for ecotoxicity) but points out some quality demands for ecotoxicity data (preferably based on standard OECD tests) and some guidelines for the use of QSARs on BCF. The CPM-selection method is to a lesser degree specific on data selection guidelines than the two other SMs mentioned above. For the two non-selection methods dealt with here, it should be mentioned that the WMPT method is very detailed in defining data sources and a hierarchy of quality. The EURAM method uses IUCLID (IUCLID 2000) as an exclusive data source, given its policy support role and the relevance of this source. Data selection guidelines will probably have to be developed within OMNIITOX for a 'new' SM, and here, the work done by Pedersen et al. (1995) on data selection strategy and quality (only ecotoxicity), and by Larsen et al. (1999a) (both ecotoxicity and human toxicity), and the WMPT approach, could be a good starting point/basis.

14) Method should be theory driven as well as data driven. According to Davis et al. (1997), a CRS method should as the starting point be based on a theoretical logic, which afterwards is meshed with data availability considerations. An SM should be based on a theoretical logic in accordance with the associated characterisation method to the degree necessary to give the required consistency between the ranking of the two methods. But it must be stressed that the consistency on prioritization of emissions and the need for a low data demand of the SM (as compared to the characterisation method) are more important criteria.

15) Sensitivity analysis should be performed. This point is aimed at development of CRS systems in general and is therefore also relevant when developing an SM. Sensitivity analysis may have the strongest priority when dealing with comparison between an SM and its associated characterisation method, e.g. looking for key parameters ('drivers') to minimise this to essential data and trying to find explanations for differences in prioritization of emissions.

16) Pre-selection of chemicals should be consistent with the CRS method. The pre-selection of emissions to be included in the ranking and scoring procedure may result in false negatives if this pre-selection is not well founded. Pre-selection is not included in any of the SMs described here, but, as implicitly in many LCIA applications, the EDIP-selection method includes some kind of 'pre-exclusion' mainly based on common sense (well-founded and based on long experience), e.g. water and $CaCO_3$ are not taken into account as may also be the case implicitly in other CRS methods.

17) The impact of scaling should be considered. Whether the scale used in an SM is ordinal (e.g. 1, 2, 3 …), nominal (e.g. 'yes' or 'no'), interval (e.g. Celsius scale of temperature) or ratio (having true zero point, e.g. Kelvin scale of temperature) is not that important for an SM, as long as the SM is consistent with the associated characterisation method. However, the scaling used and mathematics of combining values to calculate a score may have significant influence on the data demand and the results.

4 Developed Criteria for the Evaluation of SMs

To support the evaluation of the different methods, a set of criteria for performance of an SM is proposed from the above principles. A good SM is one that is:

- Consistent with the associated characterisation method in prioritization/ranking, methodology and substance data requirement
- Transparent, i.e. well-documented and manual calculation is possible
- Applicable to different chemical groups
- Operational with a data requirement that
  - is modest in demand on scope and quality of the substance data
  - comprises data also needed for calculation in characterisation step
  - is focused on data of high availability and with possible prediction, e.g. applying QSARs
- User friendly
  - high practicability – easy in use, preferably with end-user software existing
  - lower time demand as compared to the characterisation method
  - lower requirements to specific scientific skills of the user

A quantitative internal weighting of the criteria is of little relevance in the OMNIITOX project, since the number of existing SMs is very low and it is a stated goal of the OMNIITOX project to develop a new stand-alone SM or an SBM (maybe as a tiered approach) used as a kind of combined SM and simple characterisation method in support of the BM. There is thus no need for identification of the best among existing methods. A ranking of the criteria provides, however, useful guidance for the further development of SMs or simple characterisation methods used to support more advanced ones. The following ranking is recommended:

1. Validity of the method
   a) appropriately prioritizes the chemical emissions which are evaluated as significant in the associated characterisation step (no false negatives)
   b) low in false positives
2. Applicable to different chemical groups, lower in data demand than the characterisation method, and based on data of high availability
3. User friendly and transparent
   a) lower in time demand than the characterisation and easy to use
   b) skilled scientific background not needed, as far as appropriate

5 Evaluation of the Chosen Methods

The three SMs and the other CRS methods are evaluated against the developed criteria. The result of this evaluation is shown in **Table 7**.

Table 7: Results of the evaluation of the SMs and the two other CRS methods

Criteria	EDIP-selection	Priofactor	CPM-selection	EURAM	WMPT
1a. Consistency in prioritization (validity)	+	+++	n.a.	n.r.	n.r.
2a. Applicable to different chemical groups	++++	+	+++	+	++
2b. High data availability	+++	++	++	+	+++
2c. Low data demand	++++	++	++	+	+
2d. Data useable in characterisation	+	+++	+++	n.r.	n.r.
3a. Low in time demand and easy to use	+++	++	++	+	(++)
3b. Skilled scientific background not needed	+++	++	++	+	+

++++: Very high degree of fulfilment
+++: High degree of fulfilment
++: Moderate degree of fulfilment
+: Low degree of fulfilment
n.a.: Not assessed
n.r.: Not relevant

6 Discussion

The Hasse diagram technique and the CART analysis have not been assessed using the developed criteria and are therefore not included in Table 7. This is because these approaches represent frameworks rather than operational methods in an LCA context. Parameters used in these approaches are not predefined and this makes it impossible to apply most of the criteria. It is however possible to assess transparency and user friendliness to some degree, as both methods are well documented and other practical examples do exist. The underlying methodologies and available studies suggest that these approaches may help reduce the data requirements and type compared to the needs of the characterisation methods Once the methods have been applied to develop the SMs, these will typically be straightforward to use. Manual use may be undesirable, but the methods could be implemented in straightforward spreadsheets.

As shown in Table 7, none of the evaluated methods have a very high or even high fulfilment of all criteria. All have weaknesses and strengths. Here we focus on the parts of the different methods that are strong in the sense of performance as an SM. A more detailed analysis of pros and cons can be found in Larsen et al. (2002).

The EDIP-selection method is in principle applicable to all chemical groups as based on R-phrases. This basis also gives rise to high data availability (very high if QSAR calculated data are included – especially for the ecotoxicity part). The methodology is based on a very simple scoring system and it is therefore easy to use, low in time demand and specific scientific skilled background can be considered minimal.

The Priofactor method has a high consistency with the associated characterisation method. In the evaluation example quoted in this paper, it only comes up with a few false positives and a few false negatives. The false negatives only account for below 1% (ecotoxicity) or below 4% (human toxicity) of the total impact, as calculated by the associated characterisation method. The main reason for the high consistency is probably that this SM, to a certain degree, is based on the same methodology and principles as the characterisation method, but makes use of acute data instead of chronic. Some of the (perhaps less significant) key parameters are excluded and the emitted amount is included. The data needed for the Priofactor therefore has a high usability with the associated characterisation method, i.e. the EDIP method.

The CPM-selection method distinguishes between organics and inorganics (primarily metals) and includes special parameters for inorganic chemicals, like covalent bonding and redox sensitivity, which is not seen in any of the other methods described here. This method therefore has a relatively high applicability to different chemical groups. As is the case in all the other methods, amphiphilic and dissociating chemicals are not specifically addressed, i.e. they are treated like any other organic chemical. Similar to the Priofactor, the CPM-selection method uses the same methodology/principles as the associated CPM-characterisation method, but in a more simple way, i.e. acute toxicity data instead of chronic, etc.

For the two evaluated non-SMs, the main feature that distinguishes them from the three evaluated SMs is the way in which the fate part is handled. Both of them apply multimedia fate models, i.e. Mackay level I for EURAM and Mackay level III for WMPT, which have a higher data demand (especially level III) than the more simple key parameter based approaches used in the SMs. However, this may not prove to be a hindrance if QSARs and simple data guidelines are used.

In general, it can be stated that the methods evaluated here are semi-quantitative apart from the Priofactor where the ecotoxicity part must be considered as almost fully quantitative. Only the Priofactor and the EURAM method take the emitted amount into account, and only the CPM-selection method takes the special chemistry of the inorganic compounds into considerations. However, how to account for emitted quantity using the WMPT and similar methods in an LCA context, and also for addressing substances such as metals independently have been demonstrated, see section 2.5.

7 Conclusion, Recommendations and Outlook

In conclusion, it is recommended that the principles on how to develop and to select chemical ranking and scoring systems should be considered when developing the approach for selection (simplified methods, SMs) in LCIA of toxic emissions. In addition, a number of more specific recommendations are presented for developing new SMs:

- emitted amount, as quantified in the inventory results of a specific LCA-study, should be taken into account
- very high data availability for the underlying substance data is a prerequisite (based on e.g. R-phrases, K_{ow} and/or QSARs)
- method should be low in false positives and create no false negatives, or false negatives should only account for an insignificant part of the impact potential as calculated by the associated characterisation method

It is recommended that further work on selection includes a comparison with the use of the characterisation method for selection based on factors calculated with an extensive use of QSAR for estimation of the substance input parameters. Other types of selection approaches should be tested in parallel and, therefore, the following methods (or similar ones) are recommended to be included in the further work:

- EDIP-selection
- Priofactor
- CPM-selection
- EURAM
- WMPT
- Hasse diagram technique
- CART?

The Hasse diagram technique may be used as a 'baseline' CRS method (excluding value choices or subjective rules) when comparing the ranking of the different methods. The CART analysis has only been demonstrated in the context of persistence (fate), but a statistical approach may be beneficial for an SM associated with a coming newly developed OMNIITOX characterisation method (BM) and CART could become relevant in this context.

Experience from application of the few existing SMs is very limited. Of the approaches classified as SMs, only the EDIP-selection method and the Priofactor have been evaluated against the associated characterisation method and only on a single case inventory. In a broader sense, some Chemical Ranking and Scoring (CRS) approaches have been tested against more sophisticated approaches and related insights could prove beneficial.

On the basis of the developed criteria for performance of SMs and the recommended issues to be taken into account when developing new SMs, it is recommended that the research on selection focuses on the following issues:

- Is it possible to use simple data with very high availability (e.g. R-phrases, QSAR calculations) and simultaneously achieve high consistency with the associated characterisation method?
- What are the key parameters for a stand alone SM (e.g. persistence, bioaccumulation, toxicity and emitted amount) to include in an SM and how? Can it be done without subjective/expert choices (e.g. Hasse diagram technique) or are such choices essential?
- Is explicit multimedia fate modelling necessary or, as generally considered, is a simple key parameter approach sufficient to achieve high consistency with the associated characterisation method?
- Will a statistical approach like CART analysis, linear regression or other approaches like mega variate data analysis be appropriate to achieve high consistency with the associated characterisation method?

A framework for developing and evaluating SMs has been presented together with methods which are intended to act as selection methods. No conclusive recommendations are given on which route to follow to derive an SM, but it remains clear that, in order to facilitate inclusion of the toxicity-related impact categories (i.e. ecotoxicity and human toxicity) in LCA studies on a level similar to the well implemented impact categories (e.g. global warming), there is a need for further research on, and experience with use of, selection methods.

Acknowledgement. The authors wish to thank the anonymous reviewer for a well structured and relevant review. The authors also gratefully acknowledge the financial support of the European commission through the 'Sustainable and Competitive Growth'-research programme given to the OMNIITOX project and the financial support from the Danish Ministry of Science Technology and Innovation given to KEMI (Centre for chemicals in industrial production).

Glossary

BCF	BioConcentration Factor
BDF	BioDegradation Factor
BM	Base Model
CART	Classification And Regression Tree analysis
CPM	Competence Centre for Environmental Assessment of Products and Materials Systems
CRS	Chemical Ranking and Scoring
EC_{50}	Effect Concentration (50% of test organism affected)
EDIP	Environmental Design of Industrial Products
EPA	(US) Environmental Protection Agency
EU	European Union
EURAM	EU Risk Ranking Method
HDT	Hasse Diagram Technique
K_d	Soil adsorption coefficient
LC_{50}	Lethal Concentration (50% of test organism dead)
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
$LogK_{ow}$	The logarithm of the Octanol/Water partition coefficient
N.C.	Not Classified
PBT	Persistence, Bioaccumulation and Toxicity
pKa	Dissociation constant for acids (and bases)
QSAR	Quantitative Structure Activity Relationship
R-phrases	Risk phrases
SBM	Simple Base Model
SM	Selection Method
WMPT	Waste Minimization Prioritization Tool

References

Bennett DH, McKone TE, Kastenberg W (2001): CART Screening level analysis of persistence: A case study. In: Lipnick R L, Jansson B, Mackay D, Petreas M (editors) (2001): Persistent, bioaccumulative and toxic chemicals II: Assessment and new chemicals. ACS symposium series 773. Published by American Chemical Society, Washington, DC. ISBN 0-8412-3675-5

Bennett DH, McKone TE, Kastenberg W (2000): Evaluating multimedia persistence: Classification and regression tree analysis. Environ Toxicol Chem 19, 810–819

Brüggemann R, Bücherl C, Pudenz S, Steinberg CEW (1999): Application of the concept of partial order on comparative evaluation of environmental chemicals. Acta hydroch hydrob 27 (3) 170–178

Brüggemann R, Halfon E, Welzl G, Voigt K, Steinberg CEW (2001): Applying the concept of partial ordered sets on the ranking of near-shore sediments by a battery of tests. J Chem Inf Comp Sci 41 (4) 918–925

Bunke D, Gensch C-O, Möller M, Rüdenauer I, Ebinger F, Graulich K (2003): Assessment of Toxicological Risk due to Hazardous Substances: Scoring of Risk Phrases. Int J LCA 8 (1) 6–7

Davis G, Fort D, Hansen BG, Irwin F, Jones B, Jones S, Socha A, Wilson R, Haaf B, Gray G, Hoffman B (1997): Framework for Chemical Ranking and Scoring Systems. Chapter 1 in: Chemical ranking and scoring: Guidelines for relative assessment of chemicals, Swanson M B and Socha A C (eds.), pp. 1–29. SETAC-US. Proceedings from the Pellston workshop on Chemical ranking and scoring, 12–16 February, 1995. Sandestin, Florida

de Koning A, Guinée J, Pennington DW, Sleeswijk A, Hauschild M, Molander S, Nyström B, Pant R, Schowanek D (2002): Methods and typology report Part A: Inventory and classification of LCA characterisation methods for assessing toxic releases. Contribution to Work-package 7 of the OMNIITOX Project as part A of appropriate deliverable D11

EC (1996): Environmental Risk Assessment. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances (ed EC), pp 241–504. Office for Official Publications of the European Communities, Luxembourg

EC (2001): Adapting to technical progress for the 28th time Council Directive 67/548/EEC on the approximation of laws, regulation and administrative provisions relating to the classification, packaging and labelling of dangerous substances (Commission Directive 2001/59/EC, August 6)

EEC (1967): Approximation of laws, regulations and administrative provision relating to the classification, packaging and labelling of dangerous substances (Council Directive 1967/548/EEC, June 27)

Eisenberg JN, McKone TE (1998): Decision tree method for the classification of chemical pollutants: Incorporation of across-chemical variability and within-chemical uncertainty. Environ Sci Technol 32 (21) 3396–3404

Eriksson Å (1999): A comparative study of four models for ecotoxicological impact assessment in LCA – A case study of tyre emissions. Honour thesis in environmental science. Tutor Sverker Molander. June 1999. Göteborgs Universitet, Sweden

Fomsgaard I, Sørensen PB (1999): The Hasse diagram. In: Comparing Environmental Risk indicators for pesticides. Results of the CAPER project. Centre for Agriculture & Environment, The Netherlands. Report CLM 426-1999. ISBN 90-5634-106-5

Guinée JB, de Koning A, Pennington DW, Rosenbaum R, Hauschild M, Olsen SI, Molander S, Bachmann T M, 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

Halfon E, Galassi S, Brüggemann R, Provini A (1996): Selection of priority properties to assess environmental hazard of pesticides. Chemosphere 33 (8) 1543–1562

Hansen BG, Van Haelst AG, Van Leeuwen K, Van der Zandt P (1999): Priority setting for existing chemicals: European Union risk ranking method. Environ Toxicol Chem 18, 772–779

IUCLID (2000): International Uniform Chemical Information Database. Public data on high volume chemicals. (existing chemicals). Year 2000 ed. European Chemicals Bureau. Ispra, Italy

Larsen HF, Birkved M, Hauschild M, Pennington D, Guinée JB (2002): Inventory of LCIA selection methods for assessing toxic releases. Methods and typology report part B. Contribution to Work-package 7 of the OMNIITOX Project as part B of appropriate deliverable D11. EC Project contract G1RD-CT-2001-00501 <http://www.omniitox.net/>

Larsen HF, Christensen FM, Rasmussen JO, Helweg C, Olsen SI (1999b): Screening tool for prioritization of chemicals to be included in a LCA study. Presented at the 9th Annual Meeting of SETAC-Europe, 25–29 May 1999 in Leipzig, Germany. Abstract No. 4c/001

Larsen HF, Christensen FM, Rasmussen JO, Helweg C, Olsen SI (1999a): CETOX-LCA-Handbook, LCA on 'chemical-heavy' products. CETOX, Hørsholm, Denmark

Lerche D, Sørensen PB, Larsen HS, Carlsen L, Nielsen O-J (2002): Comparison of the Combined Monitoring-based and Modelling-based Priority Setting Scheme with Partial Order Theory and Random Linear Extension for Ranking of Chemical Substances. Chemosphere 49 (6) 637–649

Lerche D, Sørensen PB, Brüggemann R (2003): Improved estimation of the ranking probabilities in partial orders using random linear extensions by approximation of the mutual ranking probability. J Chem Inf Comp Sci 43 (5) 1471–1480

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

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

Pedersen F, Tyle H, Niemelä JR, Guttmann B, Lander L, Wedebrand A (1995): Environmental Hazard Classification – Data collection and interpretation guide (2nd edition). TemaNord 1995:581. Nordic Council of Ministers

Pennington DW, Bare JC (2001). Comparison of chemical screening and ranking approaches: The Waste Minimization Prioritization Tool (WMPT) vs. Toxic Equivalency Potentials (TEPs). Risk Analysis 21 (5) 897– 913

Pennington DW, Bare JC, Knodell R, Carroll G, Martin T (2003): Evaluating Pollution Prevention Progress (P2P). Clean Technologies and Environmental Policy, in press

Sørensen PB, Mogensen BB, Gyldenkærne S, Rasmussen AG (1998). Pesticide leaching assessment method for ranking both single substance and scenarios of multiple substance use. Chemosphere 36 (10) 2251–2276

US EPA (1997) Notice of availability of waste minimization software and documents. EPA530-C-97-003, Federal Register, 62:33868

US EPA (1998) Notice of availability of draft RCRA waste minimization PBT chemical list. 530-Z-98-009, Federal Register, 63:216

van de Meent D, Struijs J, Sijm D (2002): Simple recipe for calculating multi-substance toxic pressure as indicator of ecological impact of toxic substances. Presented at the 12th Annual Meeting of SETAC-Europe, 12–16 May 2002 in Vienna, Austria. Abstract No. 65-07

Wenzel H, Hauschild M, Alting L (1997): Environmental Assessment of Products, First edn. Chapman & Hall

Received: October 9th, 2003
Accepted: August 15th, 2004
OnlineFirst: August 16th, 2004

4 Ranking performance of selection methods

This Chapter is a verbatim version of the following paper submitted to the International Journal of LCA:

Larsen HF, Hauschild M (2004). Selection Methods in LCIA: Comparison of Chemical Ranking and Scoring Methods for use as Selection Methods. *Submitted to Int J LCA.*

Selection Methods in LCIA:

Comparison of Chemical Ranking and Scoring Methods for use as Selection Methods

Henrik Fred Larsen*, Michael Hauschild

Department of Manufacturing Engineering and Management, Technical University of Denmark (DTU) Building 424, DK-2800, Lyngby, Denmark. Tel: +45 45 25 48 00. Fax: +45 45 93 55 56

* **Corresponding author** (hfl@ipl.dtu.dk)

Abstract

Goal, Scope and Background. The aim of this study is to test the performance of existing Selection Methods (SMs) and other Chemical Ranking and Scoring (CRS) methods against key property based characterisation methods. The paper presents the comparison of chemical ranking as performed by existing SMs from Life Cycle Impact Assessment (LCIA) (EDIP-selection, Priofactor, CPM-selection) and a risk ranking method (EURAM) with the characterisation factors for ecotoxicity impact calculated by two key property based LCIA characterisation methods (EDIP, CPM). A selection method is a CRS method which is used in LCIA for selecting or prioritizing those chemical emissions from a life cycle inventory, which contribute significantly to the toxicity impact as calculated by the characterisation method to which the selection method is associated.

Methods. The ranking from the included methods is compared and tested against each other for statistically significant differences. The comparison focuses on amphiphilic substances and dissociating substances. In the comparison differences in ranking between the different methods are identified, and causes to the observed differences are analysed. Furthermore, the ability of the relatively simple CRS methods to rank in the same way as the key property based LCIA characterisation method EDIP, which is broadly accepted and used by LCA practitioners, is examined.

Results and Discussion. The results of the comparison show a very good statistical correlation between the ranking of the EDIP method and the other methods and in general a good statistical correlation between all methods tested.

Conclusion and Recommendations. The observed good correlation between the methods is probably due to a common perception of what makes a substance ecotoxicologically problematic which is reflected in the PBT approach (focus on Persistence, Bioaccumulation and Toxicity) included in all tested methods. However, an analysis of outliers in the comparison puts focus on characteristics of the different methods which may cause deviating rankings for substances exhibiting certain combinations of intrinsic properties and hence identifies targets for optimisation.

Outlook. An optimized selection method must be able to handle all substances in an inventory of an LCA. Analysis of non-dissociating/non amphiphilics and inorganic substances should therefore also be included.

Keywords: Amphiphilic substances; chemical ranking and scoring (CRS); dissociating substances; life cycle impact assessment (LCIA); selection methods; simple characterisation methods

Background

Today (2004) few product Life Cycle Assessment (LCA) studies include ecotoxicity and human toxicity in the impact assessment. However, when ecotoxicity and human toxicity are included, it is typically in an incomplete way (Larsen et al. 2004b, Larsen et al. 2004a, Bunke et al. 2003). The reason for this seems to be that in many cases a high number of chemical emissions from the inventory potentially contribute to the toxicity related impact categories and only for a small part of them, characterisation factors are provided by the applied impact assessment method. Therefore, the LCA practitioner has to calculate additional characterisation factors or omit the substances from the impact assessment. This calls for a method, which on a screening level can select/prioritise those chemical emissions that contribute significantly to the toxicity related impact categories. Such a method is called a selection method (SM) (Larsen et al. 2004a, detailed discussion in Larsen et al. 2002). Its overall aim is to focus the more time and data demanding characterisation effort for the toxic impact categories on the most significant chemical emissions in the inventory. Experience from application of the few existing selection methods is very sparse (Larsen et al. 2004a) and the need for research within this area therefore seems urgent. The comparative analysis presented here is focusing on ecotoxicity impacts and substances belonging to the groups of amphiphilics (e.g. surfactants) or dissociating chemicals (acids/bases), i.e. groups of substances with a special combination of intrinsic properties. It addresses the differences and similarities between the ranking obtained by the different methods and in particularly looks into the correlation between the ranking obtained by selection methods and their associated characterisation method with special focus on the EDIP characterisation method.

1 Description of the methods

The methods included in the comparison are schematically described in **Table 1**, and the EDIP-selection and the CPM-selection are for reasons of transparency further described in **Fig. 1** and **Fig. 2** respectively. A full description and a qualitative evaluation of their performance as selection method of all these methods (except EDIP) and of three other methods (Hasse diagram technique, CART and WMPT) can be found in Larsen et al. (2004a) and further detailed in Larsen et al. (2002). The characterisation part of the EDIP method is described in details in Hauschild et al (1998). Only aquatic ecotoxicity is included in this paper.

For the CPM method, a NOEC (No Observed Effect Concentration) value is used as effect parameter but no rules are given in the documentation (Eriksson, 1999) on how to determine a representative NOEC value. Eriksson uses a PNEC (Predicted No Effect Concentration) value based on the lowest NOEC value in combination with the assessment factors from the EDIP characterisation method in the calculations. This approach is also used here.

The comparison is not based on an inventory and data on emitted amounts is hence not included. In their intended use, the EDIP method and the Priofactor take into account the emitted amount of each substance mapped in the inventory. This is also the case with the EURAM method when used in risk ranking. For the other methods included this is not the case. But if emitted amount were included (e.g. just by multiplication) a higher dispersion in their ranking would be achieved.

EDIP-selection score:

Ecotox Impact Score = EXPS · ETS

Exposure score (*EXPS*)

Emission expected	Classified as R53 or R58	*EXPS*
Yes	Yes	8
Yes	No	4
No	Yes	4
No	No	1

R53: May cause long-term adverse effects in the aquatic environment
R58: May cause long-term adverse effects in the environment

Ecotoxicity score (*ETS*)

Criteria	R50 or R50/53	R51/53	R52 or R52/53	N.C.
ETS	4	2	1	0

R50: Very toxic to aquatic organisms
R51: Toxic to aquatic organism
R52: Harmful to aquatic organisms
R53: May cause long-term adverse effects in the aquatic environment
N.C.: Not Classified

Fig. 1: Criteria for the calculation of the EDIP-selection score (Ecotox Impact Score) for a given chemical

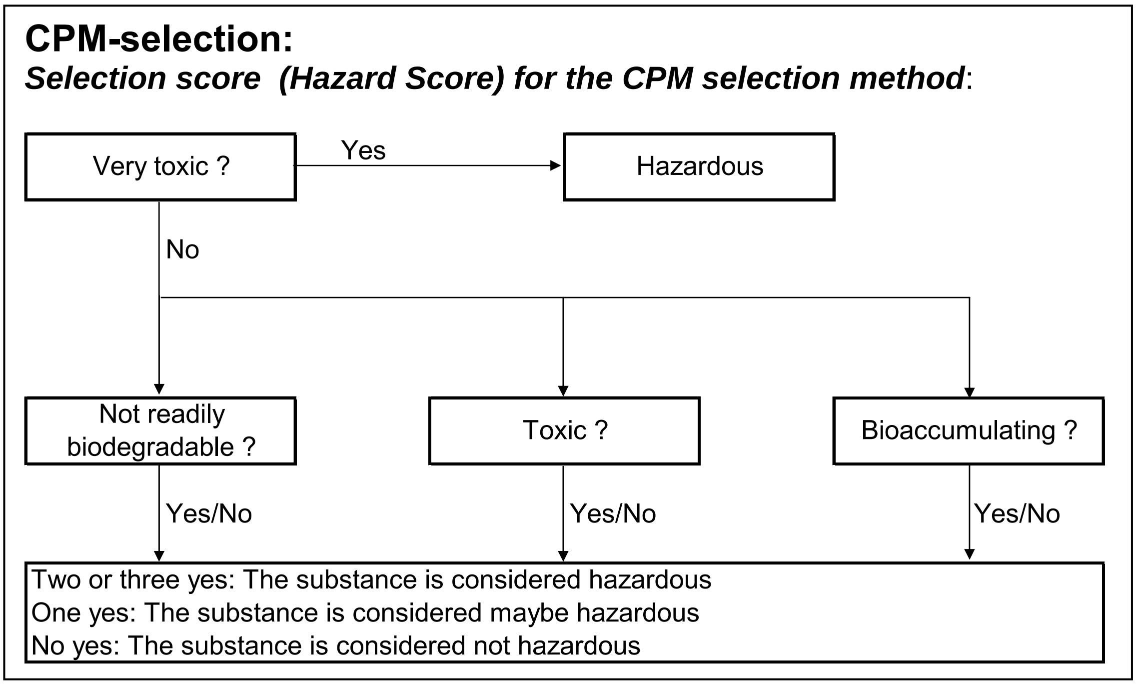

Fig. 2: Decision tree for the CPM-selection Hazard Score (see **Table 1** for further details) for a given chemical

Table 1: Characteristics of the methods

Method	Factor type	Factor name	Mathematical formula	Includes				Range of factor/score
				Effect	Biodegradation	Bioaccumulation	Distribution	
EDIP	Characterisation factor	EF_{etwc} (Equivalency Factor)	$f_{wc} \cdot BIO \cdot logBCF/PNEC_{wc}$	$PNEC_{wc}$ PNEC for chronic effects in water	BIO Ready, inherent or not inherent Range: 0.2; 0.5; 1.0	Log BCF (only included if above 1 and effect is based on acute data as in this case)	Distribution factor (f_{wc}) based on Henry's law constant and $T_{1/2}$ in air Range: 0; 0.2; 1.0	0 → ∞
CPM	Characterisation factor (organics)	IF (Impact Factor)	$LogK_{ow}/(NOEC \cdot DEG)$	NOEC Actually $NOEC_{chronic}$ for water (PNEC used)	DEG Percent ready biodegraded Range: 0.01 - 100	Log K_{ow}	÷	- ∞ → ∞
Priofactor	Selection factor	Ecotox-sub-priofactor	$BDF \cdot BCF/EC_{50}$	EC_{50} Actually $EC_{50(acute)}$ for water	BDF Ready fulfil 10d window, ready not fulfil 10d window, inherent, not inherent Range: 0.1; 0.3; 0.5; 1.0	BCF	÷	0 → ∞
EDIP-selection	Selection score (aquatic)	Ecotox Impact Score	EXPS· ETS	Ecotoxicity score (ETS), see **Fig. 1**. R50; R51; R52 (Risk phrases, based on $EC_{50(acute)}$ for water)	Exposure score (EXPS), see **Fig. 1**. R53 (based on readily biodegradable or not)	Exposure score (EXPS), see **Fig. 1**. R53 (based on bioaccumulative or not)	÷	0; 1; 2; 4; 8; 16; 32
CPM-selection	Selection score (organics)	Hazard Score	See decision tree in **Fig. 2**	Very toxic (EC_{50}<1mg/l) Toxic (EC_{50}<100mg/l) Not toxic (EC_{50}>100mg/l) (all based on $EC_{50(acute)}$)	Ready Yes/no	Bioaccumulative No: BCF<100 or $logK_{ow}$<3 Yes: BCF>=100 or $logK_{ow}$>=100	÷	Not hazardous Maybe hazardous Hazarduos
EURAM	Risk Ranking Score	AS Aquatic Score	$(1.37\ (\log(50 \cdot Dist_{env} \cdot Deg) + 1.301)) \cdot (0.7(-2 \cdot \log PNEC) + AP)$	PNEC PNEC for chronic effects in water	Deg Degradation: Ready, inherent, persistent Range: 0.1; 0.5; 1.0	AP Accumulation Potential values (range: 0; 1; 2; 3) based on cut-off values for logBCF	$Dist_{env}$ Fraction of emitted substance ending up in compartment, in this case water. Based on Mackay level 1 fugacity model and EURAM unit world	0 - 100

2 Description of data used

The 27 substances included in the comparison comprise organic salts, amphiphilics (e.g. surfactants) and organic acids/bases, see **Table 2**. These substances form part of a test set of around 80 different organic (Margni et al. 2002) and inorganic substances (Koning and Guinée 2002) covering all relevant combinations of different substance properties through representatives of different substance groups, i.e. non-dissociating organics, dissociating organics, amphiphilics, metals and other inorganics. This test set has been developed within the EU project OMNIITOX[1] for a structured comparison of characterisation methods and selection methods.

The data on ecotoxicity and chemical/physical properties (i.e. intrinsic properties) for each substance are shown in **Table 1** and **Table 2** in Appendix A. Measured values are preferred but if missing, (Q)SARs on physical/chemical properties (EPIwin 2001, especially for Henry's Law constant and half life in air, $T_{1/2}$) and ecotoxicity (ECOSAR 2001, only one case) are included. Only data on acute ecotoxicity are included.

3 Results

For all included methods factors/scores were calculated for each substance. The resulting factors/scores were ranked and the results are shown in **Table 2**.

With the aim of investigating whether or not it is possible to show any significant differences in the ranking obtained with the different methods, a non-parametric test i.e. the Spearman Rank Correlation Coefficient (Rinaman et al. 1996) was used. The null hypothesis tested was: The methods (tested pair wise) do not rank the tested substances in the same way. As the EDIP-selection method and the CPM selection method only rank in seven (here only four) and three levels respectively (not 27 levels as the others), these two methods were excluded. The result of the correlation test is shown in **Table 3**.

A graphical presentation of the correlation between the ranks of the EDIP method and the three other methods is shown in **Fig. 3**. Outliers which differ with more than 10 in rank are indicated by the name of the substance.

---

[1] **OMNIITOX** is a EU-project under the Competitive and Sustainable Growth-programme, running from 2001 to 2004. OMNIITOX will facilitate decision making regarding potentially hazardous compounds by improving methods and developing information tools necessary for impact assessment of toxic chemicals within LCA and risk assessment. Project partners are Technical University of Denmark; Leiden University, The Netherlands; University of Stuttgart, Germany; École Polytechnique Fédérale de Lausanne (EPFL), Switzerland;
Chalmers University of Technology, Sweden; European Chemicals Bureau, JRC, Ispra, Italy; Volvo Technology Corporation, Sweden; Procter & Gamble EUROCOR, Belgium; Stora Enso AB, Sweden; Antonio Puig, S.A. Spain; Randa Group S.A, Spain. More information about OMNIITOX can be found at www.omniitox.net.

Table 2: Ranks of the 27 substances by the different methods

Substance	**Ranking order for aquatic ecotoxicity impact score or factor**					
	EDIP	**EDIP-selection**	**Priofactor**	**CPM**	**CPM-selection**	**EURAM**
Pentachlorophenol	1	1	1	2	1	2
Hydramethylnon	2	1	7	1	1	18
Carbendazim	3	1	6	3	1	1
Basic Violet 3	4	1	15	4	1	19
Potassium N-methyldithiocarbamate	5	1	17	7	1	5
4,6-Dinitro-o-cresol	6	1	8	6	1	3
2,3,4,6-Tetrachlorophenol	7	1	5	13	1	11
3,6,9,12,15-Pentaoxahentriacontan-1-ol	8	1	3	14	1	7
Endothall, dipotassium salt	9	1	2	8	1	4
Dimethyldioctadecylammonium chloride	10	1	10	5	1	22
Maneb	11	1	12	9	1	8
Zineb	12	1	9	27	1	6
Dalapon	13	19	20	11	1	13
3,6,9,12,15-Pentaoxaheptacosan-1-ol	14	1	11	17	1	10
Decanoic acid	15	1	4	16	1	9
2,4-Dichloro phenol	16	15	16	10	1	12
Glyphosate	17	15	22	15	1	15
4-(1-Pentylheptyl)benzene sulphonic acid	18	15	14	18	1	25
Direct Blue 15	19	20	24	12	1	26
Pyridine	20	20	20	21	21	14
Sodium dodecyl sulphate	21	20	18	19	21	23
4-Nitro phenol	22	20	13	22	1	16
Diethanolamine	23	20	23	25	21	17
N,N-Dimethylaniline	24	15	19	20	21	20
Cyclohexanamine	25	20	25	23	21	21
MCPA sodium salt	26	20	26	26	21	24
4-Nitro benzoic acid	27	20	27	24	27	27

Table 3: Spearman's Rank Correlation Coefficient (R^2) and significance levels in brackets

Method	EDIP	Priofactor	CPM	EURAM
EDIP	1	0.77 (< 0.001)	0.86 (< 0.001)	0.68 (< 0.001)
Priofactor	0.77 (< 0.001)	1	0.56 (< 0.01)	0.71 (< 0.001)
CPM	0.86 (< 0.001)	0.56 (< 0.01)	1	0.43 (< 0.05)
EURAM	0.68 (< 0.001)	0.71 (< 0.001)	0.43 (< 0.05)	1

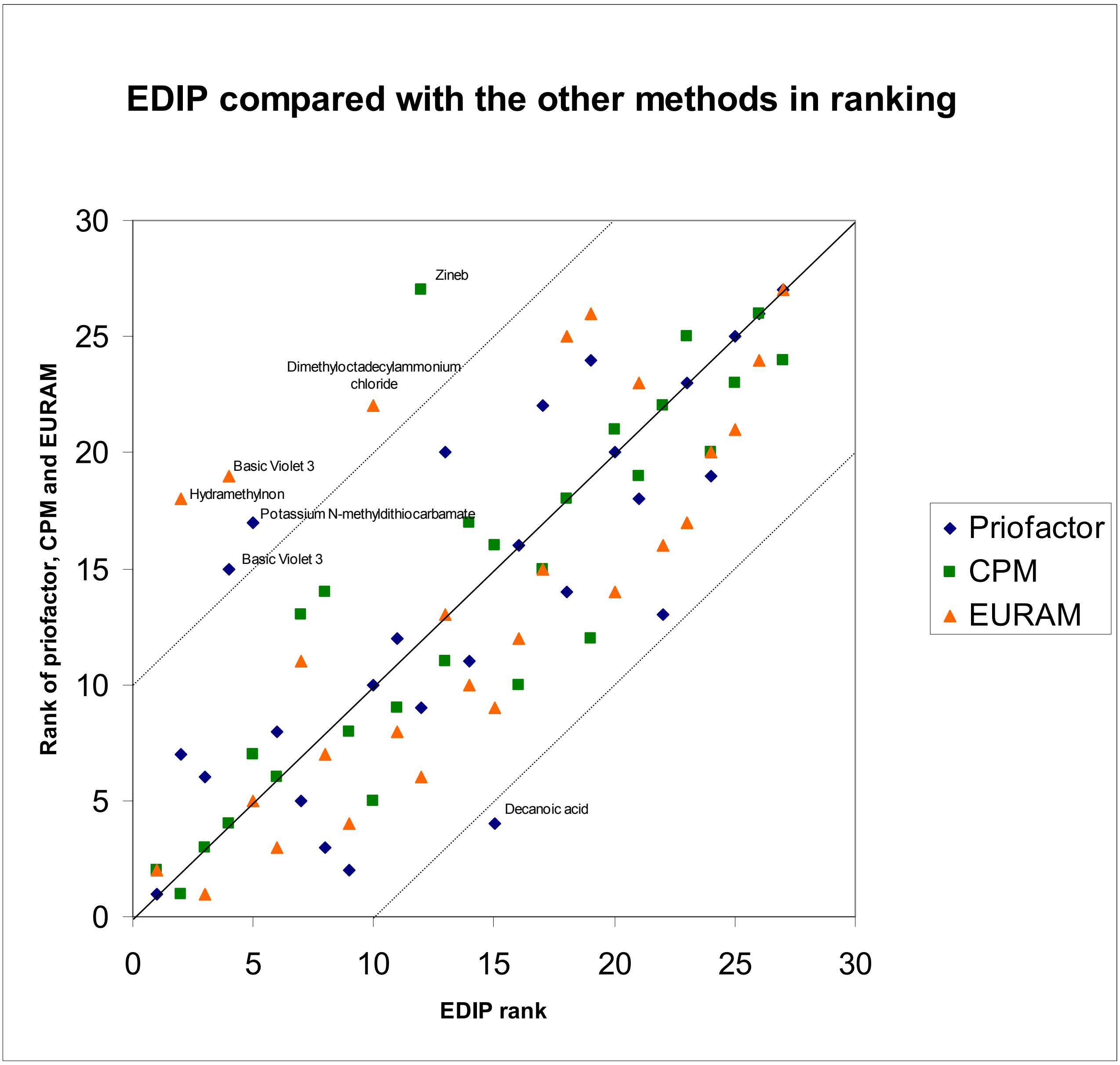

Fig. 3: EDIP ranking of the 27 substances against ranking by the Priofactor, EURAM and CPM method

4 Discussion

As is evident from **Table 2** the EDIP-selection method ranks well in accordance with the associated characterisation method (i.e. the EDIP method). This is reflected by the fact that the 12 substances ranking highest by the EDIP method also are given the highest rank level (i.e. 1) in the EDIP-selection method even though it only ranks substances in four levels in this case. The other selection method associated with the EDIP method, the Priofactor, has the same dispersion as the EDIP method. If we again look at the 12 substances given the highest EDIP rank the Priofactor also ranks these highest except in two cases. The 18 substances given the highest ranking by the CPM method are also given the highest rank by the associated selection method, i.e. the CPM-selection method. But the substance (i.e. zineb) given the lowest CPM rank is given the highest CPM-selection rank and the substance (i.e. 4-nitrophenol) given CPM rank 22 is given the CPM-selection rank 1. So here there is obviously a difference between the ranking of the characterisation method and its associated selection method which is probably due to the fact that the selection method only ranks in three levels.

If we use the EDIP ranking as a reference to prioritise the nine substances (i.e. one third of the total number) with the highest rank, the results in **Table 2** shows that the EDIP-selection and the CPM-selection have no exceptions i.e. potential false negatives and potential false positives when compared to the EDIP ranking. The Priofactor and the CPM method each has two exceptions (i.e. basic violet and potassium N-methyldithiocarbamate, and 2,3,4,6,-tetrachlorophenol and 3,6,9,12,15-pentaoxahentriacontan-1-ol, respectively) and the EURAM methods three exceptions, i.e. hydramethylnon, basic violet and 2,3,4,6-tetrachlorophenol. If we do the same for the nine substances which are given the lowest rank by the EDIP method, we see that the EDIP-selection and the CPM method each has one exception (N,N-dimethylaniline and direct blue 15, respectively) whereas both the CPM-selection and the Priofactor each has two exceptions, i.e. direct blue 15 and 4-nitrophenol, and sodium dodecyl sulphate and 4-nitrophenol, respectively. The CPM method has one exception (direct blue 15) and the EURAM method three exceptions, i.e. pyridine, 4-nitrophenol and diethanolamine.

Despite the differences in ranking by the methods described above it is not possible by using Spearman's Rank Correlation Coefficient to come up with any statistical significant (at the 0.05 level) difference in the ranking obtained by the four tested methods which rank in 27 levels, see **Table 3**. All correlation coefficients are thus significant at the 0.05 level while e.g. the correlations between the EDIP method and both the Priofactor and CPM method are stronger ($\alpha < 0.001$) than the correlation between the CPM method and the EURAM method ($\alpha < 0.05$).

Even though there is good significant correlation between the ranking of the EDIP method and the ranking of the Priofactor, CPM method and EURAM, some substances differ quite a lot in ranking as shown in **Fig. 3**. Those substances where the difference in ranking is more than 10 are analysed and possible reasons behind the observed difference are discussed below.

Basic Violet 3. This substance is given the rank 4 by the EDIP method but 15 by the Priofactor and 19 by EURAM. The main reason for the higher ranking in EDIP compared to the Priofactor ranking is that the PNEC in EDIP is based on one acute EC_{50} (0.1 mg/l, only measured value available) and therefore an application factor of 1000 is used whereas the Priofactor just uses the EC_{50} value directly. So in this case the difference is due to low data availability on acute ecotoxicity effects leading to the use of a high overall acute (laboratory level) to chronic (ecosystem level) ratio or application factor. The reason for the very high difference in ranking between the EDIP and the EURAM method is not related to the effect part (the same PNEC is used in both cases). The main reason here is caused by differences in factors for distribution. As it is assumed that the substance is emitted to water - combined with the fact that it does not evaporate from water (i.e. Henry's law constant very low, <1.0E-08 atm·m^3/mol) - the EDIP method assigns a distribution factor (f_{wc}) of 1 meaning that the full ecotoxicity impact of the substance is elicited in water. The Mackay level 1 distribution model used in EURAM does not take into account to which compartment the substance is emitted. Due to this fact combined with a high soil adsorption coefficient for the substance (i.e. 82000 l/kg) the EURAM method assign a distribution coefficient ($Dist_{env}$) of 0.01 to Basic Violet 3, meaning that only 1% of the substance is present in water and the rest is present in soil. So in this case it makes a large difference for the ranking whether or not the ranking method takes mode of entry into account.

Hydramethylnon. This substance is given the rank 2 by the EDIP method but rank 18 by the EURAM method. As for Basic Violet 3 the reason is also that the EURAM method does not take mode of entry into account.

Dimethyloctadecylammoniumchlorid. In this case the substance is given the rank 10 by the EDIP method but rank 22 by the EURAM method. As for Basic Violet 3 and hydramethylnon, again the main reason for the difference is whether or not the ranking method takes mode of entry into account. For this substance there is, however, also another difference which compensates somewhat for the 'mode of entry effect' as compared to Basic Violet 3 and hydramethylnon. Since the ecotoxicity effect assessment in this case is based on one (i.e. 0.1 mg/l) out of three acute EC_{50} values, the EDIP method uses an application factor of 100 whereas the EURAM method uses a more conservative factor of 1000. So differences in the application factors used do play a minor compensating role in this case.

Zineb. Zineb is given the rank 12 by the EDIP method but the CPM method assigns it the rank 27. Even though the substance is rather toxic (PNEC=0.0097 mg/l) and not ready biodegradable it gets the lowest CPM rank because its $\log K_{ow}$ value is negative, i.e. -0.39. Hence, the higher the toxicity, the lower the rank for substances with a negative $\log K_{ow}$. This characteristic of the CPM method (see the expression for the CPM score in **Table 1**) is especially a problem for substances which have a specific toxic mode of action (and hence typically a high toxicity), and which are at the same time relatively water soluble and hence have negative $\log K_{ow}$ values. This combination of properties is observed for a pesticide like zineb being a fungicide of the dithiocarbamate type.

Potassium N-methyldithiocarbamate. This fungicide is given the rank 5 by the EDIP method but 17 by the Priofactor. The main reason for the higher ranking in EDIP as compared to the Priofactor is that the PNEC in EDIP is based on lowest acute EC_{50} (i.e. 0.18 mg/l) among two values (no measured or QSAR value available for algae), and therefore an application factor of 1000 is used, whereas the Priofactor just uses the lowest EC_{50} value directly. As demonstrated for Basic Violet 3, the difference is due to low data availability on acute ecotoxicity effects leading to the use of a high application factor.

Decanoic acid. This fatty acid is given the rank 15 by the EDIP method but ranks as number 4 in the Priofactor. The underlying cause of this difference is found in the ways the two methods deal with bioaccumulation. For decanoic acid no measured BCF has been available and the measured $\log K_{ow} = 4.1$ is used for both the EDIP and the Priofactor estimations. The EDIP method prefers measured BCF values and if not available best (Q)SAR or alternatively $\log BCF = \log K_{ow} - 1$. In this case the EPIwin suite QSAR (BCFWIN) is used because it takes into account whether or not the substance is ionic (pKa for decanoic acid is 4.9 so more than 99% is dissociated at pH=7). The EPIwin estimated BCF equals 3. The Priofactor also prefers measured BCF values but if not available QSARs described in the TGD (EC 1996) which do not take dissociation into account are recommended for this method. The BCF estimated by the QSARs from the TGD equals about 600. So there is a factor of (600/3)=200 in difference between the BCF values used in the two methods. Even if the same BCF value was used in both cases there would still be differences in ranking by the two methods because the Priofactor puts a higher weight on bioaccumulation (multiplication by BCF, i.e. linear scale) than the EDIP method (multiplication by the logarithm to BCF, i.e. log-scale). Hence, the higher the BCF, the higher the difference will be between the ranking of the EDIP method and Priofactor if all other factors are kept the same.

5 Conclusion

The results indicate that for the special substance groups amphiphilics and dissociating substances, there is a good correlation between the ranking of the characterisation method EDIP and its associated selection methods, the EDIP-selection and the Priofactor. Yet, a larger dispersion among the scores of the substances in the EDIP-selection would be desirable (e.g. by multiplying with emitted amount) in order to differentiate better between emissions to include and emissions to exclude in the characterisation step. The correlation between the simpler characterisation method CPM and its associated selection method, i.e. CPM-selection is also good for the highest CPM ranks but not so good for the lowest ranking substances. As for the EDIP-selection, a larger dispersion of the CPM-selection scores is desirable. When comparing the ranking of the EDIP method with the ranking of the Priofactor, CPM and EURAM, a good statistical significant correlation ($\alpha<0.001$) was found in all cases. These results indicate that even though CPM and EURAM have not been designed to act as selection methods for the EDIP, a common perception of what makes a substance ecotoxicologically problematic underlies all three methods. This is also revealed in the expressions of the three methods which all include similar combinations of biodegradability (or persistence), bioaccumulation potential and toxicity (PBT). Nevertheless, some outliers have been identified, and through analysis of these, characteristics of the individual methods have been identified which for certain combinations of substance properties may result in false negatives or false positives as compared to EDIP. These characteristics include:

- the influence of data availability on size of application factors for conversion of acute effect data to chronic values
- whether or not mode of entry is taken care of in the fate modelling
- reversing of the effect of toxicity on ranking by negative $\log K_{ow}$ values when $\log K_{ow}$ is a direct factor in the expression
- the way BCF is estimated and included in the calculation of the factor

6 Further research

An optimized selection method must be able to handle all substances in the LCA inventory. Analysis of non-dissociating/non amphiphilics and inorganic substances should therefore be also included. Furthermore, the selection method should be calibrated against the specific characterisation method, which it is supposed to work with. Further work on selection methods for use in LCIA is still ongoing (July 2004) in the OMNIITOX project.

Acknowledgement

The authors gratefully acknowledge the financial support of the European commission through the Sustainable and Competitive Growth -research program given to the OMNIITOX -project and the financial support from the Danish Ministry of Science, Technology and Innovation given to KEMI (Centre for chemicals in industrial production).

References

Bunke D, Gensch C-O, Möller M, Rüdenauer I, Ebinger F, Graulich K (2003): Assessment of Toxicological Risk due to Hazardous Substances: Scoring of Risk Phrases. Int J LCA 8 (1), 6-7

CERI (2003): Chemical Evaluation and Research Institute (CERI), Japan 1-4-25 Koraku Bunkyo-ku Tokyo112-0004. http://qsar.cerij.or.jp/cgi-bin/DEGACC/index.cgi?e

ChemFate (2002): ChemFate Database. First published 1983. Syracuse Research Corporation 301 Plainfield Road, Suite 350 Syracuse, New York 13212-2510. http://esc.syrres.com/efdb/Chemfate.htm

de Koning A , Guinée J B (2002): Selection of metals and inorganics for the test set of substances. Contribution to Work-package 7 of the OMNIITOX Project. EC Project contract G1RD-CT-2001-00501. Institute of Environmental Science, Leiden University (internal report)

EC (1996): Environmental Risk Assessment. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances (ed EC), pp. 241-504. Office for Official Publications of the European Communities, Luxembourg

EEC (1967): Approximation of laws, regulations and administrative provision relating to the classification, packaging and labelling of dangerous substances (Council Directive 1967/548/EEC, June 27)

ECOSAR (2001): ECOSAR classes for Microsoft Windows. ECOSAR v.0.99g. US-EPA. USA, April 2001. www.epa.gov/oppt/

ECOTOX (2002): ECOTOXicology Database system. US EPA. http://www.epa.gov/ecotox/

EPIwin (2001): EPIwin suite v3.10. United States Environmental Protection Agency Office of Pollution Prevention and Toxics (OPPTS) 1200 Pennsylvania Avenue, NW Mail Code 7401M Washington, DC 20460. http://www.epa.gov/opptintr/exposure/docs/epiwin.htm

Eriksson Å (1999): A comparative study of four models for ecotoxicological impact assessment in LCA – a case study of tyre emissions. Honour thesis in environmental science. Tutor Sverker Molander. June 1999. Göteborgs Universitet, Sweden

Hauschild M, Wenzel H, Damborg A, Tørsløv J (1998): Ecotoxicity as a criterion in the environmental assessment of products. In: Hauschild M, Wenzel H (eds): Environmental Assessment of Products: Volume 2: Scientific background, pp. 203-314. Chapman & Hall

Howard P H (1991): Handbook of environmental fate and exposure data for organic chemicals Vol. III. Lewis Publishers. ISBN: 0-87371-328-1

HSDB (2003): HSDB on TOXNET, U.S. National Library of Medicine and National Institute of Health. http//toxnet.nlm.nih.gov/

IUCLID (2000): European Chemical Bureau (2000): IUCLID CD-ROM Year 2000 edition. Public data on high volume chemicals. ISBN 92-828-8641-7

Larsen H F, Birkved M, Hauschild M, Pennington D, Guinée J B (2004a): Evaluation of selection methods for toxicological impacts in LCA. Recommendations for OMNIITOX. *Int J LCA 9(5), 307-319*

Larsen H F, Hansen M S, Hauschild M (2004b): Ecolabelling of printed matter. Part II: Life cycle assessment of model sheet fed offset printed matter. *Environmental Project No. ?* (in press). Ministry of Environment and Energy, Denmark. Danish Environmental Protection Agency

Larsen H F, Birkved M, Hauschild M, Pennington D, Guinée J B (2002): Inventory of LCIA selection methods for assessing toxic releases. Methods and typology report part B. Contribution to Work-package 7 of the OMNIITOX Project as part B of appropriate deliverable D11. EC Project contract G1RD-CT-2001-00501

Mackay D, Ma K-C, Shiu W Y (2000): Physical-Chemical Properties and Environmental Fate Handbook. CRC press. ISBN: 0849321921

Madsen T, Boyd H B, Nylén D, Pedersen A R, Pedersen G I, Simonsen F (2001). Environmental and Health Assessment of Substances in Household Detergents and Cosmetic Detergents Products. Environmental Project No. 615, 2001. Danish Environmental Protection Agency. http://www.mst.dk/

Margni M, Pennington D, Birkved M, Larsen H F, Hauschild M (2002): Test set of organic chemicals for LCIA characterisation method comparison. Contribution to Work-package 7 of the OMNIITOX Project. DRAFT September 2002. EC Project contract G1RD-CT-2001-00501 (internal report)

N-CLASS (2003). N-CLASS Database. Physical/chemical, health and environmental effect classification for substances placed on Annex I of Council Directive 67/548/EEC (on the classification, packaging and labelling of dangerous substances) Database administrator: J. Falck, KemI. The present database is a web version of the N-CLASS Database that earlier were issued in TemaNord 1999:538. The Nordic Council of Ministers. www.kemi.se/nclass

Pagga U, Brown D (1986): The degradation of dyestuffs. Part II. Behaviour of dyestuffs in aerobic biodegradation tests. Chemosphere 15 (4), 479-491

OECD (1993): Guidelines for testing of chemicals. http://www.oecd.org

PhysProp (2002): PhysProp Database. First published 1993. Syracuse Research Corporation 301 Plainfield Road, Suite 350 Syracuse, New York 13212-2510. http://esc.syrres.com/interkow/physdemo

Rinaman C W, Heil C, Strauss M T, Mascagni M, Sousa M (1996): Probability and Statistics. Chapter 7 in Standard Mathematical Tables and Formulae. Editors: Zwillinger D (chief), Krantz S G, Rosen K H. 30 ed. CRC

SciFinder (2001). SciFinder Scholar 2001. Chemical Abstract Service 2540 Olentangy Road P.O. Box 3012 Columbus, Ohio 43210 United States of America

Swanson M B, Socha A C (1997): Executive Summary in: Chemical ranking and scoring: Guidelines for relative assessment of chemicals, Swanson M B and Socha A C (eds.), pp. xix - xxv. SETAC-US. Proceedings from the Pellston workshop on Chemical ranking and scoring, 12-16 February, 1995. Sandestin, Florida

Glossary and definitions

Acronyms

BCF	Bioconcentration factor
BDF	BioDegradation Factor. Criteria based on OECD test No. 301 and 302 (OECD 1993), see **Table 1**
BIO	BIOdegradation. Criteria based on OECD test No. 301 and 302 (OECD 1993), see **Table 1**
CART	Classification And Regression Tree analysis
CPM	Competence Centre for Environmental Assessment of Products and Materials Systems
CRS	Chemical Ranking and Scoring
DEG	DEGradation: Percent ready biodegraded as defined by OECD test No. 301 (OECD 1993)
Deg	Degradation. Criteria based on OECD test No. 301 and 302 (OECD 1993), see **Table 1**
dw	Dry weight
EC_{50}	Effect Concentration (50% of test organism affected)
EDIP	Environmental Design of Industrial Products
EURAM	EU Risk Ranking Method
K_d	Soil adsorption coefficient
K_{oc}	Adsorption coefficient for organic carbon
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
$LogK_{ow}$	The logarithm of the Octanol/Water partition coefficient
N.C.	Not Classified
NOEC	No Observed Effect Concentration
OMNIITOX	Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments
pK_a	Dissociation constant for acids (and bases)
PNEC	Predicted No Effect Concentration
(Q)SAR	(Quantitative) Structure Activity Relationship
R-phrases	Risk phrases
SM	Selection Method
$T_{1/2}$	Half-life
WMPT	Waste Minimization Prioritization Tool

Definitions

Selection method	A method to select (prioritise) those emissions (chemicals) from the inventory of a specific LCA-study that are most likely to contribute - according to a specific characterisation method - significantly to the impact categories on ecotoxicity and human toxicity.
CRS-method	A Chemical Ranking and Scoring (CRS) method can be described as “a tool for assessing chemicals by considering health effects, environmental effects or other hazards, persistence, and exposure. Chemical ranking and scoring either produces a relative ranking of chemicals or assigns chemicals to specific groups or categories” (Swanson and Socha 1997).
Characterisation method	A method or model used to derive characterisation factors.

Appendix A. Data on test set

Table 1: Data on test set: Type, acute ecotoxicity and assigned R-phrases (values in *italics* are estimated)

Name	CAS No.	Type	Lowest EC_{50} acute among algae(A), fish (F) and crustacean (C) (mg/l)	Assigned R-phrases
Direct Blue 15	2429-74-5	Organic salt	*46* [a] (A,F,C)	N.C., N.C.[b]
Endothall, dipotassium salt	2164-07-0	Organic salt	0.14 [c] (A,F,C)	R50, R53 [d]
Basic Violet 3	548-62-9	Organic salt	0.1 [e] (A,F,C)	R50, R53 [b]
MCPA sodium salt	3653-48-3	Organic salt	230 [c] (A,F,C)	N.C., N.C.[b]
Maneb	12427-38-2	Organic salt	0.32 [e] (A,F,C)	R50, R53 [b]
Potassium N-methyldithiocarbamate	137-41-7	Organic salt	0.18 [e] (F,C)	R50, R53 [d]
Zineb	12122-67-7	Organic salt	0.97 [e] (A,F,C)	R50, R53 [b]
Sodium dodecyl sulphate	151-21-3	Amphiphilic	1.8 [f] (A,F,C)	N.C., N.C.[d]
4-(1-Pentylheptyl)benzene sulphonic acid	23003-92-1	Amphiphilic	0.9 [f] (A,F,C)	R50, N.C.[d]
3,6,9,12,15-Pentaoxaheptacosan-1-ol	3055-95-6	Amphiphilic	0.46 [f] (A,F,C)	R50, R53 [d]
3,6,9,12,15-Pentaoxahentriacontan-1-ol	4478-97-1	Amphiphilic	0.05 [f] (A,F,C)	R50, R53 [d]
Dimethyldioctadecylammonium chloride	107-64-2	Amphiphilic	0.1 [g] (A,F,C)	R50, R53 [b]
4-Nitro benzoic acid	62-23-7	Organic acid/base	500 [g] (A,F,C)	N.C., N.C.[d]
4-Nitro phenol	100-02-7	Organic acid/base	4.7 [g] (A,F,C)	N.C., N.C.[b]
Dalapon	75-99-0	Organic acid/base	11 [e] (F,C)	R52, R53 [b]
Pentachlorophenol	87-86-5	Organic acid/base	0.018 [e] (A,F,C)	R50, R53 [b]
2,4-Dichloro phenol	120-83-2	Organic acid/base	2 [g] (A,F,C)	R51, R53 [b]
Decanoic acid	334-48-5	Organic acid/base	0.3 [g] (A,F,C)	R50, R53 [d]
4,6-Dinitro-o-cresol	534-52-1	Organic acid/base	0.066 [e] (A,F,C)	R50, R53 [b]
2,3,4,6-Tetrachlorophenol	58-90-2	Organic acid/base	0.14 [e] (A,F,C)	R50, R53 [b]
Diethanolamine	111-42-2	Organic acid/base	2.2 [e] (A,F,C)	N.C., N.C.[b]
Hydramethylnon	67485-29-4	Organic acid/base	0.07 [e] (F,C)	R50, R53 [d]
N,N-Dimethylaniline	121-69-7	Organic acid/base	5 [g] (A,F,C)	R51, R53 [b]
Pyridine	110-86-1	Organic acid/base	1.1 [e] (A,F,C)	N.C., N.C.[b]
Cyclohexanamine	108-91-8	Organic acid/base	20 [g] (A,F,C)	N.C., N.C.[b]
Carbendazim	10605-21-7	Organic acid/base	0.007 [e] (A,F,C)	R50, R53 [b]
Glyphosate	1071-83-6	Organic acid/base	1.3 [e] (A,F,C)	R51, R53 [b]

N.C.: No Classification

[a] ECOSAR (2001)

[b] N-CLASS (2003)

[c] HSDB (2003)

[d] Evaluated by the authors according to the criteria defined in EU Council Directive 67/548/EEC (EEC, 1967) including its amendments

[e] ECOTOX (2002)

[f] Madsen et al. (2001)

[g] IUCLID (2000)

Table 2: Data on testset: Biodegradation, bioaccumulation and physical/chemical data (values in *italics* are estimated)

Name	Biodegradability	BCF	LogK_{ow}	Henry's law constant (atm·m^3/mol)	$T_{1/2}$ in air (days)	pKa	K_{oc}[a] (l/kg dw)
Direct Blue 15	Not inherent [b]	*3* [p]	*0.71* [c]	< *1.0E-08* [d]	*0.32* [e]	-	*2.0E+09* [f]
Endothall, dipotassium salt	*Not ready* [g]	*3* [p]	*1.9* [h]	< *1.0E-08* [d]	*0.53* [e]	-	*10* [f]
Basic Violet 3	*Not ready* [g]	*3* [p]	0.51 [c]	< *1.0E-08* [d]	*0.024* [e]	-	*4.1E+06* [f]
MCPA sodium salt	*Not ready* [g]	1[i]	*-1.3* [c]	< *1.0E-08* [d]	*1.1* [e]	-	*29* [f]
Maneb	*Not ready* [g]	10 [i]	*0.62* [c]	< *1.0E-08* [d]	*0.050* [e]	-	*550* [j]
Potassium N-methyldithiocarbamate	*Not ready* [g]	*3* [p]	*0.48* [h]	*3.1E-07* [d]	*0.11* [e]	-	*4.0* [f]
Zineb	*Not ready* [g]	170 [k]	*-0.39* [h]	< *1.0E-08* [d]	*0.073* [e]	-	*10* [f]
Sodium dodecyl sulphate	Ready [l]	7 [l]	1.6 [l]	< *1.0E-08* [d]	*0.72* [e]	-	*10000* [f]
4-(1-Pentylheptyl)benzene sulphonic acid	Ready [m]	32 [m]	*2.5* [n]	< *1.0E-08* [d]	*0.65* [e]	-	*16000* [f]
3,6,9,12,15-Pentaoxaheptacosan-1-ol	Ready [m]	120 [m]	*3.6* [n]	< *1.0E-08* [d]	*0.12* [e]	-	*10* [f]
3,6,9,12,15-Pentaoxahentriacontan-1-ol	Ready [m]	390 [m]	*5.7* [n]	< *1.0E-08* [d]	*0.11* [e]	-	*18* [f]
Dimethyldioctadecylammonium chloride	Not ready [l] Inherent [l]	23 [c]	*3.8* [c]	< *1.0E-08* [d]	*0.16* [e]	-	*1.0E+10* [f]
4-Nitro benzoic acid	Ready [l]	*3* [p]	1.9 [l]	< *1.0E-08* [d]	*18* [e]	3.4 [c]	*17* [f]
4-Nitro phenol	Ready [l]	280 [l]	2.0 [l]	4.2E-10 [c]	*2.5* [e]	7.1 [j]	*310* [f]
Dalapon	*Not ready* [g]	3 [o]	0.76 [j]	*2.5E-07* [d]	*19* [e]	1.7 [o]	*2.3* [j]
Pentachlorophenol	Not ready [l]	780 [o]	5.2 [o]	2.5E-08 [c]	*19* [e]	4.7 [o]	1300 [j]
2,4-Dichloro phenol	Not ready [l] Inherent [l]	38 [l]	3.0 [l]	*5.5E-06* [d]	10 [c]	4.5 [l]	350 [l]
Decanoic acid	Ready [l]	*3* [p]	4.1 [l]	*1.3E-06* [d]	*0.96* [e]	4.9 [c]	*87* [f]
4,6-Dinitro-o-cresol	*Not ready* [g]	*37* [o]	2.1 [o]	1.4E-06 [c]	*35* [e]	4.3 [o]	260 [j]
2,3,4,6-Tetrachlorophenol	Not ready [q]	60 [q]	4.5 [c]	*8.8E-06* [d]	*39* [e]	5.2 [c]	6600 [j]
Diethanolamine	Ready [l]	*0.05* [j]	-2.2 [l]	< *1.0E-08* [d]	*0.12* [e]	9.0 [j]	*4.0* [j]
Hydramethylnon	*Not ready* [g]	*12* [p]	2.3 [c]	< *1.0E-08* [d]	*0.079* [e]	-	*6.3E+08* [f]
N,N-Dimethylaniline	Ready [l]	12 [l]	2.3 [c]	*7.7E-05* [d]	0.072 [c]	5.2 [c]	*77* [f]
Pyridine	Ready [j]	*3* [p]	0.63 [o]	1.1E-05 [c]	29 [c]	5.2 [c]	5 [j]
Cyclohexanamine	Ready [l]	*2* [p]	1.2 [l]	4.2E-06 [c]	*0.19* [e]	10.6 [j]	*40* [f]
Carbendazim	Not ready [q]	2.1 [q]	1.5 [o]	< *1.0E-08* [d]	*0.053* [e]	4.2 [o]	220 [j]
Glyphosate	*Not ready* [g] Inherent [l]	0.63 [l]	0.002 [l]	< *1.0E-08* [d]	*0.14* [e]	2.3 [o]	2600 [j]

[a] K_d (soil) estimated as 0.02*K_{oc}

[b] Pagga and Brown (1986)

[c] PhysProp (2002)

[d] HENRYWIN v3.10 and/or VP/WSol (EPIwin 2001)

[e] AopWin v1.90 (EPIwin 2001)

[f] PCKOCWIN v1.66 (EPIwin 2001)

[g] BIOWIN v4.00 (EPIwin 2001)

[h] KOWWIN v1.66 (EPIwin 2001)

[i] HSDB (2003)

[j] ChemFate (2002)

[k] Howard (1991)

[l] IUCLID (2000)

[m] Madsen et al. (2001)

[n] SciFinder (2001)

[o] Mackay et al. (2000)

[p] BCFWIN v2.14 (EPIwin 2001)

[q] CERI (2003)

5 Ecotoxicity effect indicators

This Chapter is a verbatim version of the following paper submitted to the International Journal of LCA:

Larsen HF, Hauschild M (2004). Evaluation of ecotoxicity effect indicators for use in LCIA. *Submitted to Int J LCA.*

Evaluation of ecotoxicity effect indicators for use in LCIA

Henrik Fred Larsen[*]**, Michael Hauschild**
Department of Manufacturing Engineering and Management, Technical University of Denmark (DTU) Building 424, DK-2800, Lyngby, Denmark
* **Corresponding author** (hfl@ipl.dtu.dk)

Abstract

Goal, Scope and Background. The paper describes different ecotoxicity effect indicator methods/approaches. The approaches cover three main groups, viz. PNEC approaches, PAF approaches and damage approaches. Ecotoxicity effect indicators used in life cycle impact assessment (LCIA) are typically modelled to the level of impact indicating the potential impact on 'ecosystem health'. Existing indicators modelled all the way to damage are poorly developed and even though relevant alternatives from risk assessment exist (e.g. recovery time and mean extinction time) these are unfortunately at a very early development stage and only few attempts have been made to include them in LCIA.

Methods. The approaches are described and evaluated against a set of performance criteria.

Results and Discussion. The results of the evaluation of the two impact approaches (i.e. PNEC and PAF) show both pros and cons for both of them. The assessment factor-based PNEC approach has a low data demand and uses only the lowest value (e.g. lowest NOEC value). Because it is founded in tiered risk assessment, and hence making use of conservative assessment factors, it is not optimal, in its present form, to use in the comparative framework of LCIA seeking best estimates. The PAF approaches have a higher data demand but use all data and can be based on effect data (PNEC is no-effect-based) making them non-conservative and more suitable for LCIA. However, indiscriminate use of effect data is probably making the PAF-approaches no more environmentally relevant than the assessment factor-based PNEC approach but the PAF approaches can at least in theory be linked to damage modelling. All approaches for damage modelling included here, except for the 'media recovery' depending directly on the exposure model, have a high environmental relevance but very low data availability. They are all at a very early stage of development.

Conclusion, Recommendations and Outlook. An analysis of the different PAF approaches shows that the crucial point is, according to which principles and on which data, the hazardous concentration to 50% of the included species (i.e. HC50) is estimated. The ability to estimate many characterisation factors on ecotoxicity is important if the ecotoxicity impact category is to be included in LCIA in a proper way. However, the number of effect data which is available for the relevant chemicals, is typically low. So, besides the coupling to damage modelling, the main challenge within the further development and improvement of ecotoxicity effect indicators is to find an optimal method to estimate HC50 based on few data.

Keywords: Damage approaches; ecotoxicity effect indicators; hazardous concentration (HC50); life cycle impact assessment (LCIA); PAF approaches; PNEC approaches

Introduction

The purpose of this paper is to present a qualitative review of existing methods of ecotoxicity assessment. The analysis also includes a review of possible damage models. The work described has been done as part of the OMNIITOX[2] project. It

---

[2] **OMNIITOX** is an EU-project under the Competitive and Sustainable Growth Programme, running from 2001 to 2004. OMNIITOX will facilitate decision making regarding potentially hazardous compounds by improving methods and developing information tools necessary for impact assessment of toxic chemicals within LCA and risk assessment. Project partners are Technical University of Denmark; Leiden University, The Netherlands; University of Stuttgart, Germany; École Polytechnique Fédérale de Lausanne (EPFL), Switzerland; Chalmers University of Technology,

includes an inventory of existing and some proposed ecotoxicity effect indicator methods/approaches for use in life cycle impact assessment (LCIA). An ecotoxicity effect indicator (EEI) is here defined as the 'effect part' of a characterisation factor for ecotoxicity. For example a characterisation factor (CF) for 1 kg emitted of a given chemical can be expressed as the effect indicator (e.g. EEI = 1/PNEC) multiplied by the 'fate part' (dC) as shown in equation 1. A synonym for the effect indicator is effect factor as used by Pennington et al. (2004). The included approaches are described and evaluated against performance criteria, and recommendation on improvements and further development are outlined.

The methods used for EEIs within both risk assessment and LCIA fall into two main approaches.

- Assessment Factor (AF) based approaches (Predicted No Effect Concentration, PNEC approaches)
- Species Sensitivity Distribution (SSD) based approaches (Potentially Affected Fraction of species, PAF approaches)

In LCIA the PNEC approaches are modelled to the level of impact on the ecosystem, i.e. a midpoint in the environmental mechanism or impact chain (ISO 2000, Udo de Haes and Lindeijer 2002). For one of the PAF approaches, i.e. the marginal PAF increase approach in Eco-indicator 99 (Goedkoop and Spriensma 2001a, 2001b), attempts have been made to model all the way to damage or endpoint in the form of the Potentially Disappeared Fraction of species (PDF of species), here designated as Potentially Vanished Fraction of species (PVF) to avoid confusion with Probability Distribution Function (PDF) used later on in this paper. Further, the AMI method (based on the average PAF increase approach) links to damage on the same basis as the Eco-indicator 99 method but uses a different general conversion factor from PAF to PVF (Jolliet et al. 2003).

Even though attempts are done to model all the way to damage by use of general conversion factors, the existing methods typically calculate a midpoint indicator used to indicate potential impact on ecosystems or potential impact on 'ecosystem health'. Although, as stated by Calow (1998), "we are not yet able to define general criteria of 'ecosystem health'", the biological diversity (i.e. species diversity) is here considered as a measure of 'ecosystem health'. Pratt and Cairns (1996) states that "the relationship between diversity and ecological 'stability' remains elusive" but "predictions and empirical evidence suggest that species richness is a useful measure of biological diversity that responds predictably to a number of stressors".

To be able to transform a midpoint or impact indicator into an endpoint or damage indicator (expressing the results in terms of changes in biodiversity), a damage model is required. For damage models, the following three potential approaches are identified.

- Recovery time approach
- Species extinction approach (Mean Extinction Time, MET)
- Changes in genetic diversity

These approaches are all at an early stage of development.

Sweden; European Chemicals Bureau, JRC, Ispra, Italy; Volvo Technology Corporation, Sweden; Procter & Gamble EUROCOR, Belgium; Stora Enso AB, Sweden; Antonio Puig, S.A. Spain; Randa Group S.A, Spain. More information about OMNIITOX can be found at www.omniitox.net.

1 PNEC-based impact approaches

At present the PNEC approach making use of assessment factors is used in many of the existing LCIA methods, e.g. USES-LCA (Huijbregts et al. 2000) and EDIP (Hauschild et al. 1998). It is also the recommended approach in generic risk assessment according to the Technical Guidance Document (TGD) on risk assessment from the European Commission (EC 2003a).

The ecotoxicity potential of an emission, i.e. the characterisation factor multiplied by the emitted amount, can be expressed in different ways as illustrated by the USES-LCA method (ecotoxicity potential expressed as an emission of a reference substance, dichlorobenzene) and the EDIP method (ecotoxicity potential expressed as a dilution volume).

Sub-approaches that can be identified under the PNEC approach include:

- PNEC-based solely on acute ecotoxicity data (EC_{50}s)
- PNEC-based on chronic ecotoxicity data if possible (No Observed Effect Concentrations, NOECs)
- PNEC-based on $HC5_{NOEC}$ from SSDs

Even though PNEC is based on acute data in many estimations (because of data lack), chronic data is typically preferred when available. The PNEC approach based on an $HC5_{NOEC}$ value overlaps with the PAF approaches because the PNEC value in this case is estimated as the hazardous concentration to 5% of included species ($HC5_{NOEC}$), i.e. the concentration where the NOEC value is exceeded for 5% of the species in the SSD (van Straalen and van Leeuwen 2002). Actually, the PNEC-based Dutch Environmental Quality Criteria (EQC) are estimated in this way (de Bruijn et al. 1999) as well as the PNEC in the USES-LCA method (Huijbregts 2001) when sufficient data are available, i.e. at least 4 NOEC values according to de Bruijn et al. (1999).

Within LCIA a characterisation factor (CF) for ecotoxicity can be expressed as the change in the ecotoxicity effect indicator (EEI) due to a change in the environmental concentration (dC) for every kilogram emitted of a certain substance. When the effect indicator is derived from an assessment factor-based PNEC approach, the expression becomes:

$$\mathrm{CF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{1}{\mathrm{PNEC}} \cdot \mathrm{dC}\ , \tag{1}$$

and if PNEC is SSD based (i.e. PNEC = $HC5_{NOEC}$) then

$$\mathrm{CF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{1}{\mathrm{HC5_{NOEC}}} \cdot \mathrm{dC} \tag{2}$$

An example of an $HC5_{NOEC}$ is shown in **Fig. 1**.

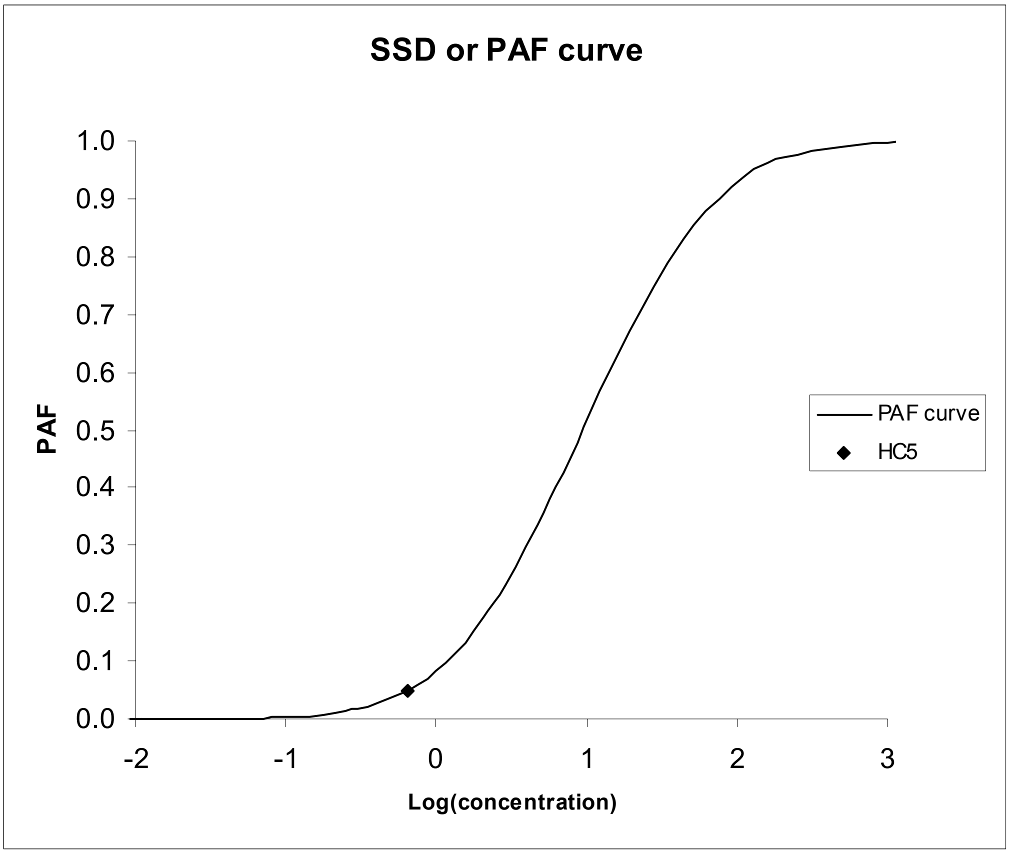

Fig. 1: Example of a species sensitivity distribution (SSD) curve or PAF curve illustrating the relationship between the environmental concentration of a toxicant and PAF, i.e. the cumulative probability of exceeding e.g. NOECs for a certain fraction of species in the community/ecosystem in question. The concentration at which the fraction p of species are having their NOEC exceeded is denoted the hazardous concentration at level p, i.e. HCp. The concentration (in this example $10^{-0.19}$), at which 5% (PAF=0.05) of the species are having their NOEC exceeded, is denoted $HC5_{NOEC}$.

2 PAF-based impact approaches

The Potentially Affected Fraction of species (PAF) can be defined as the fraction of species in an (generic) ecosystem/community that is expected to be (potentially) affected above its no-effect level (e.g. NOEC or a predefined level, e.g. EC_{50}) at a given environmental concentration of a toxicant or other stressor (adopted from Traas et al. (2002)).

The PAF approach is based on the principles of Species Sensitivity Distribution (SSD) which is a statistical distribution describing the variation among a set of species in toxicity of a certain substance or mixture, see Fig. 1. This distribution can be based on different distribution functions (e.g. lognormal or log-logistic, both based on parametric statistics) and on different data, e.g. NOECs or EC_{50}s (Posthuma et al. 2002a). As an alternative, it is possible to avoid the assumption of any distribution function by using non-parametric statistics, i.e. the median combined with e.g. bootstrap technique for confidence limits (Newman et al. 2002).

The SSD approach or PAF approach is used or proposed used in the following identified ways in LCIA:

- Multi substance PAF (msPAF) or combi-PAF approach
- ‘Marginal PAF increase’ approach (tangential or marginal gradient)

- ‘Average PAF increase’ approach, HC5 (secantial or average gradient)
- ‘Average PAF increase’ approach, HC50 (secantial or average gradient)

The different PAF approaches are described in Section 2.1 and in more detail in Appendix A.

2.1 Marginal PAF increase approach

The multi substance PAF (msPAF) method is within LCIA used as part of the ‘marginal PAF increase approach’ in the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b) and in this case called combi-PAF.

The main principles in the msPAF method are the following: For each of the substances or toxicants in the data set in question, a single substance PAF is calculated, see Appendix A, Section A1. Instead of using the concentration units (e.g. µg/l) for the NOEC values (we assume that it is a NOEC-based SSD) these are scaled to dimensionless hazard units (HU) by dividing each NOEC value by the median (actually the geometric mean, GM) of the NOEC values, done set by set for each toxicant. We hereby achieve that 1 HU is equal to a concentration where the NOEC is exceeded for 50% of all species tested for all included toxicants. If we then want to estimate the potentially affected fraction of species due to a mixture exposure (we know the environmental concentration of each toxicant) we have to scale each concentration to HU in the same way as the NOEC values. If all the toxicants in the mixture have the same Toxic Mode of Action (TMoA), e.g. narcotic, we can use the principles of Concentration Addition (CA) and just add the number of HU. But if different TMoA are involved we have to use the more complicated procedure for Response Addition (RA), see Appendix A, Section A2. Huijbregts et al. (2002) and Pennington et al. (2004) have described how to use RA in connection with the ‘marginal PAF increase’ approach and the ‘average PAF increase’ approach respectively.

In the ‘marginal PAF increase’ approach, the EEI is expressed as the marginal increase in the msPAF of the community/ecosystem SSD in question, due to exposure from an emitted toxicant. The aim is to express the potential impact from an emitted toxicant by the marginal increase in the number of species having their NOEC values exceeded taking the background impact (i.e. the number of species already having their NOEC exceeded) into account, see Fig. A3 in Appendix A. Based on investigations in The Netherlands comprising background concentrations of toxicants and SSDs for different compartments, the Eco-indicator 99 (Goedkoop and Spriensma 2001a, 2001b) sets up a general msPAF curve called combiPAF assuming that effects from all toxicants can be considered as concentration additive (CA). As shown by Huijbregts et al. (2002) this assumption can give an error higher than a factor 100 on the characterisation factor, mainly due to differences in TMoA and thereby differences in the scale parameter value (β) for the individual PAF curves, see Appendix A. As the estimated average background impact level in The Netherlands is 22% (i.e. 22% of the species having their NOEC exceeded) the point on the msPAF-curve corresponding to msPAF = 0.22 is chosen as the working point (Goedkoop and Spriensma 2001a, 2001b). When calculating the marginal increase in msPAF (i.e. dmsPAF) due to a marginal increase in the environmental concentration, the slope (i.e. slope factor γ) of the tangent to the working point is used. At the working point msPAF = 22% this slope factor amounts to 0.59. This gives the following general equation:

$$\mathrm{CF} = \mathrm{dmsPAF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{\gamma}{\mathrm{HC50}_{\mathrm{NOEC}}} \cdot \mathrm{dC} \qquad (3)$$

If γ is equal to 0.59 then:

$$CF = \frac{0.59}{HC50_{NOEC}} \cdot dC \qquad (4)$$

$HC50_{NOEC}$ is in this case the geometric mean (GM) of the single substance SSD values (i.e. NOECs) of the substance in question.

The reason for dividing by HC50 in equation 3 and 4, and the following equations on CF, is that the increase in concentration (dC) must be expressed in HUs on which the slope is defined, see Fig. A3 in Appendix A.

2.2 'Average PAF increase' approaches

2.2.1 HC5-based approach

Instead of using a tangential gradient, as in the 'marginal PAF increase' approach, Pennington et al. (2004) argue for using a secant gradient ('average PAF increase' approach) especially at low exposure concentrations (below HC5) where the shape of the PAF curve becomes very uncertain and dependent on the distribution model chosen. The secant or average gradient is a linear gradient between the origin (of the PAF curve) and a chosen working point on the curve corresponding to for example PAF = 0.05, assuming that the background impact level is below PAF = 0.05. The general characterisation factor equation for this approach is:

$$CF = dPAF = EEI \cdot dC = \frac{0.05}{(HC5/HC50)/HC50} \cdot dC \qquad (5)$$

As shown by Pennington et al. (2004) the factor (HC50/HC5) may be expressed as $10^{2.94\beta}$ (where β is the scale parameter) leading to the following general equation:

$$CF = \frac{0.05 \cdot 10^{2.94 \cdot \beta}}{HC50} \cdot dC \qquad (6)$$

2.2.2. $HC50_{EC50}$-based approach

As recently proposed as best available practice in LCA by Pennington et al. (2004), and as implemented in the method for Assessment of the Mean Impact on ecosystems, AMI (Payet and Jolliet 2003, Payet et al. 2003), PAF = 0.5 may be used as working point for the average gradient (see example in Fig. A3 in Appendix A). In the AMI method, two statistical estimators have been explored for the assessment of the average toxicity of chemicals. A non parametric estimator, using the median as the $HC50_{EC50}$ value combined with bootstrap statistics for the estimate of its uncertainty (Payet and Jolliet 2003), and an estimator based on the assumption of lognormal distribution of data using the GM as $HC50_{EC50}$ and the student's t-statistics for its confidence interval (Payet et al. 2003). In this case the PAF curve is based on EC_{50} values for chronic toxicity (instead of NOEC values as in e.g. the Eco-indicator 99 method). Background impact level is assumed not to be relevant in probably almost all cases. For the average PAF increase approach based on $HC50_{EC50}$ the general characterisation factor equation is:

$$CF = dPAF = EEI \cdot dC = \frac{0.5}{HC50_{EC50}} \cdot dC \qquad (7)$$

3 Damage approaches

The description below, of the three damage approaches, is based on Payet and Larsen (2004).

3.1 Recovery time approach

Of the damage approaches, the 'recovery time approach' used as 'media recovery' is actually used in the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b) and the IMPACT 2002+ method (using AMI) (Jolliet et al. 2003) when estimating the potentially vanished fraction of species (PVF).

The media recovery model is based on the assumption that the media quality is linked directly to the biodiversity. Species are considered as disappeared as soon as the toxicant concentration in the ecosystem reaches a certain level, and considered as reappeared when the toxicant disappears by e.g. degradation. This model is thus directly linked to the fate modelling. This is the easiest way to link the PAF and the PVF and it is based on two rough assumptions:

- The assumption of the equivalence time between disappearance and recolonization of species. This requires at least some knowledge about the life history of species which is not available for most of the species present in the environment.
- The assumption of the equivalent diversity before and after the toxic impact. This assumption would not be valid for a large scale assessment where the reduction of populations would lead to an important genetic drift and therefore a reduction of genetic diversity.

These working assumptions have not been tested yet, and the models are currently at research level.

Nevertheless, these models may be linked to the PAF-based impact approaches because PVF may be expressed as a function of PAF depending on the toxicant concentration on one hand and the time of exposure on the other hand. Both the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b) and the AMI method (Jolliet et al. 2003) express the results of ecotoxicological impact in PAF units. In order to translate the result into an endpoint indicator, Eco-indicator 99 assumes a factor 10 of increase in concentration of exposure to express the result in PVF instead of PAF. This factor of 10 is necessary since NOEC values are used for building the msPAF curve. The AMI method uses the same basis but considers the fraction of affected species based on chronic EC_{50} values instead of the NOECs, and therefore a factor 2 instead of 10 is applied for translating the PAF to PVF, thus inherently assuming that half of the species exposed above their EC_{50} level will become extinct. However, the factor is disputable since other works assume that a 50% effect on for example reproduction will always result in extinction of the population after a hundred years of exposure (Snell and Serra 2000).

3.2 Time to extinction approach

The environmental threats should not cause immediate extinction of a population but shorten the expected time to extinction (Hakoyama and Iwasa 2000). Based on stochastic population models, some models, like the Mean Extinction Time (MET), have been developed to quantify the expected survival of species exposed to a habitat size reduction or an environmental pollution (Lande 1998). Among the consequences of a toxicant effect is a reduction in the growth rate of the population. The estimation of this decrease can be translated into a MET risk, corresponding to the decrement of the intrinsic growth rate which can be assessed with a mathematical model (Tanaka and Nakanishi 2000). These models may include both the normal environmental fluctuation in population growth rate and the random catastrophes. The required parameters for this sort of models are generally:

- Reproduction rate, based on the life history of the organisms

- Carrying capacity of the media, which is used to assess the initial population size

Only one attempt has yet been done to include these models in LCIA (Itsubo et al. 2003).

3.3 Genetic diversity

Instead of using biodiversity as basis for the endpoint/damage modelling, use of genetic diversity could be a good alternative solving some of the problems with diversity within species contra diversity between species and the problem with vulnerability of species after repeated exposure to toxicants. Facilitating the interpretation of the changes in genetic diversity, a model has recently been presented, linking the phenotypic diversity and the ecosystems' functioning. This model could provide a way to translate the changes in genetic diversity (which is directly linked with the phenotypical variance reduction) in terms of modification of ecosystems' functioning (Norberg et al. 2001). The strength of the study is to focus on the functional group of species as the basic unit of ecosystems, looking at its sensitivity to the changes in diversity. Multispecies models are reduced to three equations that represent the total biomass in the community, the average phenotype, and the phenotypic variance. This model has the strengths of linking the evolutionary dynamic to the ecosystem functioning (Tilman 2001), and of expressing the results in terms of quantitative change in biomass production in the ecosystems. Such a model is promising, but the data are not available enabling the computation of the reduction in biomass production due to the average phenotype and the reduction in phenotypic variance resulting from toxic pressure.

4 Assessment criteria

The different approaches are evaluated against the following criteria, which are mainly based on Hauschild and Pennington (2002):

Scientific validity: This is based on whether the method/approach including its assumptions and interpretation is generally accepted in the relevant international scientific community, and the modelling assumptions compatible with the methodological requirements of LCA.

Environmental relevance: The indicator can be more or less relevant for the effect we want to indicate, i.e. effects on (an) ecosystem(s). As an example an indicator only taking one acute value (e.g. LC50) into account is less environmental relevant than an indicator taking chronic data on several taxa from three trophic levels in to account. It should be possible to interpret the result in terms of either impact (midpoint) or damage (endpoint) depending on how far the indicator is modelled along the environmental mechanism.

Reproducibility: To what extent will the method, its description and interpretation allow different practitioners to come up with the same substance-specific indicators considering also the variability of the input data.

Data demand: The number and kind of data needed for calculating the indicator is crucial for how easy it actually is to produce indicators (e.g. difficult accessible data will demand more time) and for the number of chemicals for which the calculation is possible (no relevant data, no indicator).

Data availability: If the data needed for the method has a low availability, only a limited number of indicators can actually be calculated.

Quantification of uncertainty: Is it possible to calculate/estimate the uncertainty of the indicators calculated by the method? Knowing the uncertainty will give an indication of the reliability of the result.

Transparency: For the method to be generally accepted and understood by the user it is important that it is transparent. It should not be too complex but explainable to the practitioner. It should be well-documented and manual calculation possible.

Spatial differentiation: To what degree is it possible to include spatial differentiation for a given approach?

5 Results

The result of the evaluation of the PNEC- and PAF-based approaches are shown in **Table 1** and for the damage approaches in **Table 2**.

Table 1: Assessment of PNEC- and PAF-based approaches

Criteria	PNEC-based approaches				PAF-based approaches		
	AF-based PNEC (only acute data)	**AF-based PNEC (only chronic data)**	**AF- based PNEC (chronic (preferred) and acute data)**	**SSD-based PNEC ($HC5_{NOEC}$)**	**Marginal PAF increase (fixed β value)**	**Average PAF increase, HC5 (fixed β value)**	**Average PAF increase, HC50**
Scientific validity	++	+	++	++	+++	+	++
Environmental relevance	+	+++	++(+)	+++	+++	+++	+++
Reproducibility	++	+(+)	+(+)	++	++(+)	++	+++
Transparency	++++	++++	+++(+)	++	+(+)	++	+(+)
Low data demand	++++	++++	+++(+)	++	+	++	++
High data availability	++++	++	++++	+(+)	+	+	+(+)
Spatial differentiation possible	+	+(+)	+(+)	++	+++	++ [a]	+(+)
Quantification of uncertainty included	+	+	+	++ [c]	+ [c]	+ [c]	++++ [b]

++++: Very high degree of fulfilment
+++: High degree of fulfilment
++: Moderate degree of fulfilment
+: Low degree of fulfilment

a: β not fixed
b: Implemented in AMI (Payet et al. 2003)
c: Not implemented but possible

Table 2: Assessment of damage approaches

Criteria	Recovery time [a]	Mean extinction time	Genetic diversity
Scientific validity	+(+)	+	+
Environmental relevance	++(+)	+++(+)	++++
Reproducibility	++	(+)	(+)
Transparency	+(+)	+	(+)
Low data demand	++	+	(+)
High data availability	++	+	(+)
Spatial differentiation possible	n.a.	n.a.	n.a.
Quantification of uncertainty included	n.a.	n.a.	n.a.

++++: Very high degree of fulfilment
+++: High degree of fulfilment
++: Moderate degree of fulfilment

+: Low degree of fulfilment
n.a.: Not assessed
a: As media recovery

6 Discussion

6.1 AF-based PNEC approaches

A general problem when using the AF-based PNEC approach (see equation 1) in LCIA is that it was created as a tool for risk assessment, which typically is a tiered procedure making use of conservative estimates. For the sake of comparison we seek best estimates in LCIA and the use of conservative assessment factors can result in high bias on the ecotoxicity effect indicators. Furthermore, the PNEC approach is based on the lowest ecotoxicity value and therefore sensitive to the database used if not all available data (i.e. all data sources) are included.

The main problem when using an AF-based PNEC approach based only on acute data is that it has a low environmental relevance. Besides local situations with high exposure, the only kind of effects that we can expect to occur in the "real" ecosystems are chronic. LCA typically deals with chronic exposure while the available ecotoxicity data mostly are acute data. If we try to solve this problem by extrapolating acute data to chronic data (typically by applying a factor of 10) we face a problem with different kinds of TMoA within and between different kinds of chemicals and interspecies differences resulting in different acute to chronic ratios (ACRs). These may be up to a factor 500 if based on acute and chronic average toxicity over species (de Zwart 2002) and if based on single species in the range of 0.79 - 5,500 (Forbes and Calow 2002). The inclusion of chronic data may therefore improve the environmental relevance significantly.

The AF-based PNEC approach based solely on chronic data to some degree solves the problem with lack of environmental relevance of the approach based only on acute data. But in this case we run in to the problem that the number of chemicals with sufficient chronic data is very limited. For about 1000 to 1500 chemicals only chronic data are available whereas acute data are available for about 6000 to 10000 chemicals (rough estimates based on de Zwart (2002), Allanou et al. (1999), data availability in ECOTOX (2002) and more). If EU's REACH system for registration and reporting of data on chemicals (EC 2003b) is implemented in the coming years, the number of chemicals where ecotoxicity data become available will probably increase significantly but primarily due to a higher number of acute data.

By combining the two above mentioned approaches in an AF-based PNEC approach were chronic data is preferred (the way it is typically done today) we still have problems related to extrapolation from acute to chronic and environmental relevance in the cases were we are forced to use acute data. In addition, we acquire a problem with biased ecotoxicity indicators because some are based on acute data (far from the PNEC endpoint and with high uncertainty) and others on chronic data (close to the endpoint and with less uncertainty). This is especially a problem if conservative extrapolations factors are used, and this is typically the case today.

The SSD-based PNEC approach (see equation 2) has the potential of being more environmentally relevant than the AF-based approaches because all available chronic data are exploited instead of a single one (the lowest) as in the AF-based approaches. But if the data used do not represent the ecosystem we want to relate our estimates to (i.e. based on haphazard ecotoxicity data with no relevance for the trophic structure etc.) and/or if assessment factors are used anyway to estimate chronic values from acute ones, this approach is most probably not more environmentally relevant than the AF-based PNEC approaches. Another problem with the SSD-based PNEC approach as compared to the AF-based approaches, is that the data demand is higher on chronic data where the availability is low. At least 4 NOEC values (de Bruijn et al. 1999) or to have a stable result more than 10 NOEC values (van Straalen and van Leeuwen 2002) are needed to derive $HC5_{NOEC}$, as opposed to 2 – 3 NOEC values for obtaining the lowest AF in the AF approaches including chronic data (e.g. Hauschild et al. 1998, EC 2003a). The higher data demand for $HC5_{NOEC}$ is reflected in the generic risk assessment recommendations in the EU TGD (EC 2003a) stating that if $HC5_{NOEC}$ is used for estimating PNEC, at least 10 NOEC values are needed covering at least 8 different taxonomic groups. The estimation procedure of the SSD-based PNEC approach is less transparent than that of the

AF-based approach, but quantification of uncertainty can be included, if it is tested or assumed that the data fits the distribution function used.

6.2 PAF-based approaches

All the PAF-based approaches are making use of the SSD framework and are therefore associated with its advantages and drawbacks. Two general problems are mentioned above i.e. the haphazard use of ecotoxicity data and the high demand on data of low availability. Another problem is that for maybe around 50% of the chemicals with available data, the SSD does not follow the parametric distribution functions typically used i.e. lognormal (Newman et al. 2002). The non-parametric version of the AMI method (Payet and Jolliet 2003) avoids the last mentioned problem by using a distribution-free non-parametric SSD method making use of the median and bootstrap technique for calculating confidence limits. Advantages of the PAF approaches are that inclusion of mixtures are possible and that modelling to endpoint (damage) seems at least theoretically possible. If spatial differentiation is considered, the inclusion of the species sensitivity may also be of some advantage as compared to the AF-based PNEC approach. The marginal PAF increase approach (see equation 3) seems most powerful in spatial differentiation because of the possibility to define the spatially differentiated background level by choosing different working points on the msPAF curve, see Fig. A3 in Appendix A.

Because the marginal PAF increase approach includes background impact level, it has a huge data demand on background concentration of toxicants and background PAFs (to define the working point) in order to create the multi substance PAF curve (i.e. determine the β value), if it is going to cover more than just the Netherlands. When the msPAF curve is created, the data demand is reduced to at least 4 NOEC values for each chemical (Goedkoop and Spriensma 2001a, 2001b). This data demand of 4 NOEC values on each chemical is only met for a maximum of 200 chemicals (de Zwart 2002). In the eco-indicator 99 method making use of this approach it has only been possible to calculate ecotoxicity effect indicators for about 40 substances (Goedkoop and Spriensma 2001a, 2001b). However, the fact that this approach includes background impact and that it at least in theory is possible to estimate the impact level for different places (countries, habitats e.g. forests, agricultural land etc.) makes this approach more relevant for spatial differentiation than the others.

The average PAF increase approach with working point at HC5 (see equation 5) has a lower data demand than the marginal PAF increase approach for the creation of the msPAF curve because it does not include background impact (i.e. it is assumed that the background impact is below PAF=0.05). For estimation of the ecotoxicity effect indicator on each chemical, the data demand is the same as for the marginal approach, if we assume that a fixed β value is used and that the msPAF curve is NOEC-based. The fact that the β value is dependent on the TMoA may cause more than a factor 100 error in the estimated effect indicator in both the marginal PAF increase approach (Huijbregts et al. 2002) and the average PAF increase approach based on $HC5_{NOEC}$ (Pennington et al. 2004) if a fixed β value is used. If it is not accepted to use a fixed β value and an exact one is not known, the $HC5_{NOEC}$ value has to be determined (see equation 5) in the average PAF increase approach based on $HC5_{NOEC}$. In this case the data demand becomes the one needed to determine the $HC5_{NOEC}$, i.e. at least 10 NOECs to have a stable result as described above.

The average PAF increase approach based on $HC50_{EC50}$ (equation 7) is not dependent on a β value because it is assumed that the increase in PAF, due to an increase in the concentration of the toxicant, can be described by an average linear gradient starting from (1, 0.5) and having a slope of 0.5 on a standardised PAF curve showing the concentration of the toxicant on the X-axis in hazard units (HUs), see Fig. A3 in Appendix A. As compared to an average gradient based on HC5, taking variation on β values into account, the uncertainty of assuming an average gradient based on HC50 is below a factor 10 for most chemicals as shown by Pennington et al. (2004). This estimation is based on an interval of 0.2 – 0.7 for acute β values covering the main part of the 89 chemicals tested by de Zwart (2002). However, at least 17 of the tested chemicals have acute β values above 0.7. Furthermore, the range of the chronic β values is higher, with at least 19 chemicals having chronic β values above 0.7 and at least 7 having chronic β values below 0.2. Actually, the observed range in chronic β values by de Zwart (2002) is 0.02 – 1.65 but extreme values (at least above 1.25) are to be considered as artefacts due to a very poor data foundation, i.e. typically only 3 – 10 species tested, and not the 25 – 50 needed to reach a stabilized β value (de Zwart 2002).

The $HC50_{EC50}$ -based average PAF increase approach is implemented in the AMI method (Payet and Jolliet 2003, Payet et al. 2003). In this case chronic EC_{50} values are used instead of chronic NOEC values as typically used in PAF approaches. In this way a general problem with that NOEC values is avoided, i.e. the problem that a NOEC value is determined as the highest measured value which is not statistically different from a control value in a laboratory test. The determined NOEC value is therefore dependent on the test design used (e.g. the concentrations that were actually tested), and as a consequence not necessarily just below the lowest concentration where the chronic effect actually occurs for the organism tested. Contrary to all the other approaches on EEIs, the AMI method includes quantification of uncertainty. The non-parametric version of the AMI method (Payet and Jolliet 2003), using the median for estimating $HC50_{EC50}$, needs as a minimum 5 chronic EC_{50}s for the bootstrap technique to estimate confidence limits. Procedures for estimating the median-based $HC50_{EC50}$ and the confidence limits on only three acute data (representing three taxonomic groups) are described but based on assessment factors. As an alternative to the non-parametric version, the parametric version of AMI (Payet et al. 2003), assuming lognormality of data and using the geometric mean for estimating $HC50_{EC50}$, can be applied with minimum three different EC50s from 3 different taxonomic groups and both acute and chronic data may be used. The AMI method suffers from the general low availability of chronic data, and the use of assessment factors (acute to chronic) is needed. Furthermore, confidence limits based on only three data values typically becomes quite wide making the statistically differentiation between substances impossible. The fact that most chronic data are expressed as NOEC values creates the need for a ‘new’ kind of assessment factors to be used when estimating chronic EC_{50} values from NOEC values. Finally, it should be noticed that the use of the geometric mean of the EC50s improves the stability of the indicator regarding the species tested and makes it less sensitive to differences in the actual ecotoxicity data used (e.g. data from different databases). Hereby the reproducibility is improved.

6.3 Damage-based approaches

All the three approaches for damage modelling (see Table 2), except for the ‘media recovery’ depending directly on the fate model, have a high environmental relevance but very low data availability. They are all at a very early research stage, especially the approach on genetic diversity. Despite this fact, the recovery time approach used as media recovery has been used in some attempts to include damage modelling in the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b), and most recently in the AMI method (Jolliet et al. 2003). The damage approaches are further evaluated in Payet and Larsen (2004).

7 Conclusion and recommendations

Based on the evaluation described, different directions for improvement and further development of existing approaches, and development of new ones, exist. There seems to be at least three main directions to go:

- Improving the assessment factor-based PNEC approach making it less risk assessment based and more suitable for LCIA. The goal will be produce non-conservative assessment factors including uncertainty (confidence limits) and if possible taking toxic mode of action into account. However, the problem with stability of the indicator depending on the choice of the database still remains.

- Improving the chemical coverage and the environmental relevance of the 'PAF related' approaches. The main problem here seems to be data lack and that the way this approach has been used till now does not reflect effects on the ecosystem in a more accurate way than the assessment factor-based PNEC approach. The goal will be to make procedures for a more environmentally relevant application (e.g. more realistic, not haphazard representation of species on each trophic level). There is also a need to improve the chemical coverage by fitting the approach to a low data availability, and further to utilize, improve and develop the inclusion of mixtures and damage modelling.
- Further development of the 'media recovery 'damage approach or development of new damage-based indicator based on the 'time to extinction' approach or 'changes in genetic diversity'.

For Damage modelling, the 'media recovery' approach seems to be the most realistic way to go if a method is to be functional for LCIA within the near future. This approach can be coupled with the PAF approaches but needs further development on e.g. the connection between media recovery and recovery/recolonization of species populations. Taking into account that the two other damage approaches are at an even earlier development stage than the 'media recovery' model, and that the availability of the needed data is very poor, it is probably not realistic to reach practical useable methods based on these approaches in the near future. However, from a theoretical point of view, the approaches based on mean extinction time and genetic diversity are very attractive and further dealt with in Payet and Larsen (2004).

For the assessment factor-based PNEC approaches the main problem is that they are founded in tiered risk assessment and therefore conservative, which is not compatible with the comparative framework of LCIA. A way to deal with this problem could be to try to develop non-conservative assessment factors taking the huge work on acute to chronic ratios all ready done (e.g. Chapman et al.1998, Solbe et al. 1998, Länge et al.1998, Forbes and Calow 2002) as a starting point, and maybe try to differentiate the assessment factors by TMoA. However, as the PNEC approach is no-effect based (i.e. NOEC based) it will still suffer from the uncertainty of measured NOEC values due to variation in test design and the potential dependence of the lowest toxicity value on the choice of database to characterize the toxicity of the substance.

If we accept to use a fixed β value in equation 6, which is the most appropriate if the method is going to be functional in a normal LCIA context, then, despite the described differences in theoretical foundation, all PAF approaches described here lead to the following general characterisation factor equation:

$$\mathrm{CF} = \mathrm{dPAF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{k}{\mathrm{HC50}} \cdot \mathrm{dC} \tag{8}$$

The constant k in equation 8 may be 0.59, as in the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b), 0.5, as in the average HC50-based approach or 0.2 - 43, as in the average HC5-based approach (Pennington et al. 2004). So, in the comparative approach applied in LCIA, there will be no difference in practise between the PAF approaches, as long as the same value for HC50 and the same value for change in concentration (dC) are used. The key element in the effect indicator part (k/HC50) of equation 8 therefore becomes HC50.

The crucial point in the determination of a PAF-based ecotoxicity effect indicator is therefore the data used and the principles applied for determining the HC50 value of each toxicant. As mentioned above, the HC50 may be estimated by use of e.g. NOEC values or EC_{50} values and based on the non-parametric median or the parametric geometric mean. Furthermore, the actual data used may for example reflect haphazard representation of species on each trophic level or a more realistic and consciously chosen representation of the structure of the ecosystem/community in question. The choice of data and estimation principle may have significant influence on the outcome especially when the number of available data on each toxicant is low, which is the typical case within LCIA handling many chemical emissions. These issues are addressed in Larsen and Hauschild (2004).

Acknowledgement

Thanks to Jérôme Payet for stimulating discussions and comments on the draft paper. The authors also gratefully acknowledge the financial support of the Danish Ministry of Science, Technology and Innovation given to KEMI (Centre for Chemicals in Industrial Production).

References

Aldenberg T, Jaworska J, Traas TP (2002): Normal Species Sensitivity Distributions and Probabilistic Ecological Risk Assessment. Chapter 5 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 49-102. Lewis, Boca Raton, FL, USA

Allanou R, Hansen BG, van der Bilt Y (1999): Public Availability of Data on EU High Production Volume Chemicals http://ecb.jrc.it/

Bruijn JCT de, van Leeuwen K, van der Plassche E, Sijm D, van der Weiden M (1999): Environmental Risk Limits in The Netherlands. Part I. Procedures in: Environmental Risk Limits in The Netherlands. Könemann H (ed.), pp. 1-33. Report No. 601640 001. RIVM, Bilthoven, The Netherlands

Calow P (1998): General Principles and Overview. Chapter 1 in: Handbook of Ecotoxicology. Calow P (ed.), pp. 1-5. Blackwell Science, Oxford, Great Britain

Campbell RC (1974): Statistics for biologists. Second edition. Cambridge University Press, Cambridge, Great Britain

Chapman PM, Fairbrother A, Brown, D (1998): A critical evaluation of safety (uncertainty) factors for ecological risk assessment. Environ Toxicol Chem 17 (1) 99-108

EC (2003a): Environmental Risk Assessment. Chapter 3 (Part II) in: Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances, Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Institute for Health and Consumer Protection. European Commission. ECB, JRC, Ispra, Italy

EC (2003b): Proposal for a Regulation of the European Parliament and of the Council concerning the Registration, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency and amending Directive 1999/45/EC and Regulation (EC) {on Persistent Organic Pollutants}. COM (2003) 644, Brussels, 29 October 2003

ECOTOX (2002): ECOTOXicology Database system. US EPA: http://www.epa.gov/ecotox/

Forbes VE, Calow P (2002): Extrapolating in Ecological Risk Assessment: Balancing Pragmatism and Precaution in Chemical Controls Legislation. BioScience 52 (3) 249-257

Goedkoop M, Spriensma R (2001a): The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Report. Third edition. Pré Consultants, Amersfoort, The Netherlands http://www.pre.nl

Goedkoop M, Spriensma R (2001b): The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Annex. Third edition. Pré Consultants, Amersfoort, The Netherlands http://www.pre.nl

Hakoyama H, Iwasa Y (2000): Extinction risk of a density-dependent population estimated from a time series of population size. J Theor Biol 204, 337-359

Hauschild M, Pennington D (2002): Indicators for Ecotoxicity in Life-Cycle Impact Assessment. Chapter 6 in: Life-cycle Impact Assessment: Striving Towards Best Practice, Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds.), pp. 149-176. SETAC-Europe, Brussels, Belgium

Hauschild M, Wenzel H, Damborg A, Tørsløv J (1998): Ecotoxicity as a criterion in the environmental assessment of products. Chapter 6 in: Environmental Assessment of Products: Volume 2: Scientific background, London, Hauschild M, Wenzel H (eds.), pp. 203-314. Chapman & Hall, London, Great Britain

Huijbregts M (2001): Uncertainty and variability in environmental life-cycle assessment. Ph.D. Thesis University of Amsterdam. ISBN 90-76894-05-1

Huijbregts M, Thissen U, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000): Priority assessment of toxic substances in life cycle assessment. Part I: Calculation of toxicity potentials for 181 substances with the nested multi-media fate, exposure and effects model USES-LCA. Chemosphere 41 (2000) 541-573

Huijbregts M, Van de Meent D, Goedkoop M, Spriensma R (2002): Ecotoxicological Impacts in Life Cycle Assessment. Chapter 20 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II G W, Traas T P (eds.), pp. 421-433. Lewis, Boca Raton, FL, USA

ISO (2000): ISO 14042: Environmental management – Life cycle assessment – Life cycle impact assessment. International Organisation for Standardisation, Geneva, Switzerland

Itsubo N, Ii R, Abe K, Nakagawa A, Hayashi K, Inaba A (2003): Biodiversity Damage Assessment – Applying the Theory of Biology in LCIA. Slides from platform presentation (WE2/8) at the SETAC Europe 13th Annual Meeting at Hamburg, Germany, April 27 – May 1, 2003

Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer G, Rosenbaum R (2003): Impact 2002+: A New Life Cycle Impact Assessment Methodology. Int J LCA 8 (6) 324-330

Lande R (1998): Anthropogenic, ecological and genetic factors in extinction and conservation. Researches on population ecology 40 (3) 259-269

Larsen HF, Hauschild M (2004): GM-troph – a low data demand ecotoxicity effect indicator for use in LCIA. Submitted to Int J LCA

Länge R, Hutchinson T, Scholz N, Solbe J (1998): Analysis of the ECETOC Aquatic Toxicity (EAT) database. II – Comparison of acute to chronic ratios for various aquatic organisms and chemical substances. Chemosphere 36 (1) 115-127

Newman MC, Ownby DR, Mézin LCA, Powell DC, Christensen TRL, Lerberg SB, Anderson B-A, Padma TV (2002): Species Sensitivity Distributiions in Ecological Risk Assessment: Distributional Assumptions, Alternate Bootstrap Techniques, and Estimation of Adequate Number of Species. Chapter 7 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 119-132. Lewis, Boca Raton, FL, USA

Norberg J, Swaney DP, Dushoff J, Lin J, Casagrandi R, Levin SA (2001). Phenotypic diversity and ecosystem functioning in changing environments: A theoretical framework. PNAS 98 (20) 11376-11381

Payet J, Jolliet O (2003): Comparative assessment of the toxic impact of metals on aquatic ecosystems: The AMI method. In: Life-Cycle Assessment of Metals: Issues and research directions. Alain Dubreuil (ed). SETAC, Pensacola, FL, USA

Payet J, Larsen HF (2004): Endpoint Modelling for the Life Cycle Impact Assessment on Ecosystems. In prep.

Payet J, Pennington D, Hauschild M, Jolliet O (2003). Comparative Assessment of toxic Impact on Aquatic Ecosystems: The AMI method (Assessment of the Mean Impact). Submitted to Environ Toxicol Chem

Pennington D, Payet J, Hauschild M (2004): Aquatic ecotoxicological indicators in life-cycle assessment. Environ Toxicol Chem 23 (7) 1796-1807

Posthuma L, Traas TP, Suter II GW (2002a): General Introduction to Species Sensitivity Distribution. Chapter 1 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 3-10. Lewis, Boca Raton, FL, USA

Posthuma L, Suter II GW, Traas TP (2002b): Species Sensitivity Distribution in Ecotoxicology. Lewis, Boca Raton, FL, USA

Pratt JR, Cairns JJr (1996): Ecotoxicology and the Redundancy Problem: Understanding Effects on Community Structure and Function. Chapter 12 in: Ecotoxicology - A Hierarchical Treatment. Newman MC, Jagoe CH (eds.), pp. 347-370. Lewis, Boca Raton, FL, USA

Rinaman CW, Heil C, Strauss MT, Mascagni M, Sousa M (1996): Probability and Statistics. Chapter 7 in Standard Mathematical Tables and Formulae. Editors: Zwillinger D (chief), Krantz SG, Rosen KH. 30 ed. CRC, Boca Raton, FL, USA

Snell TW, Serra M (2000): Using probability of extinction to evaluate the ecological significance of toxicant effects. Environ Toxicol Chem 19 (9) 2357-2363

Solbe J, Mark U, Buyle B, Guhl W, Hutchinson T, Kloepper-Sams P, Länge R, Munk R, Scholz N, Bontinck, Niessen H (1998): Analysis of the ECETOC Aquatic Toxicity (EAT) database. I – General introduction. Chemosphere 36 (1) 99-113

Straalen NM van, van Leeuwen CJ (2002): European History of Species Sensitivity Distributions. Chapter 3 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 19-34. Lewis, Boca Raton, FL, USA

Suter II GW (2002): North American History of Species Sensitivity Distributions. Chapter 2 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 11-17. Lewis, Boca Raton, FL, USA

Tanaka Y, Nakanishi J (2000): Mean extinction time of population under toxicant stress and ecological risk assessment. Environ Toxicol Chem 19 (11) 2856-2862

Tilman D (2001): An evolutionary approach to ecosystem functioning. PNAS 98 (20) 10979-10980

Traas TP, van de Meent D, Posthuma L, Hamers T, Kater BJ, de Zwart D, Aldenberg T (2002): The Potentially Affected Fraction as a Measure of Ecological Risk. Chapter 16 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 315-344. Lewis, Boca Raton, FL, USA

Udo de Haes HA, Lindeijer E (2002): The conceptual Structure of Life-Cycle Impact Assessment. Chapter 8 in: Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds.): Life-cycle Impact Assessment: Striving Towards Best Practice, pp. 209-225. SETAC-Europe, Brussels, Belgium

Zwart D de (2002): Observed Regularities in Species Sensitivity Distribution for Aquatic Species. Chapter 8 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II GW, Traas TP (eds.), pp. 315-344. Lewis, Boca Raton, FL, USA

Glossary

AF	Assessment Factor
CA	Concentration Addition
CF	Characterisation Factor
CDF	Cumulative Distribution Function
EC_{50}	Effect Concentration (50% of test organism affected)
EDIP	Environmental Design of Industrial Products
GM	Geometric Mean
HC5	Hazardous Concentration for 5% of included species
HC50	Hazardous Concentration for 50% of included species
HU	Hazard Units
LC_{50}	Lethal concentration (50% of test organism dead)
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
MET	Mean Extinction Time
msPAF	Multi-substance PAF

NOEC	No Observed Effect Concentration
OMNIITOX	Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments
PAF	Potentially Affected Fraction of species
PNEC	Predicted No Effect Concentration
PDF	Probability Distribution Function
PVF	Potentially Vanished Fraction of species
RA	Response Addition
SSD	Species Sensitivity Distribution
TGD	Technical Guidance Document
TMoA	Toxic Mode of Action
α	Location parameter
β	Scale parameter
γ	Slope factor

Appendix A: The PAF approach

The PAF (Potentially Affected Fraction of species) approach is based on the principles of Species Sensitivity Distribution (SSD) which is a statistical distribution describing the variation among a set of species in toxicity of a certain substance or mixture. This distribution can be based on different distribution functions, e.g. triangular, log-logistic, lognormal (all parametric) or by non-parametric statistics not assuming any specific distribution, and on different data (e.g. EC_{50}s or NOECs). General issues about SSD are most recently described in Posthuma et al (2002a), Suter II (2002) and in van Straalen and van Leeuwen (2002) which are all introductory chapters in the book “Species Sensitivity Distribution in Ecotoxicology” (Posthuma et al. 2002b).

The description below includes the single substance PAF, the multi substance PAF (msPAF also called combi-PAF), the marginal PAF increase approach and the most recently proposed approach based on average PAF increase.

A1 Single substance PAF

PAF can be defined as the fraction of species in an (generic) ecosystem/community that is expected to be (potentially) affected above its no-effect level (i.e. NOEC) or a predefined level (e.g. EC_{50}) at a given environmental concentration of a toxicant or other stressor (adopted from Traas et al. (2002)).

The PAF approach is based on the assumption that the sensitivity of species living in a community (or ecosystem) can be described by a Probability Distribution Function (PDF) (e.g. a bell shaped normal distribution), see **Fig. A1** which after integration yields a Cumulative Distribution Function (CDF) as illustrated in **Fig. A2**.

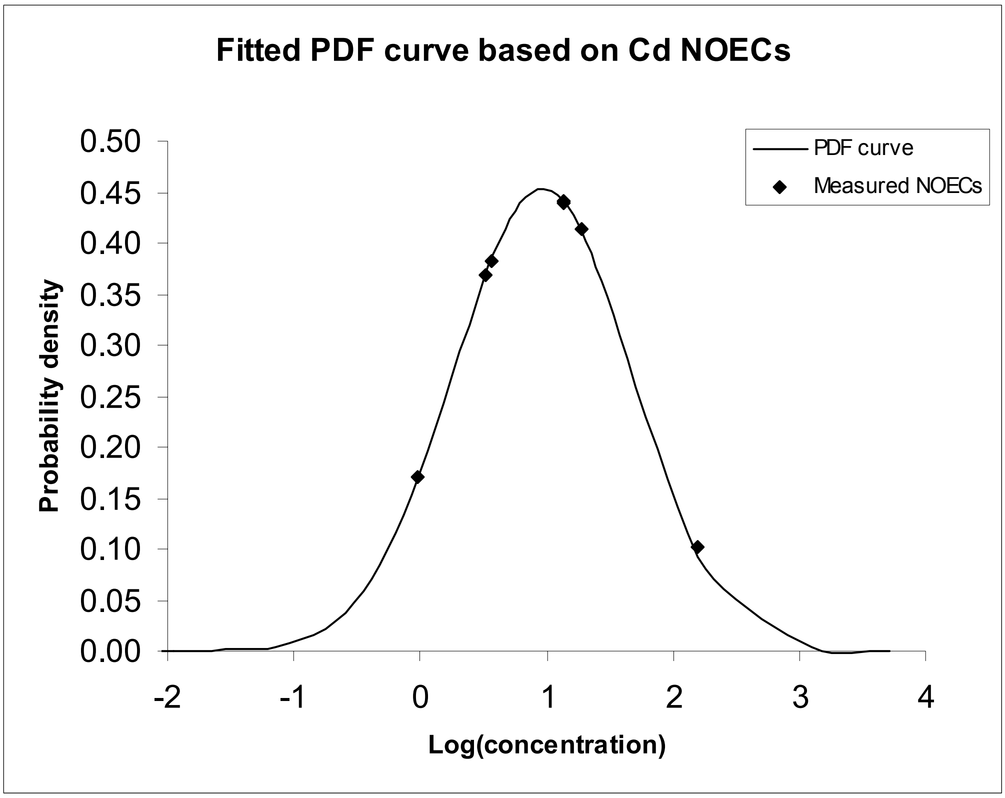

Fig. A1: An example of a fitted Probability Distribution Function (PDF, here a lognormal distribution) based on seven cadmium (Cd) NOECs for different soil species (n = 7, one point hidden in the figure). The $\log_{10}$ sample mean is 0.97 and $\log_{10}$ sample standard derivation is 0.70. The probability density (Y-axes) expresses the probability of selecting species (from the soil community in question) with a NOEC value equal to the corresponding Cd concentration. Data on Cd are taken from Aldenberg et al. (2002)

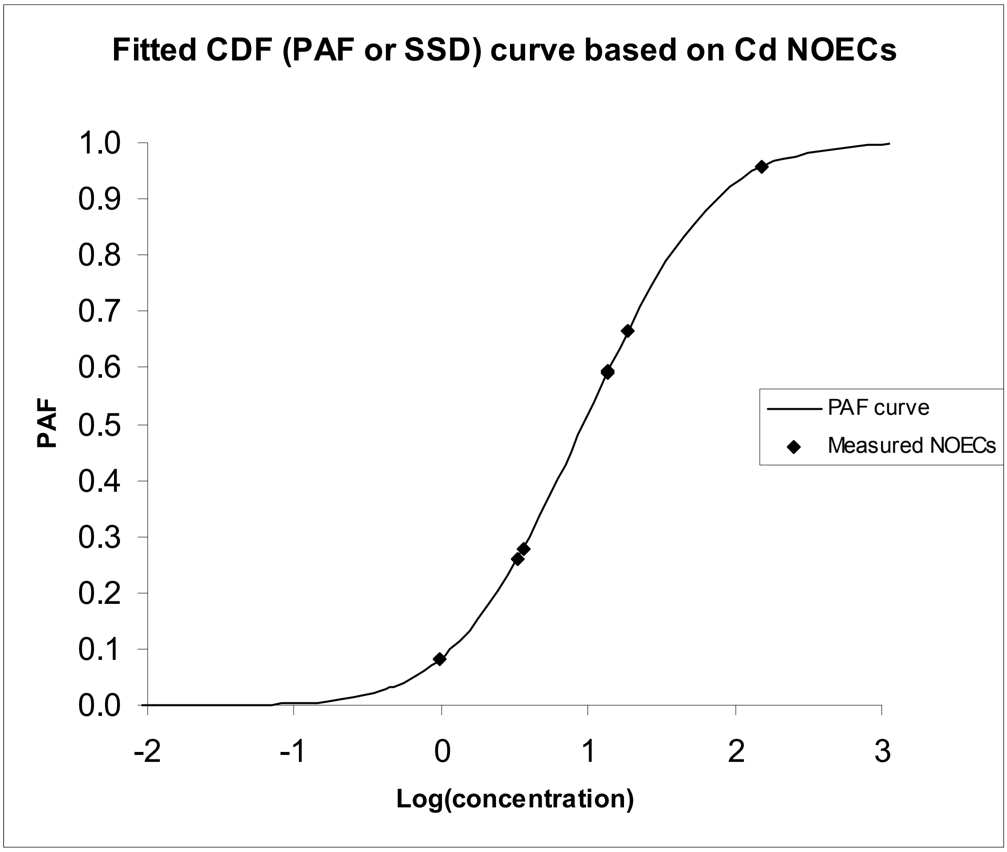

Fig. A2: Fitted lognormal CDF or PAF curve illustrating the relationship between the concentration of a toxicant (here cadmium, Cd) and PAF, i.e. the cumulative probability of exceeding NOECs for a certain fraction of species in the community/ecosystem in question (here a soil community). The dots represent measured values of NOECs for Cd in soil as in Fig.1. The concentration at which the fraction p of species are having their NOECs (or alternatively L(E)C_{50}s) exceeded is denoted the hazardous concentration at level p, i.e. HCp. For example the concentration at which 5% (PAF=0.05) of the species are having their NOEC exceeded is denoted HC5. Data on Cd are taken from Aldenberg et al. (2002)

Whether one uses a SSD function (PDF and CDF) based on a lognormal distribution or a log-logistic distribution is in principle not crucial for the shape of the curves or the outcome of the estimation of the HCp value (or PAF value) as long as the percentile (p value) used is not to low (significantly below 0.05) as shown by van Straalen and van Leeuwen (2002, Figure 3.3) and Pennington et al. (2004, Figure 4a and 4b). But of course the input data have to fit the distribution or a non-parametric method having a higher data demand has to be used as described by Newman et al. (2002).

In Fig. A1 and Fig. A2 a lognormal distribution is used as described for the PDF and CDF in e.g. Rinaman et al. (1996, pp. 583-584)

The CDF (integral of PDF) for a log-logistic distribution is shown below.

Log-logistic CDF (de Zwart 2002):

$$PAF = \frac{1}{1 + e^{-(\log C - \alpha)/\beta}} \text{, where} \qquad (A1)$$

C : Environmental concentration (of toxicant)

α : Sample mean or location parameter (estimated as $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$, where n is the number of input log data (x), e.g. log NOECs

β : Scale parameter (estimated as $\hat{\beta} = \frac{\sqrt{3}}{\pi} \cdot \sigma$, where σ is the standard deviation: $\frac{1}{\sqrt{n-1}} \cdot \sum_{i=1}^{n} (x_i - \overline{x})^2$

The PAF approach including the single substance PAF (described above) and the multi substance PAF (msPAF, described below) has most recently been described in details by Traas et al (2002).

A2 Multi Substance PAF (msPAF)

One of the advantages of the msPAF approach (also called combi-PAF) is that it is able to handle mixtures as described below. This description is mainly based on Traas et al (2002).

For each of the toxicants in the data set in question a single substance PAF is made (in principle as the example in Fig. A2). But instead of using the concentration units (e.g. µg/l) for the NOEC values (we assume that it is a NOEC-based SSD for an aquatic community) these are scaled to dimensionless hazard units (HUs) by dividing each NOEC value by the parametric median (i.e. the geometric mean) of the NOEC values, done set by set for each toxicant. We hereby achieve that 1 HU is equal to a concentration where the NOEC is exceeded for 50% of all species tested for all included toxicants. The resulting CDF is pictured with HU on the X-axes and msPAF values on the Y-axes, and the curve type resembles the one in Fig. A2.

If we then want to estimate the potentially affected fraction of species due to a mixture exposure (where we know the environmental concentration of each toxicant), we have to scale each concentration to HUs in the same way as the NOEC values. If all the toxicants in the mixture have the same Toxic Mode of Action (TMoA) (e.g. baseline narcotic) we can use the principles of Concentration Addition (CA) and just add the number of HU. From the CDF curve we can read the msPAF corresponding to the total number of HU. If we assume that the species sensitivity distribution can be described by a log-logistic distribution then the msPAF can be calculated in the following way:

$$\text{msPAF}_{\text{CA}} = \text{PAF}_{\text{TMoA}} = \frac{1}{1 + \text{e}^{-\log(\Sigma \text{HU}_{\text{TMoA}})/\beta_{\text{TMoA}}}} , \qquad (A2)$$

where β_{TMoA} is the average scale parameter (scale factor) over all the toxicants in the mixture.

The scale parameter for each toxicant is calculated as $(\sigma \cdot \sqrt{3})/\pi$, where σ is the standard deviation for each CDF, see equation A1.

If the mixture contains toxicants with different TMoA the estimations become more complicated. All toxicants with same TMoA are treated in groups and for each group a PAF_{TMoA} is calculated as described above for concentration addition (see equation A2). For each single toxicant with different TMoA (or unknown TMoA) a $PAF_{(TMoA)}$ is also calculated according to the principles for calculating single substance PAF, see equation A1. All these PAF values (PAF_{TMoA} and single substance PAF) are then treated by the rules for Response Addition (RA):

$$msPAF_{RA} = 1 - \prod_{i=1}^{n} (1 - PAF_i) \ , \qquad \text{(A3)}$$

where n is the number of PAF values.

The $msPAF_{RA}$ can in this case be designated $msPAF_{CA+RA}$ because CA precedes RA.

A3 'Marginal PAF increase' approach

The 'marginal PAF increase' approach is used in connection with LCIA in the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b) and most recently described in Huijbregts et al. (2002).

In this approach the ecotoxicity effect indicator is expressed as the marginal increase in the msPAF, (as compared to the background level msPAF) of the community/ecosystem SSD in question, due to exposure from an emitted toxicant. In other words the aim is to express the potential impact from an emitted toxicant by the marginal increase in the number of species having their NOEC values exceeded taking the background impact (i.e. the number of species already having their NOEC exceeded) into account.

The 'marginal PAF increase' approach is based on the principles of calculating an msPAF as described in Section A2. In the adoption of the approach in Eco-indicator 99 (Goedkoop and Spriensma 2001a, 2001b) it is assumed that because all possible TMoAs are already present in the environment an emitted toxicant will imply concentration addition to a mechanism already present. The method used in Eco-indicator 99 is therefore only based on CA. This assumption may result in an error of above a factor 100 (Huijbregts et al. 2002). The method is making use of Dutch investigations on SSDs for different compartments (e.g. freshwater) which includes measured existing environmental concentrations of toxicants (mainly pesticides and metals) and hereby the calculation of the background msPAF values. Based on these investigations the Eco-indicator 99 method sets up a general log-logistic msPAF curve (called combi-PAF) with the scaling to HU as described in Section A2. An average β value (scale factor) of 0.4 and a background msPAF value of 22% (geometric mean of msPAF background values for water and soil in the Netherlands) defining the working point is used in this method.

The working point is the point on the PAF curve that corresponds to the background impact on the community/ecosystem in question, i.e. the number of HU all ready present corresponding to a certain msPAF value.

In the 'marginal PAF increase' approach the increase in PAF due to the emission of a toxicant is not directly calculated from the actual PAF curve (i.e. CDF). To ensure linearity (proportionality) in the calculation and use of the characterisation factor, the slope (slope factor, γ) of the tangent to the curve at the working point is used instead i.e. a tangential or marginal gradient. The marginal gradient used in the Eco-indicator 99 method (working point at PAF = 0.22) together with another marginal gradient and an average gradient (described in Section A4) both at working point 0.5, are shown in **Fig. A3**.

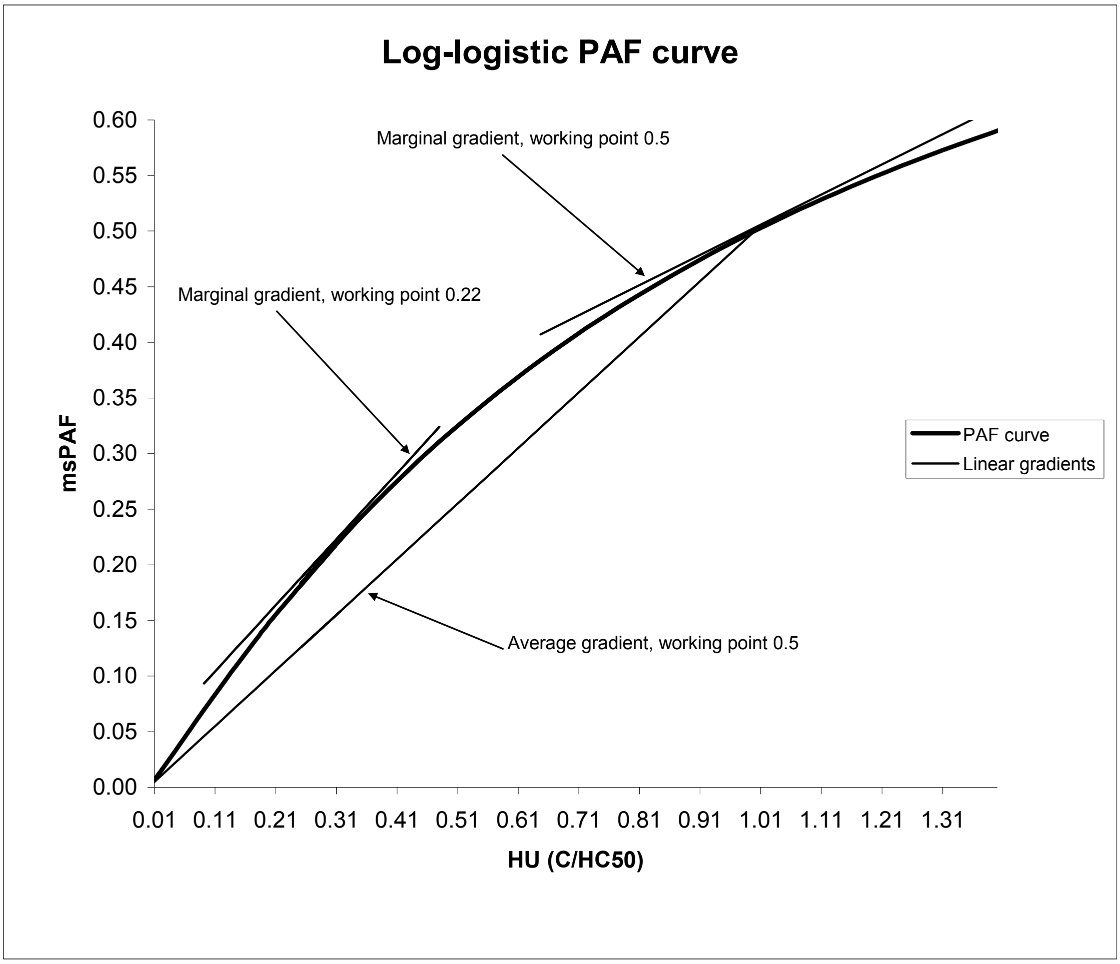

Fig. A3: Log-logistic PAF curve with concentration (C) shown on a linear scale as hazard units, HU (C/HC50). The marginal gradient with working point at PAF = 0.22 and having a slope of 0.59 is the one used in the Eco-indicator 99 method. The marginal gradient and the average gradient both with working point at PAF = 0.5 have slopes of 0.27 and 0.50 respectively. The msPAF curve is defined by a β value of 0.4 as used in Eco-indicator 99.

In this marginal approach the PAF increase per HU is dependent on the slope of tangent (marginal gradient) which is dependent on the placing of the working point as shown in Fig. A3. In Eco-indicator 99 the working point (PAF = 0.22) is defined by the average background impact (background PAF) as described above. The difference in the size of the slope (γ) if the working point is placed at PAF = 0.05 instead of PAF = 0.50 is about a factor 3 when β is set to 0.4 as in the Eco-indicator 99 method. If the β value is set to 0.7 (highest average value within different TMoA (de Zwart 2002)) the difference becomes a factor of 22. So the location of the working point can have a relatively high impact on the slope depending on the kind of TMoA involved.

So, in the Eco-indicator 99 method the working point is defined by an msPAF value of 22% and the tangent to that point on the generalised msPAF curve has a slope (γ) of 0.59. The characterisation factor (CF) defined as the marginal increase in msPAF due to a marginal increase in the concentration of a toxicant can be calculated in the following way:

$$CF_{CA} = dmsPAF = \frac{\gamma}{10^{\alpha}} \cdot dC \qquad (A4)$$

where α is the location parameter, estimated by the sample mean of the $\log_{10}$ transformed species toxicity values (i.e. NOEC values for the toxicant in question) and dC is the concentration increase calculated by the fate model, in this case USES-LCA (Huijbregts et al. 2000). So, to be able to calculate the 'effect part' (i.e. $\gamma / 10^{\alpha}$) of equation A4 only the mean of the NOEC values for the toxicant in question is needed. This mean (α) can be calculated as the geometric mean (GM) of the NOECs:

$$\mathrm{GM} = \sqrt[1/n]{\prod_{i=1}^{n} x_i} \text{ , where n is the number of NOEC values } (x_i) \qquad \text{(A5)}$$

The number of NOEC values (n) is specified to 4 in Goedkoop and Spriensma (2001a, 2001b). The minimum requirement of 4 NOEC values (from minimum 4 different taxonomic groups) is also used in the Netherlands for estimation of Environmental Quality Criteria (EQC) by log-logistic probability distribution (de Bruijn et al. 1999, Traas et al. 2002). As stated in Aldenberg et al. (2002) and de Bruijn et al. (1999) it should be tested whether or not the NOEC values fit the probability distribution (i.e. log-logistic) by e.g. Kolmogorov-Smirnov test before this statistical extrapolation method is used.

Huijbregts et al. (2002) have modified the 'marginal PAF increase' approach described above by including the principles of response addition (RA) (see equation A3) with the aim of taking different TMoA into account. When doing that they come up with an equation for a characterisation factor that can be expressed in the following way:

$$\mathrm{CF}_{\mathrm{CA+RA}} = \mathrm{dmsPAF} = \frac{1-\mathrm{msPAF}}{1-\mathrm{PAF}} \cdot \frac{\gamma}{10^{\alpha}} \cdot \mathrm{dC} \qquad \text{(A6)}$$

where msPAF is the background msPAF (e.g. 0.22 as in Eco-indicator 99 method mentioned above) and PAF is the single substance PAF value for the toxicant in question (calculated according to equation A1).

A4 'Average PAF increase' approaches

Instead of using a tangential gradient, as in the 'marginal PAF increase' approach, Pennington et al. (2004) argue for using a secant or average gradient, especially at low exposure concentration (below HC5) i.e. in the area where the shape of the CDF curve becomes very uncertain. As shown in Fig. A3 the average gradient is a linear gradient starting from the chosen working point (e.g. msPAF = 0.5) and having a slope (e.g. 0.5) determined by the working point.

If we assume that the background PAF is below 0.05 but use this value as a working point for an average gradient the equation becomes (Pennington et al. 2004).

$$\mathrm{CF}_{\mathrm{CA}} = \mathrm{dmsPAF} = \frac{0.05}{(\mathrm{HC5}/\mathrm{HC50})/\mathrm{HC50}} \cdot \mathrm{dC} \qquad \text{(A7)}$$

The slope is in this case 0.05/(HC5/HC50).

As recommended as best available practice in LCA by Pennington et al. (2004) and as implemented in the AMI method (Payet et al. 2003) the average gradient may be based on HC50 (working point, PAF = 0.5). In this case the equation for the characterisation factor becomes:

$$CF_{CA+RA} = dmsPAF = \frac{0.5}{HC50} \cdot dC \qquad (A8)$$

So in this case the slope is 0.5 as illustrated in Fig. A3.

As illustrated by the example in **Fig. A4** the estimation of HC5 (needed in equation A7) is much more uncertain than the estimation of HC50.

By choosing the average gradient based on HC50 (equation A8) a distinction between CA and RA is not necessary – all toxicants can be handled according to CA as shown by Pennington et al. (2004).

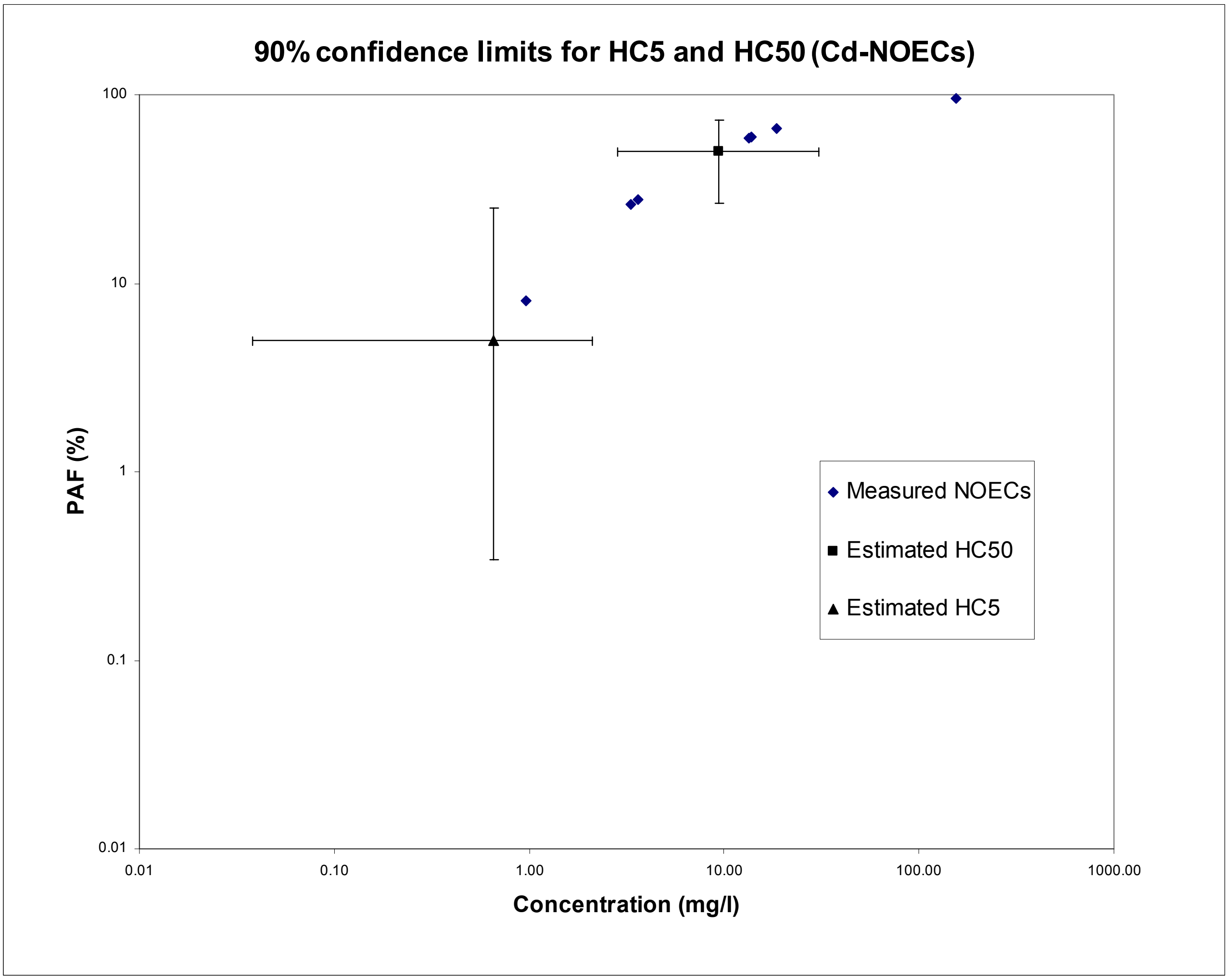

Fig. A4: An example illustrating the 90% confidence limits (i.e. 5th percentile and the 95th percentile) for both PAF and concentration, for HC50 and HC5 estimated on the basis of seven cadmium (Cd) NOECs for different soil species (n = 7, one point hidden in the figure), fitted to a lognormal distribution. The horizontal limits for HC5 are estimated on basis of the law of extrapolation (Aldenberg et al. 2002, p. 61-62 and Table 5.A1) and the vertical limits for both HC5 and HC50 on basis of the uncertainty of the fraction affected (Aldenberg et al. 2002, p. 65 and Table 5.A2). The horizontal limits for HC50 are estimated on basis of student’s t-distribution (Campbell 1974, Table A12). Data on Cd are taken from Aldenberg et al. (2002).

6 GM-troph: An ecotoxicity effect indicator based on three data values

This Chapter is a verbatim version of the following paper submitted to the International Journal of LCA:

Larsen HF, Hauschild M (2004). GM-troph – A low data demand ecotoxicity effect indicator for use in LCIA. *Submitted to Int J LCA.*

GM-troph

- A low data demand ecotoxicity effect indicator for use in LCIA

Henrik Fred Larsen[*], **Michael Hauschild**

Department of Manufacturing Engineering and Management, Technical University of Denmark (DTU) Building 424, DK-2800, Lyngby, Denmark

* **Corresponding author** (hfl@ipl.dtu.dk)

Abstract

Goal, Scope and Background. The development and further improvement of ecotoxicity effect indicators (EEIs) for use in life cycle impact assessment (LCIA) has only been going on for about two decades. In this paper we focus on the development of an effect-based (i.e. EC_{50}-based) average indicator, the GM-troph. The indicator is estimated by use of the hazardous concentration for 50% of the covered species ($HC50_{EC50}$) and is able to work on only three acute data values, which is often the data availability for a substance in LCIA.

Methods. The study includes both a theoretical description and a test on real data of three different effect-based average approaches (arithmetic mean, geometric mean and median) focusing on their statistical robustness. The real data set is composed of ecotoxicity effect data for eleven different substances representing seven different toxic modes of action (TMoA).

Results and Discussion. The theoretical considerations and the test on real data show that the geometric mean is the most robust average estimator for $HC50_{EC50}$, especially in the dominating situation where data availability is limited to a few data points. Test on the difference between estimating the average toxicity (i.e. $HC50_{EC50}$) on the level of species EC_{50}s and on the level of taxa or trophic levels (i.e. with geometric means of EC_{50}s within taxa or trophic levels used as input data) indicate that in some cases of unequal representation in number of species between taxa, estimations based on the species level may be biased.

Conclusions and Recommendations. Based on these results, the following recommendations are given for the choice of estimation principle for the EEI: The indicator shall be based on $HC50_{EC50}$ estimated as the geometric mean of three (average) EC_{50} values, covering the three main taxa, plants, invertebrates and vertebrates, which represent the three trophic levels of the ecosystem, primary producers, primary consumers and secondary consumers. In practice, the EEI shall be based on data from laboratory test with algae, invertebrates (crustacean) and fish. Instead of using the normally very wide 95% confidence limits, it is recommended to use the range given by the observed maximum and minimum values as limits around the $HC50_{EC50}$. Further, it is recommended to use EC_{50}(chronic) values when possible. Often, only acute data will be available, and here the use of best estimate assessment factors is recommended to extrapolate from acute to chronic values. As a starting point, an acute to chronic ratio of 10 between $HC50_{EC50}$(acute) and $HC50_{EC50}$(chronic) is recommended, but more research is certainly needed in this area. Due to the comparative framework of LCIA it is recommended only to use test results from laboratory tests, fulfilling certain standard conditions, i.e. applying standard organisms, measuring well defined endpoints over restricted test durations.

Outlook. The ability of a geometric mean-based $HC50_{EC50}$ to represent the toxicity of very toxic substances and toxicity towards very sensitive species has not been dealt with here, and again further research is needed. However, on the basis of the results from the tests on real data it may be anticipated that the GM-troph with its max-min limits at least to some degree accounts for the toxicity to most sensitive species among standard organism, if representative toxicity data are available.

Keywords: Average estimates; ecotoxicity effect indicators; geometric mean; hazardous concentration (HC50); life cycle impact assessment (LCIA); max-min limits

Introduction

The paper is based on the report "Implementation of the OMNIITOX Base Model. Part VIII – Implementation of the ecotoxicological effects module" by Larsen et al. (2004c), which was done as part of the OMNIITOX [3] project. The indicator described here, the GM-troph, is used in the OMNIITOX base model on calculating ecotoxicity characterisation factors.

In recent years the research on ecotoxicity effect indicators (EEIs) has intensified. Some important output from this work has been used as a basis for the development of the approach proposed here. The general frame has been defined by the SETAC Task Group on Ecotoxicity (Hauschild and Pennington 2002, Pennington et al. 2004). Further in the development of EEIs, different ways have been explored for the estimation of average toxicity and its associated uncertainty, using non-parametric statistics (Payet and Jolliet 2003) or using parametric statistics (Payet et al. 2003). Most recently Larsen and Hauschild (2004a) have done an evaluation of different EEI approaches including damage approaches and putting focus on data availability. This paper describes further development of an unbiased average estimate of the toxicity of chemicals based on a modest data requirement, with an improvement of the selection of the data input and principles of estimation, and the calculation of the uncertainty for the effect indicator.

Based on the general framework of life cycle assessment (LCA) and especially life cycle impact assessment (LCIA) (ISO 2000; Udo de Haes and Lindeijer 2002) and the work done until now on EEIs (se above), some general constraints relevant for the EEI approaches may be outlined:

- A general condition for the LCIA models is that the impact category indicator must be additive.
- In contrast to (tiered) risk assessment the indicator shall be a best estimate, i.e. not a conservative estimate.
- Emissions of a toxicant mapped in a life-cycle inventory (LCI) is to be regarded as a single pulse without time duration and therefore time and space are integrated in the assessment giving further restrictions to the modelling.
- In ordinary LCAs the activities releasing toxicants to the environment are usually not precisely located, and therefore site-specific approaches cannot easily be used. Most often we have to rely on large-scale averages of environmental conditions.
- The large number of substances covered by an LCI calls for a model that relies on relatively few input data in order to make the data gathering feasible.
- The data availability regarding ecotoxicological effect data for the majority of substances on the market puts severe restrictions on the data demand of the EEI model.
- The assessment of impact (or damages) on ecosystems in LCA requires the compatibility between the fate model and the effect model. The two models can for example be connected as shown in equation 1 for the characterisation factor

---

[3] **OMNIITOX** is a EU-project under the Competitive and Sustainable Growth-programme, running from 2001 to 2004. OMNIITOX will facilitate decision making regarding potentially hazardous compounds by improving methods and developing information tools necessary for impact assessment of toxic chemicals within LCA and risk assessment. Project partners are Technical University of Denmark; Leiden University, The Netherlands; University of Stuttgart, Germany; École Polytechnique Fédérale de Lausanne (EPFL), Switzerland; Chalmers University of Technology, Sweden; European Chemicals Bureau, JRC, Ispra, Italy; Volvo Technology Corporation, Sweden; Procter & Gamble EUROCOR, Belgium; Stora Enso AB, Sweden; Antonio Puig, S.A. Spain; Randa Group S.A, Spain. More information about OMNIITOX can be found at www.omniitox.net.

(CF) per kg emitted contaminant, indicating the fraction of species experiencing an increase in stress for a change in contaminant concentration. The 'effect part' (i.e. the effect indicator, 0.5/HC50) is here expressed in PAF $\cdot$ m^3 $\cdot$ kg^{-1} and the 'fate part' (i.e. change in concentration, dC) can be expressed in kg $\cdot$ m^{-3} per kg emitted contaminant. In this case the characterisation factor is expressed in PAF per kg emitted contaminant. If the 'fate part' is expressed in a time integrated fraction of the emitted amount (days), as in the OMNIITOX base model, the characterisation factor is expressed in PAF $\cdot$ m^3 $\cdot$ days per kg emitted contaminant.

There seems to be two main directions to follow for the indicator, viz. the predicted no effect concentration (PNEC) approach and the potentially affected fraction of species (PAF) approach, as argued by Larsen and Hauschild (2004a). Both have pros and cons but in the comparative context of LCA, where best estimates are sought, the choice of a PAF approach based on average toxicity seems preferable, and further secures the (at least theoretical) connection to damage or endpoint modelling. This is important within LCA because it makes it possible to gather different classes of midpoint impact categories in one common endpoint category, for example the impact to ecosystems from land-use (expressed in units of biodiversity) and the ecotoxic impact to ecosystems (expressed in units of PAF). A damage model may translate the midpoint indicators into an endpoint or damage indicator expressing them in equivalent units of potentially vanished fraction of species (PVF). The compatibility between the average toxicity assessment approaches describes in this paper and the existing damage models has been studied and possibilities identified to translate the midpoint indicator based on the geometric mean into a damage indicator expressed as change in biodiversity (i.e. PVF) (Payet and Larsen 2004). This is a key issue for the further methodological development in LCA, especially for the link between the land-use, eutrophication, acidification and the impact due to toxicants (ecotoxicity).

As data availability is low in LCIA (typically three acute data values) an EEI based on average toxicity (i.e. $HC50_{EC50}$) with a working point at PAF = 0.5 on the PAF curve seems most reasonable (Larsen and Hauschild 2004a). A characterisation factor (CF) based on this type of indicator can be expressed in the following way (per kg emitted substance):

$$\mathrm{CF} = \mathrm{dPAF} = \mathrm{EEI} \cdot \mathrm{dC} = \frac{0.5}{\mathrm{HC50}_{\mathrm{EC50}}} \cdot \mathrm{dC} \tag{1}$$

The $HC50_{EC50}$ is the hazardous concentration at which 50% of the included species have their EC_{50} value exceeded (endpoint for example mortality), see Larsen and Hauschild (2004a) for further details.

The main advantages and disadvantages of choosing such an effect-based indicator as compared to a no-effect based (i.e. PNEC based) are given below:

Advantages:

- The risk of bias from the laboratory test set-up is low as compared to a no-effect based indicator, where typically the highest tested concentration, which is not statistically different in toxicity from the control concentration, is used.
- The use of a value which is estimated and placed in the centre of the concentration response curve (i.e. HC50) where uncertainty is lowest.
- Makes quantification of damage in terms of potential loss of species possible (at least in theory).

Disadvantages:

- The focus is shifted a way from protection of the function and structure of ecosystems.
- The importance of very sensitive species may be neglected.

A potential bias between ecotoxicity and other impact categories, which model lower levels of impact, may be removed by normalisation.

As shown by Larsen and Hauschild (2004a), when estimating ecotoxicity effect indicators based on the PAF approaches within the comparative framework of LCIA, the data used and the principles applied when determining the HC50 are crucial to the outcome. The main goal of this paper is to propose and document a recommendable way to estimate the HC50 value from the typical data availability of three acute data values.

1 Estimation principles

Two different estimation principles, i.e. the median and the geometric mean, are used today for estimation of an effect-based HC50 (Larsen and Hauschild 2004a). Here, we will look at these two average estimation principles but further include the arithmetic mean, and the alternative no-effect based PNEC approach (here represented by the lowest EC_{50}, termed $LowEC_{50}$ on which the PNEC would be based) for comparative reasons. First, the different estimation principles are evaluated from a theoretical point of view, and in Section 5, a test on real data is carried out.

The four estimation principles are:

- arithmetic mean (effect-based)
- geometric mean (effect-based)
- median (effect-based)
- PNEC (no-effect based)

The arithmetic mean (termed mean) is certainly the most used estimator of average in general but should not normally be used for calculating the average effect concentration within ecotoxicology because it presumes that the data set is normal distributed, which is typically not the case for toxicity (see below).

The geometric mean is typically used when estimating average toxicity for a population, e.g. in a standard laboratory test. According to Newman and Dixon (1996) an individual lethal dose (individual effective dose (I.E.D.)) exists for each individual within a population and often displays a lognormal distribution because “in biological material the variation often shows a geometrical rather than an arithmetic distribution” (cited ref. Bliss, 1935). If average within genuses (term used in classification meaning a group of closely related species) is used as data input when dealing with species sensitivity distributions (SSDs), the geometric mean is also typically used (e.g. Versteeg et al. 1999). This is also the case when the HC50 is estimated from the typical SSD approach (e.g. Aldenberg et al. 2002), which is based on one data point (e.g. NOEC or EC_{50}) from each single species in the group of species selected.

The geometric mean presumes lognormal distribution of the data set. It is possible to test for this precondition by use of tests for goodness of fit, e.g. Anderson-Darling test (Aldenberg et al. 2002). However, this is not always done (Forbes and Calow 2002a; Newman et al. 2002) which may be a problem, because, 27 of 51 data sets failed the test for lognormality, as demonstrated in Newman et al. (2002). But, for the typical case where three pieces of data is available, it will not be possible to perform any goodness of fit test with any confidence.

The failure of the data set for many substances to meet the precondition of lognormal distribution is one of the reasons why Payet and Jolliet (2003) have developed a median-based ecotoxicity effect indicator based on non-parametric statistics (median and confidence limits by bootstrapping). However, as stated in Aldenberg et al. (2002) and Newman et al. (2002), the use of non-parametric statistics (i.e. median based) requires a larger data set than if parametric statistics (i.e. geometric mean) is used. Anyway, according to the method by Payet and Jolliet (2003), the calculation of confidence limits around the $HC50_{EC50}$, estimated by bootstrapping, demands at least 5 data points and if only three are available (as the typical case here), the difference between the median and the two extremes is multiplied with a factor of two (assumed factor from extrapolation) and used as confidence limits (Payet and Jolliet 2003).

Even though the PNEC approach is used as the dominating approach within generic risk assessment today (e.g. EC 2003a) and still very much used in LCIA (e.g. Huijbregts et al. 2000, Hauschild et al.1998), it is not directly included here because it is not an average approach. Only the lowest EC_{50} value ($LowEC_{50}$), on which the PNEC by use of an assessment factor is typically based, is included for comparative reasons.

1.1 Theoretical examples

In the theoretical examples in the following it is anticipated that the test organisms included in the data set for a substance cover three trophic levels, represented by algae, crustacean and fish (see Fig. 4 and Section 3 for definition of trophic levels etc.).

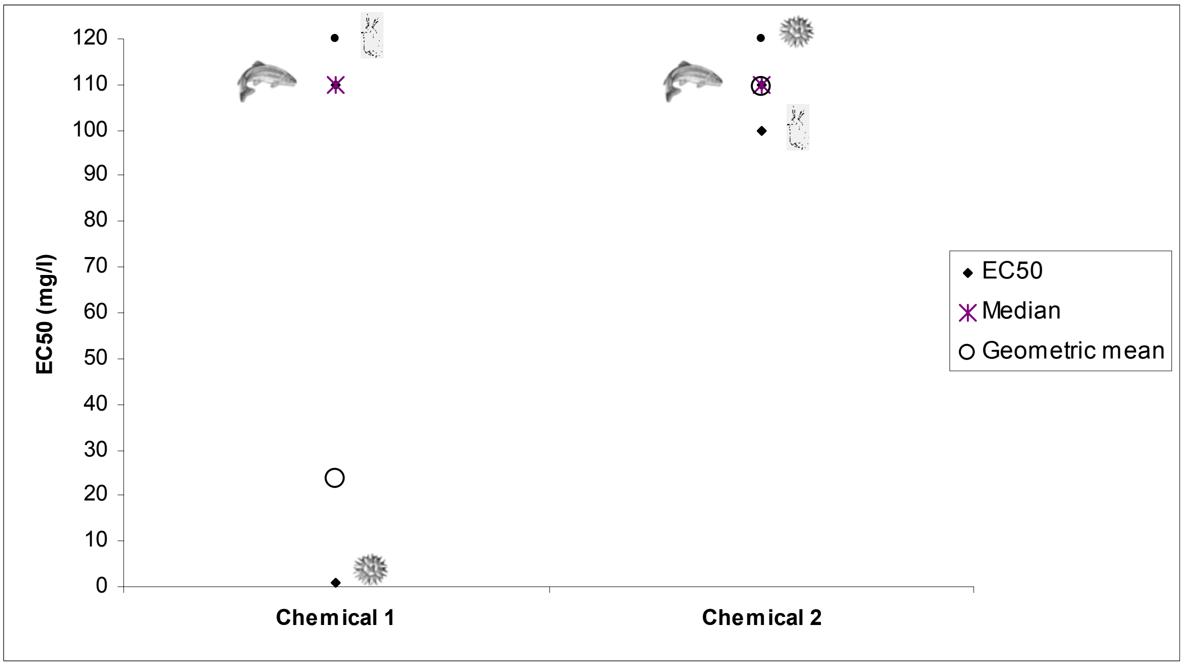

Fig. 1: Two theoretical cases illustrating the difference between the ability of the median and the geometric mean to reflect average toxicity of three EC_{50}s

If we look at the two theoretical cases (chemical 1 and chemical 2) in **Fig. 1** it is obvious that the median is not able to distinguish between the average toxicity of the two chemicals even though chemical 1 is very toxic to one of the tested organism (algae) whereas chemical 2 has low toxicity to all three tested organism. The geometric mean is, however, able to distinguish between the average toxicity of the two chemicals.

Looking at chemical 1 only and now assuming two cases of different data availability as shown in **Fig. 2**, the median shows low robustness. If the fifth data point represents one of the two not very sensitive organism groups instead of the most sensitive organism group (e.g. algae for herbicides), the median jumps from a relatively low EC_{50} value to a relatively high EC_{50} value.

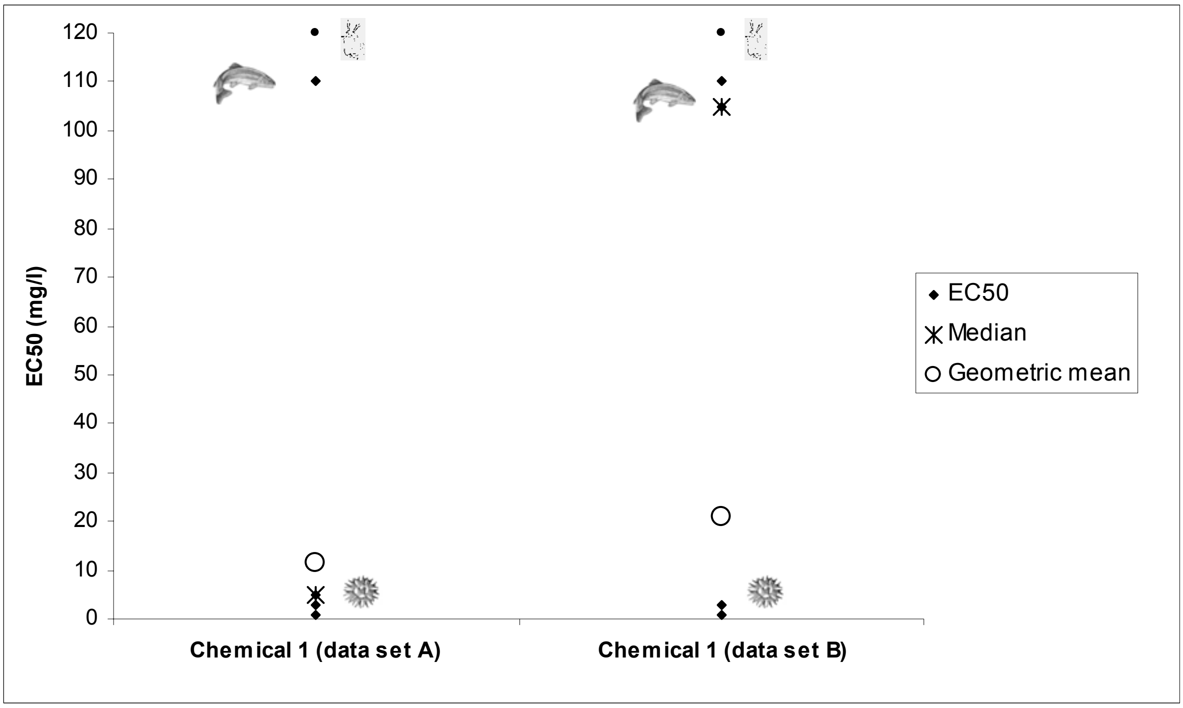

Fig. 2: Two theoretical cases of different data availability for chemical 1 illustrating the ability of the median and the geometric mean to reflect average toxicity of five EC_{50}s

Although the geometric mean is relatively robust here (see Fig. 2), there may be a problem using the individual species data as input rather than the geometric mean for each of the organism groups or taxa (general term for taxonomic units in classification) used representing trophic levels. As pointed out by Aldenberg et al. (2002), a biased species selection leads to biased estimated parameters (e.g. HC50) in SSDs. In some cases we may thus have many test data for one trophic level and only one (or a few) data for the two other trophic levels. Just calculating the geometric mean of these data (i.e. on species level) may lead to bias putting a weight on the trophic level with many measured values which may be disproportionate to ecological relevance of this trophic level and instead reflect the fact that through regulation, it has been given a high priority in ecotoxicity testing. Furthermore, “it is generally assumed that members of the same taxonomic group are more similar to each other in sensitivity than to members of other taxonomic groups” (Forbes and Calow 2002a). Nevertheless, studies on SSDs are typically based on haphazard collection of species with doubtful ecological relevance as shown by Forbes and Calow (2002a).

In **Fig. 3** a theoretical example of two chemicals (chemical 3 and chemical 4) with quite different toxicity profiles illustrates the inability of the PNEC approach (here lowEC_{50}) to distinguish. Note that PNEC is typically a factor 100 - 1000 lower than LowEC_{50} depending on the assessment factor used (Hauschild et al. 1998, EC 2003a). As can be seen in Fig. 3, the LowEC_{50} is the same for chemical 3 and chemical 4. However, chemical 3 is very toxic to all three organisms tested, whereas chemical 4 only is very toxic to one of the organisms tested (i.e. the daphnia). The PNEC approach is aiming at protecting the most sensitive species (hereby inherently assuming that the ecosystem health is protected) and is therefore not an average approach. Any way it seems reasonable to anticipate that the toxic pressure (and hereby the effect) on an ecosystem will be higher if the chemical is very toxic to organisms from all three trophic levels (chemical 3) than if this is only true for one trophic level or one species (chemical 4). It is possible that this one sensitive species is a key species and therefore very important for the structure and function of the ecosystem, but this will probably only be true in very few cases if at all, and is not the average situation which we aim for in LCIA in order to avoid a consistent bias caused by basing the ecotoxicity indicator on conservative assumptions.

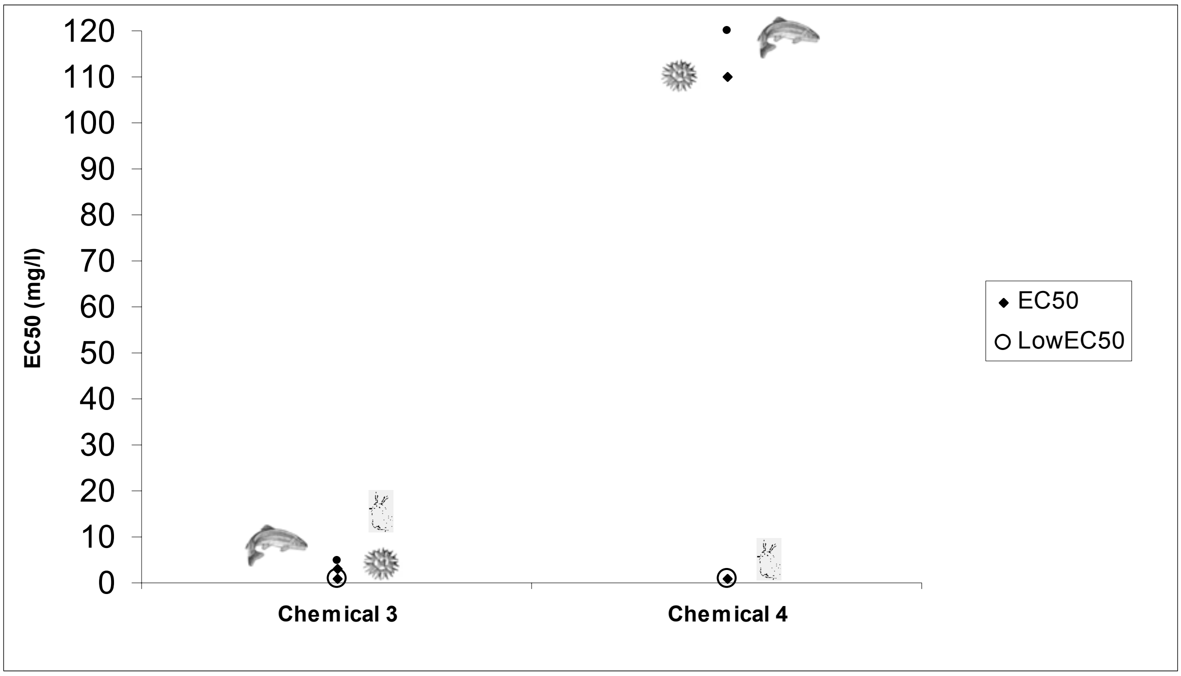

Fig. 3: Two theoretical cases illustrating the inability of LowEC_{50} to reflect average toxicity on a three EC_{50} data set

2 Environmental compartments

In this paper we will focus on the freshwater pelagic compartment for which the data availability is dominating. A proposal on how to deal with other compartments can be found in Appendix A.

3 Trophic levels

An ecosystem can be characterised by its structure and function. Structural descriptors like species diversity (species richness) and trophic structure, and functional descriptors like biomass production, energy flow and nutrient recycling may be used (Cairns et al. 1995, Sand-Jensen 2000, Pratt and Cairns 1996). Here, we focus on the trophic structure because it includes both the different life forms (e.g. autotrophic and heterotrophic organism) and to a high degree different feeding types (e.g. herbivorous and carnivorous), and to some degree the level of biological evolutionary development/complexity (e.g. micro-organism, invertebrates and vertebrates) in a structured way. Furthermore, the legal framework for the dominating part of the available ecotoxicity test data is based on the representation of trophic levels (e.g. EC 2003a).

A simplified food web with food chains for a freshwater ecosystem is shown in **Fig. 4**. The positions along the food chains are trophic levels (Whittaker 1975). In the freshwater ecosystem the different trophic levels are represented by for example the phytoplankton (primary producers), the zooplankton (primary consumers, herbivores), the planktivore fish (secondary consumers, first carnivores) and the piscivore fish (tertiary consumers, secondary carnivores).

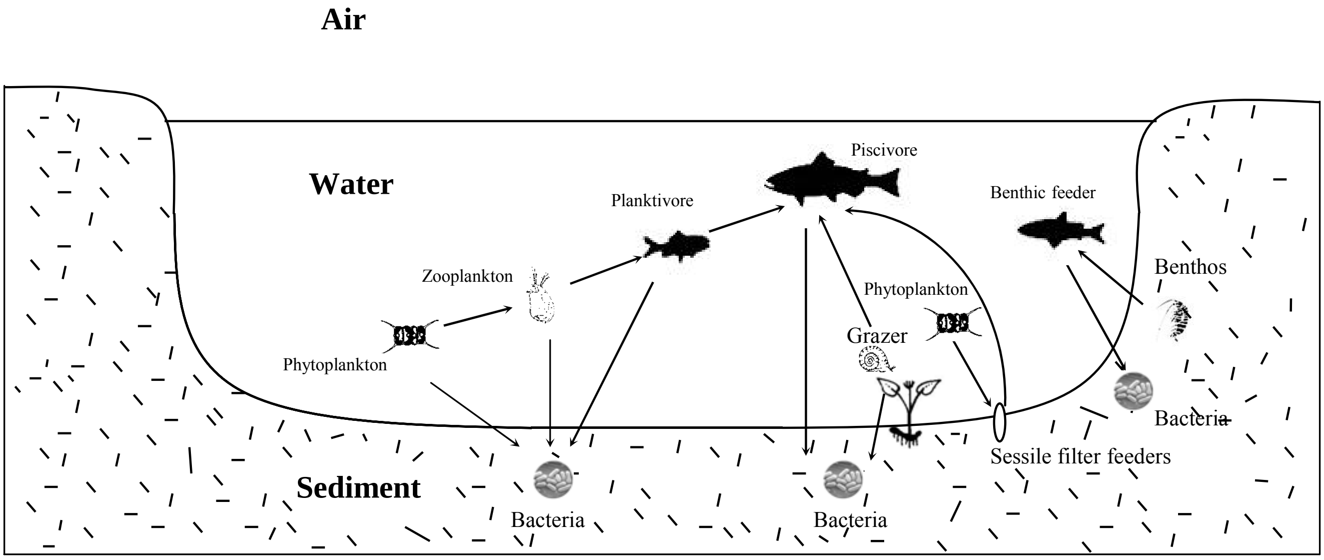

Fig. 4: Simplified food web for a freshwater ecosystem. Adapted/modified from Chapman et al. (2003), with permission

As is evident from the description in Appendix B, the laboratory ecotoxicity effect data for freshwater is dominated by test on these 3-4 trophic levels, represented by algae (phytoplankton), crustacean (zooplankton) and fish. However, as illustrated in Fig. 4, one more major trophic level exists, the reducers, here illustrated by bacteria.

The reducers are represented by micro-organisms, i.e. bacteria and fungi. Even though these organisms are at a low trophic level and may therefore serve as an early warning indicator of potential toxic effects, experience from bioassays (laboratory ecotoxicity tests) seems to indicate a general lower sensibility of these tests as compared to tests on organisms representing other trophic levels. In a review on bioassays for microbial systems (Mayfield 1998) several tests covering different approaches (e.g. growth rate, biomass, and enzyme activity) are described. Most of the evaluated tests are either characterised as not being sensitive enough to represent toxic responses in the natural environment (e.g. ATP assays and microcalorimetric assays) or not developed to a 'standardised' level (e.g. turbidostat culture system), and/or toxicity data is to a great extend lacking except for special chemicals (fungicides for fungi tests). Based on these arguments it is not recommended to include the reducers in the calculation of the ecotoxicity effect indicator.

Based on the arguments pointed out here, and the fact that within generic risk assessment, as described in e.g. the TGD (EC 2003a), three trophic levels are typically focused upon and therefore most data is available for these, the following trophic levels are recommended for inclusion in the estimation of HC50:

1. Primary producers (i.e. algae)
2. Primary consumers (i.e. invertebrates)
3. Secondary consumers (i.e. fish)

4 Endpoints

In LCA studies we typically deal with marginal concentration increases in the 'model' environment. At least if we calculate emissions for a 'small' functional unit. The emissions will therefore mostly give rise to potentially chronic effects but local emissions leading to potential acute effects may have significant importance as illustrated by for example Larsen et al. (2004b).

By choosing the chronic level we run into the problem with lack of chronic data for the main part of the tested chemicals (Larsen and Hauschild 2004a). Attempts to solve this problem are typically done by including acute data and extrapolating to chronic level by use of assessment factors (AFs). Especially within risk assessment, but also in existing LCIA methods like USES-LCA (Huijbregts et al. 2000) and EDIP (Hauschild et al. 1998), the AFs used are generally considered as conservative and used for estimating the Predicted No Effect Concentration (PNEC). However, a study by Forbes and Calow (2002b) on a limited database indicates that there could be an argument for increasing the AF used within tiered risk assessment by an order of magnitude. In the same study it is shown that acute-to-chronic ratio (ACR), on which the AFs are based, can be very different for different substances. An ACR (based on acute LC_{50} values compared with chronic LOEC values with growth rate as endpoint) of 100 – 1000 is not unusual (Forbes and Calow 2002b) most probably for substances with specific toxic mode of action (TMoA), e.g. pesticides, as opposed to a factor of well below or around 10 for substances with a non-specific TMoA (narcotics). As we are aiming at best estimate in LCA, we should avoid the use of conservative (and in some cases to low) AFs and instead use best estimate ones. For best estimate extrapolation, we need different AFs depending on the kind of TMoA of the substance in question and to obtain that, research is needed. Fortunately, for many of the known very toxic substances with specific TMoA (e.g. pesticides), chronic data already exists, but we are still faced with the problem for the main part of existing substance for which chronic toxicity is unknown. Facing the challenge of choosing between an indicator which is based solely on acute values, and an indicator based on chronic values and making use of assessment factors to a high degree, it seems preferable to choose the chronic indicator when we are aiming at obtaining a best estimate while taking the framework of LCA into account.

The endpoint for acute test results to be included in calculation of the EEI is EC_{50} (LC_{50}; IC_{50}) defined as the test concentration of the substance where 50% of the test organism dies (e.g. fish), are immobilized (e.g. *Daphnia*) or growth inhibited by 50% (algae).

For chronic tests the endpoint is also EC_{50} but here, the effects measured are chronic, e.g. inhibition of reproduction and reduced growth. For algae the endpoint (and the value) is the same as for the acute part, i.e. 50% inhibition of growth.

As the no observed effect concentration (NOEC, here defined as chronic NOEC) is the key value for estimating PNEC in risk assessment, many chronic ecotoxicity results have been published as NOECs. However, according to the standard test guidelines, also EC_{50}(chronic) should be recorded (at least for *Daphnia*) which is also done and published in some cases (ECOTOX 2003, IUCLID 2000).

Since the number of chronic EC_{50} values is relatively limited as compared to the number of NOECs, the estimation of missing EC_{50}(chronic)-values from NOECs is tempting, but also problematic. The NOEC value can be defined as "the highest concentration of the test substance that produces no statistically significant adverse effect on the exposed population of test organism when compared to an untreated control" (Chapman et al. 1996). It is therefore determined by hypothesis-testing leading to the fact that the value of NOEC needs to be one of the test concentrations. The determined value for NOEC is therefore highly dependent on the choice of test concentrations and the experimental variability (i.e. choice of test design), and may be more or less close to the 'true' highest concentration producing no adverse effect or true no effect concentration (NEC) (Solbé 1998). Several other arguments for the unsuitability of NOEC as a precise, unbiased estimate of toxicity are stated in Chapman et al. (1996) including the fact that calculation of confidence intervals is not possible for the NOEC. On the contrary, an EC_{50} estimate does not have to be one of the test concentrations, it is not dependent on the precision of the experiment, and a calculation of confidence intervals is possible. Based on these arguments and the fact that we are aiming for an effect-based indicator, it is recommended not to use NOEC values directly in the calculation of the ecotoxicity effect indicator.

As earlier stated, the indicator shall as a minimum be able to work on only one acute data value (EC_{50}) from each of the three trophic levels represented by algae, invertebrates (crustaceans) and fish. Even though this is a minimum it will be the dominating case due to data availability as described in Larsen and Hauschild (2004a). So, in most cases we are facing the challenge of estimating the most robust $HC50_{EC50}$(acute) based on three acute EC_{50}s and afterwards extrapolate this value to an $HC50_{EC50}$(chronic) value. Unfortunately, best estimate AFs for this extrapolation are not developed yet (Larsen and Hauschild 2004a), and research is needed in this area, which is outside the scope of this paper. However, as a starting point, a general assessment factor of 10 is recommended as described in Payet and Jolliet (2003). In the rest of this paper we will focus on acute values.

General considerations about choice of ecotoxicity tests in the context of LCA, and specific recommendations on test organism and test criteria to be included are described in Appendix B.

5 Estimation principles tested on real data

With the aim of finding the most robust effect indicator (i.e. $HC50_{EC50}$) based on only three data values, the different average approaches (i.e. geometric mean, median and mean) are tested on real substance examples below. The substances, which are presented in Table 1 represent different toxic modes of action (TMoA).

Table 1: Substances included in the test of different 'average approaches' to estimate $HC50_{EC50}$

Substance name	CAS No.	Type	TMoA	Lowest EC_{50}(acute) (mg/l)	Highest EC_{50}(acute) (mg/l)
2,3,4,6-Tetrachlorophenol	58-90-2	Intermediate (biocide)	?	0.09	10.1
4-Methyl-2-pentanone	108-10-1	Organic solvent	Base-line narcosis	170	780
2,4-Dichlorophenol	120-83-2	Organic solvent	Base-line narcosis	1.4	21
2-Chloroaniline	95-51-2	Intermediate	Polar narcosis	0.13	150
4-Nitrophenol	100-02-7	Intermediate	Polar narcosis	3.8	32
Dicamba	1918-00-9	Herbicide	Auxin-like growth regulator	0.061	750
Metribuzin	21087-64-9	Herbicide	Photosynthesis inhibitor	0.0117	147
Terbutylazine	5915-41-3	Herbicide	Photosynthesis inhibitor	0.0032	66
Pendimethalin	40487-42-1	Herbicide	Cell division and cell elongation inhibitor	0.0054	90.4
Azoxystrobin	131860-33-8	Fungicide	Mitochondrial respiration inhibitor	0.049	13
Dimethoate	60-51-5	Insecticide, acaricide	Cholinesterase inhibitor	0.14	560

Apart from different TMoA, the substances in Table 1 have been chosen to represent different ranges of acute toxicity within each trophic level or between the trophic levels, and different data availability. As seen from Table 1 the ratio between highest and lowest measured EC_{50} value for a substance lies from a factor 5 (4-methyl-2-pentanone) to a factor 20,000 (terbutylazine).

The TMoA indicated for each of the substances in Table 1 is taken from Russom et al. (1997) and The Pesticide Manual (Pest. Man. 1996). The EC_{50} values are mainly extracted from the US EPA database ECOTOX (2003) but also the ECB database IUCLID (2000) and data from RIVM (1999) are included. Only results from laboratory tests executed under certain standard conditions with freshwater pelagic 'standard' organisms, as described in Appendix B, are included. The tests on real data are described below and in further details in Larsen et al. (2004c).

5.1 Test for lognormality

It is here assumed that the species sensitivity distributions (overall and within each of the taxa algae, crustacean and fish, and between the taxa) for the substances depicted in Table 1, are lognormal, which is a condition for the use of geometric means. Actual tests for goodness of fit by use of the Anderson-Darling test as described in Aldenberg et al. (2002) require eight or more data points (D'Agostino1986, quoted by Aldenberg et al. 2002) and is thus only possible at the species and genus level by pooling all the taxa together. The result of the goodness of fit is shown in Table 2.

Table 2: The number of data values (EC_{50}s (acute)) at different levels for each of the included substances. Cases where a goodness of fit test can be performed (i.e. number of species or genuses ≥ 8) are shown in bold, and if lognormal distribution can not be rejected at the 5% significance level, the figure is marked with an asterisk (*). The Anderson-Darling test for goodness of fit (modified A^2 test statistics) is used according to Aldenberg et al. (2002, p. 57 and 91) and Stephens (1986, p. 122-125)

Substance	Total number of data[1]	Total number [2]		Number of algae [2]		Number of crustacean [2]		Number of fish [2]	
		Species	Genuses	Species	Genuses	Species	Genuses	Species	Genuses
2,3,4,6-Tetrachlorophenol	12	**9 ***	**8 ***	2	2	2	1	5	5
4-Methyl-2-pentanone	8	4	4	1	1	1	1	2	2
2,4-Dichlorophenol	20	**11 ***	**10 ***	3	2	1	1	7	7
2-Chloroaniline	15	6	5	3	2	1	1	2	2
4-Nitrophenol	35	**10 ***	**9 ***	3	2	1	1	6	6
Dicamba	10	5	5	2	2	1	1	2	2
Metribuzin	18	**11**	**11**	6	6	2	2	3	3
Terbutylazine	11	**10 ***	**10 ***	4	4	1	1	5	5
Pendimethalin	17	6	6	2	2	1	1	3	3
Azoxystrobin	6	6	6	3	3	1	1	2	2
Dimethoate	36	**9 ***	**9 ***	2	2	1	1	6	6

[1] Meaning total number of EC_{50} and LC_{50} data (including 'replicates' of the same species)
[2] Meaning total number of different genuses or species with EC_{50} or LC_{50} data

Due to lack of data on a sufficient number of species or genuses it has only been possible to test six of the substances for lognormal distribution of the species sensitivity, and only on the total species and total genus level - not within each of the taxa/trophic levels, i.e. algae, crustacean and fish. As shown in Table 2, lognormal distribution is only rejected for metribuzin at the 0.05 significance level ($\alpha = 0.05$). One reason for metribuzin failing the fitness test is a high representation (6) of algae species (which are highly sensitive, $EC_{50} = 0.01 - 0.15$ mg/l) as compared to only two species of crustacean ($EC_{50} = 12 – 35$ mg/l) and three species of fish ($EC_{50} = 3.4 – 97$ mg/l) for this substance. If the most sensitive algae species is excluded (i.e. $EC_{50} = 0.0117$, new most sensitive $EC_{50} = 0.0119$), lognormal distribution can not be rejected at the 0.05 significance level.

For estimation of the mean of the sensitivity distribution, it is a requirement that data are normally distributed. Testing the same six pair of data sets for normality reveals that for all but one (2,4-dichlorophenol), normal distribution is rejected at the 0.05 significance level. For 2,4-dichlorophenol the sensitivity distribution for species and genuses are only just significant at the 0.05 significance level (A^2 (modif.) equals 0.711 and 0.701 respectively, with a threshold limit of 0.752 at the 0.05 significance level) as opposed to the test for lognormality on the same substance, which shows significance at the 0.15 and 0.25 significance level for species and genuses respectively. With the rejection of the normal distribution hypothesis, the use of mean estimates on these tested pairs of data sets is in principle meaningless for all but one, and the results confirm that toxicity data are typically not normally distributed (but lognormally distributed) as stated in Section 1.

5.2 Results of the test on real data

As an example all the data collected for 2,3,4,6-tetrachlorophenol are shown in Table 3. Data, calculations, references etc. for all 11 substances can be found in Larsen et al. (2004c).

Table 3: Data for 2,3,4,6-tetrachlorophenol with geometric means (GM) on level of species, genus and trophic level (mg/l). Eight fictive scenarios (S) are constructed with all the possible combinations of highest and lowest measured EC_{50} value from each of the three trophic levels represented by the three taxonomic groups algae, crustacean and fish

Taxon	Species	EC_{50} (acute)	GM-species level	GM-genus level	GM-trophic level	S1	S2	S3	S4	S5	S6	S7	S8
Algae	*Chlorella vulgaris*	10.1	10.1	10.1	3.624	10.1	10.1	10.1	10.1				
	Selenastrum capricornutum	1.3	1.3	1.3						1.3	1.3	1.3	1.3
Crustacea	*Daphnia galeata mendotae*	0.58	0.58	0.312	0.312	0.58	0.58			0.58	0.58		
	Daphnia magna	0.29	0.167										
	Daphnia magna	0.18											
	Daphnia magna	0.09						0.09	0.09			0.09	0.09
Fish	*Poecilia reticulata*	1.085	0.807	0.807	0.475	1.085		1.085		1.085		1.085	
	Poecilia reticulata	0.6											
	Pimephales promelas	1.03	1.03	1.03									
	Oryzias latipes	0.62	0.62	0.62									
	Oncorhynchus mykiss	0.334	0.334	0.334									
	Lepomis macrochirus	0.14	0.14	0.14			0.14		0.14		0.14		0.14
Geometric mean		0.546	0.679	0.749	0.812	1.852	0.936	0.995	0.503	0.935	0.473	0.503	0.254
Median		0.590	0.620	0.713	0.475	1.085	0.580	1.085	0.140	1.085	0.580	1.085	0.140
Mean		1.362	1.675	1.830	1.470	3.922	3.607	3.758	3.443	0.988	0.673	0.825	0.510
$LowEC_{50}$		0.090	0.140	0.140	0.312	0.580	0.140	0.090	0.090	0.580	0.140	0.090	0.090

As shown in Table 3, the different scenarios (S1, S2, ….) create eight fictive data sets by combining the highest and the lowest measured value from each of the taxa into new data sets each with three values. The idea is to see how robust different approaches to estimate $HC50_{EC50}$ are to these combinations, when we - as in most cases - only know three data and not twelve as here. By taking the extreme values within each taxon we obtain the maximum variation within our fictive data sets.

The distributions of the geometric mean (GM), the arithmetic mean (Mean), the median (Median) and the lowest EC_{50} ($LowEC_{50}$) for the eight fictive scenarios in Table 3 are shown in **Fig. 5**. Furthermore, the geometric mean and the median based on either the full data set for all species (sp.) or the geometric means within each taxon or trophic level (troph) are also shown.

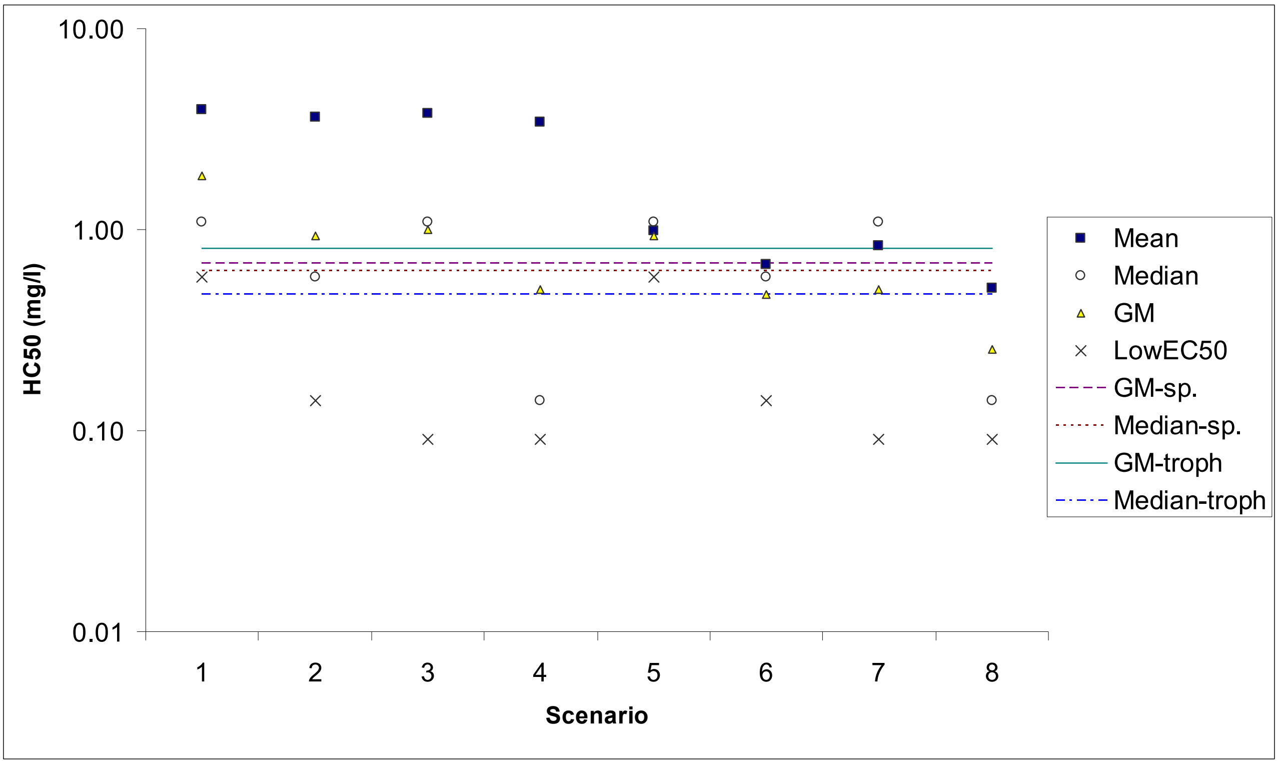

Fig. 5: Average estimates for the eight fictive scenarios for 2,3,4,6-tetrachlorophenol

From Table 3 and Fig. 5 it can be seen that the geometric mean based on the geometric means for each of the three taxa (i.e. the average on trophic level, termed GM-troph, value 0.812) and the geometric mean based on the average on species level (termed GM-sp., value 0.679) are quite close in this case (difference about a factor 1.2). The geometric mean based on the average on genus level (termed GM-genus, value 0.749) is even closer to the GM-troph. The two medians i.e. the average on the species level (termed Median-sp., value 0.620) and the average on the throphic level (termed Median-troph, value 0.475) are both lower than the GM-troph and GM-sp. (max. difference about a factor 1.7). But all these different measures of the average based on the full data set are within the 95% confidence limits of the GM-troph (0.0312 - 21.1) as well as the 95% confidence limits of the GM-sp. (0.256 – 1.80). These and the following confidence limits are estimated on basis of the t-statistics according to Campbell (1974, p. 142-144 and Table A12).

As would be expected, the mean values for the eight scenarios are generally higher than the other average measures, only exceeded by the median in two cases (scenario 5 and scenario 7), see Fig. 5. The GMs for the different scenarios are distributed around the GM-troph and the other averages based on the full data set. This is also the case for the scenario-based medians, but for 2,3,4,6-tetrachlorophenol with a small tendency to more extremes (scenario 4 and scenario 8). The scenario values for the LowEC$_{50}$ are logically the lowest values, but in two cases higher than the Median-troph (scenario 1 and scenario 5).

If we calculate the ratio between the highest HC50$_{EC50}$ and the lowest HC50$_{EC50}$ estimated within the scenarios for each of the different approaches we get 7.3 (GM), 7.8 (median), 6.4 (LowEC$_{50}$) and 7.7 (mean). In this respect, they are quite identical.

If we calculate the 95% confidence limits for the GMs we get the result shown in **Fig. 6**. Here the confidence limits are quite wide for some of the scenarios (especially scenario 2, 3 and 4) due to a high standard deviation on the GM (large difference between the two extreme values) combined with the fact that the number of data is only three.

As an alternative the 90% confidence limits and the 80% confidence limits for the GM may be estimated. The 80% confidence limits for the GM are shown in **Fig. 7** together with the 95% and the 90% confidence limits for the GM-troph.

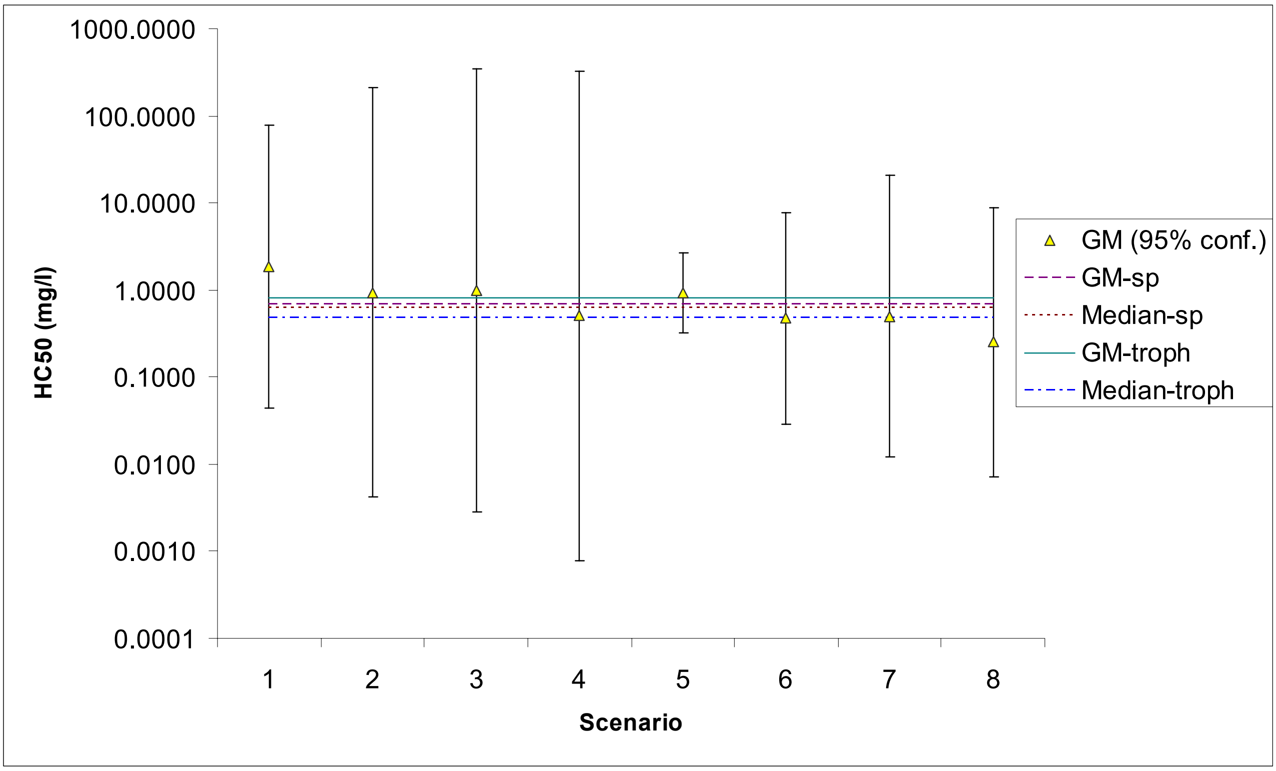

Fig. 6: Geometric means (GMs) with 95% confidence limits for the eight fictive scenarios for 2,3,4,6-tetrachlorophenol

Even after a reduction of the confidence limits to 80% for this substance, the confidence limits for all the scenarios still enclose the GM-troph as seen in Fig. 7.

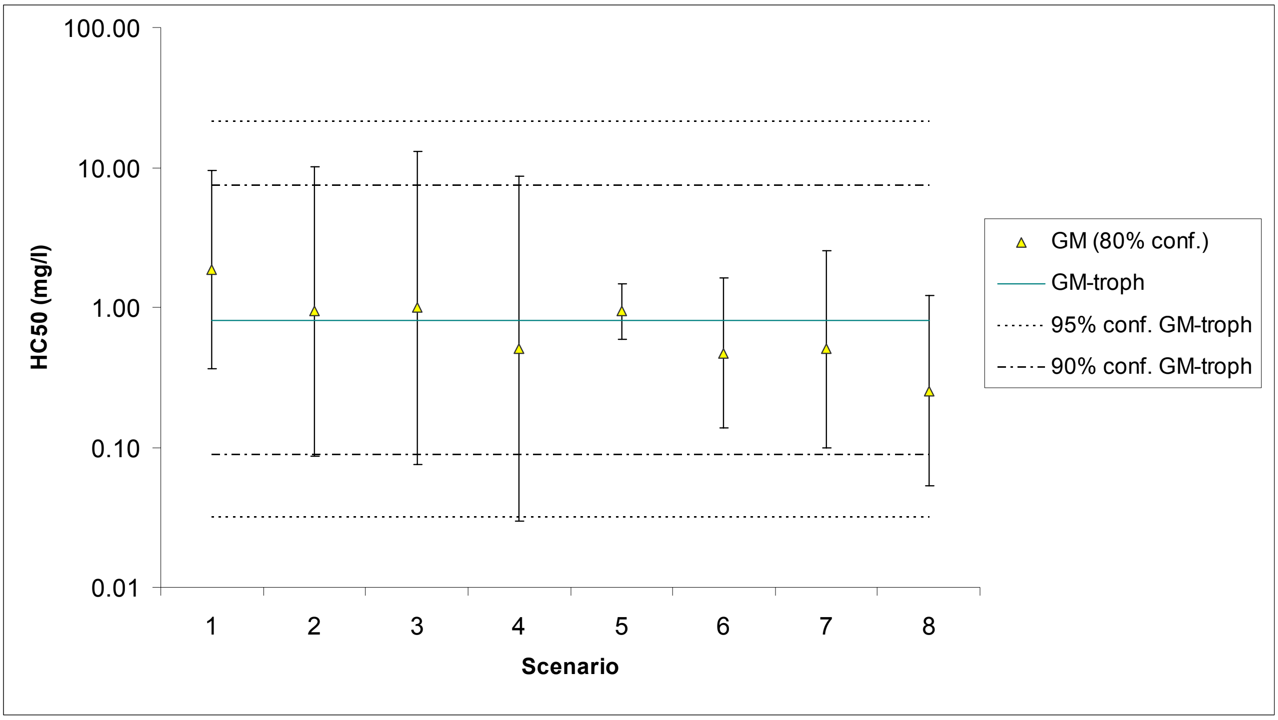

Fig. 7: Geometric means (GMs) with 80% confidence limits for the eight fictive scenarios for 2,3,4,6-tetrachlorophenol

Another way to define the limits around the geometric mean is to use the lowest value in the data set (with three observations) as the lower limit and the highest value in the data set as the upper limit. This approach is shown in **Fig. 8.** In this case, the limits for all eight scenarios also enclose the GM-troph, and the width of the confidence limits is almost identical to, or a bit more narrow than, the 80% confidence limits as shown in Fig. 7. Also shown in Fig. 8 are the max-min limits around the GM-troph defined as the highest value (upper limit) and the lowest value (lower limit) among the three GM-troph-level values (algae, crustacean, fish), see Table 3.

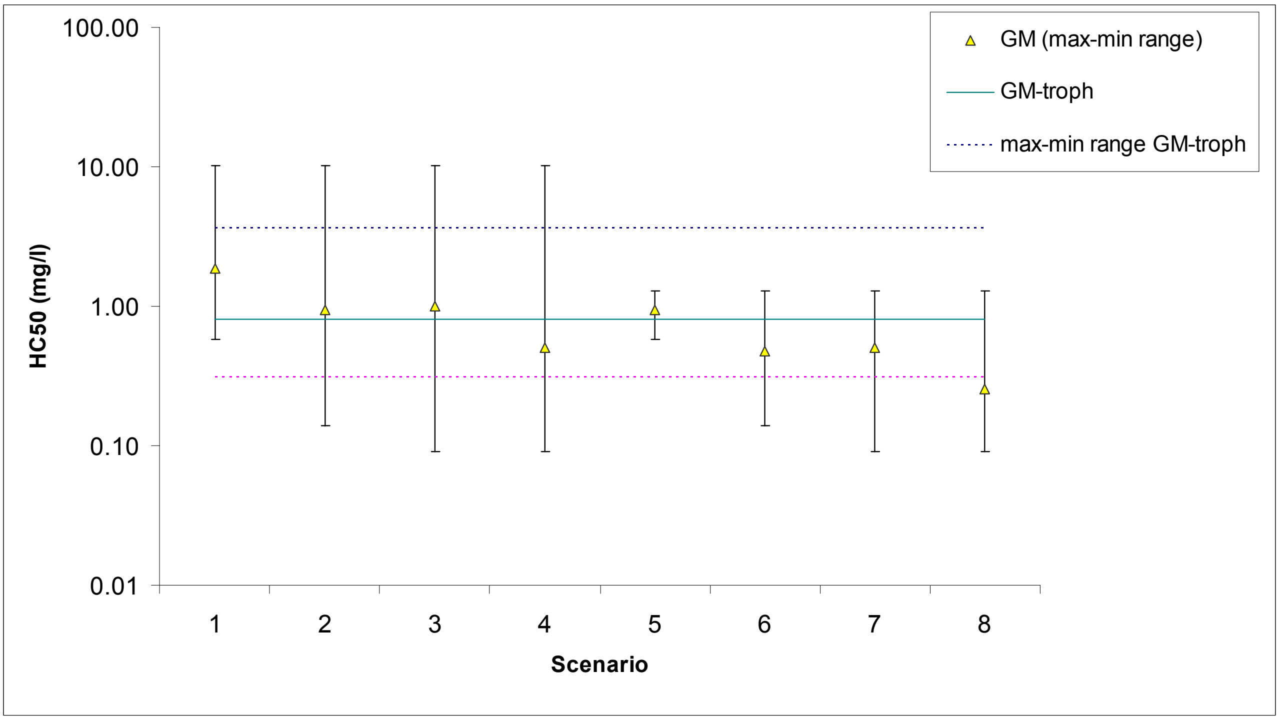

Fig. 8. Geometric means (GMs) with max-min limits for the eight fictive scenarios for 2,3,4,6-tetrachlorophenol

Table 4: Ratio between highest and lowest scenario-estimated $HC50_{EC50}$ for substances included in the test of different 'average approaches'

Substance name	Ratio between highest and lowest estimated $HC50_{EC50}$			
	GM	Median	$LowEC_{50}$	Mean
2,3,4,6-Tetrachlorophenol	7.3	7.8	6.4	7.7
4-Methyl-2-pentanone	1.2	1.0	1.0	1.3
2,4-Dichlorophenol	3.8	6.6	3.6	3.1
2-Chloroaniline	4.2	1.1	14	4.2
4-Nitrophenol	10	7.7	8.4	11
Dicamba	12	6.4	38	6.7
Metribuzin	24	29	13	32
Terbutylazine	11	13	33	3.8
Pendimethalin	38	37	5	230
Azoxystrobin	8.5	4.2	5.3	18
Dimethoate	85	840	46	29

The analyses shown above for 2,3,4,6-tetrachlorophenol are repeated for all 11 substances shown in Table 1 and reported in Larsen et al. (2004c). For every substance the ratio between the highest $HC50_{EC50}$ and the lowest $HC50_{EC50}$ estimated within the scenarios for each of the different approaches is shown in Table 4.

These ratios show that the variation in GM is higher (a factor 1.2-3.8) than the variation in the median for six of the analysed substances. For the remaining five substances the variation in the median is highest. In most cases, the ratio of the variation in the median to the variation in the GM lies at the level of a factor 1.1-1.7 but in one case (dimethoate), the ratio is about a factor of 10. This is an example of the sensitivity of the median when a shift occur in a three value data set from two low values and one high to two high values and one low as shown theoretically in Fig. 2 for a five value data set ('jumping median').

An example illustrating to some degree the theoretical case shown in Fig. 1, although the medians are not identical in this example, is provided by 4-nitrophenol and metribuzin. On a three value data set, thus representing geometric means at each trophic level (14.6; 12.0; 11.6 for 4-nitrophenol and 30.1; 20.6; 0.038 for metribuzin), the median approach gives the values 12.0 (4-nitrophenol) and 20.6 (metribuzin) indicating that 4-nitrophenol on average is more toxic than metribuzin despite the fact that metribuzin is very toxic to algae. The geometric mean on the other hand gives the values 12.7 (4-nitrophenol) and 2.86 (metribuzin) indicating a higher average toxicity of metribuzin.

The calculated averages on the species (or genus) level and the trophic level are in most of the cases here quite close. But, in some of the investigated cases, the difference in the number of species represented at each trophic level leads to large difference in average toxicity. One example is metribuzin for which the GM-troph is four times higher (2.9/0.73 = 4.0)) than the GM-sp. or GM-genus. The main reason for this difference is that the substance is especially toxic to algae which are represented by six species/genuses whereas crustaceans only are represented by two species/genuses, and fish only by three species/genuses. The effect is even more pronounced when comparing the Median-sp. or Median-genus with the Median-troph giving rise to a ratio of 140 in difference (21/0.15 = 140).

If we look at the results of the different approaches used to calculate confidence limits around the geometric mean for all 11 substances, it can generally be concluded that:

- 95% confidence limits around GM-troph are in most cases very wide making the differentiation between the average toxicity among chemicals impossible
- Though more narrow than the 95% confidence limits, the 90% confidence limits around GM-troph are still relatively wide
- Even the 80% confidence limits around the GM-troph are a bit wider or as narrow as limits based on the min-max values of the three data GM-troph data set (based on one value from each trophic level)
- The limits based on min-max values are relatively narrow for the substances tested here and in all but one case (i.e. 4-nitrophenol, not shown), all eight fictive scenarios overlap with the GM-troph calculated on the basis of the full data set (see example in Fig. 8)
- In the case of 4-nitrophenol not even the 95% confidence limits around the GM (scenario 1 and scenario 8) overlap with the GM-troph and for these two extreme scenarios the estimated GMs are 45 mg/l and 4.4 mg/l and with a GM-troph value of 13 mg/l this gives rise to an ‘error’ of a factor 3-4.

The GM-troph and the associated min-max limits for all 11 substances are shown in **Fig. 9.**

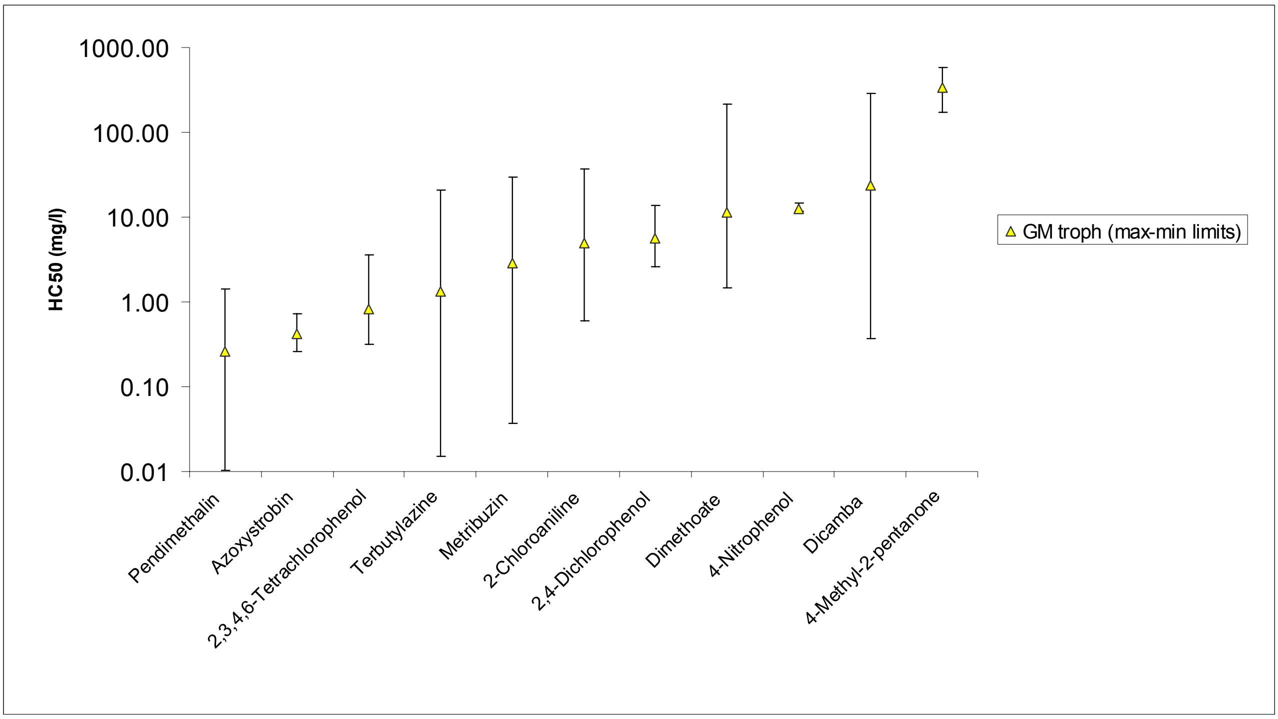

Fig. 9: GM-troph with min-max limits for the 11 included substances (mg/l)

6 Conclusion, recommendations and outlook

On the basis of theoretical and practical analyses of the different average approaches, including different ways of calculating (confidence) limits for the data sets of typically three observations (one from each of the three trophic levels), the following is recommended for the EEI:

- The indicator should be based on the GM-troph calculated as the geometric mean of the three EC_{50} values, one from each trophic level represented by algae, invertebrates (crustaceans) and fish.

- If more than one EC_{50} value from each trophic level is available then the GM-troph should be calculated as the geometric mean of the geometric means for each trophic level (GM-trophic-levels). The GM-trophic-levels is calculated as the geometric mean of the GM-genus-level which again are calculated as the geometric mean of the GM-species-level which in their turn are calculated as the geometric mean of the single EC_{50} values for each species as shown for 2,3,4,6-tetrachloropehol in Table 3.
- As limits around the GM-troph, the lowest EC_{50} value should be used as the lower limit, and the highest EC_{50} value as the upper limit in data sets with only three EC_{50} values, i.e. one from each trophic level.
- If more than one EC_{50} value from each trophic level is available then the max-min limits around the GM-troph should be based on the three GM-trophic-level values, i.e. the lowest GM-trophic-level value is used as the lower limit and the highest GM-trophic-level value as the upper limit.

By using the GM-troph it is suggested to put equal weight on each of the three trophic levels instead of relying on an arbitrary species representation with weights indirectly determined by for example regulatory priority and therefore doubtful ecological relevance. So, by making a conscious choice of equal weights to each of the trophic levels, we try to avoid the possible bias from data sets with highly unequal number of tested species/genuses among the three trophic levels, which would occur if GM-sp. (or GM-genuses) were used instead. As suggested by Forbes and Calow (2002a), a way to increase the ecological relevance when dealing with the species sensitivity distribution approach might be to assign weights to the input values from each taxon (or trophic level) reflecting the relative abundance of different taxa in the community/ecosystem in question. Combining this approach with theories of functional redundancy of species (Pratt and Cairns 1996) could be a very interesting research area for the further development of the EEI.

As recommended it is not proposed to determine a statistically estimated uncertainty as basis for the limits around the GM-troph even though the number of input data is higher than three in some cases. This is proposed in order to use the same approach for all substances and because the max-min approach is simple and seems to work fine (at least for the 11 substances tested). Furthermore, in most cases only three relevant data values are available anyway. The results obtained here indicate that the max-min range of the three-data GM-troph (no matter the database) in practice includes the 'true' GM-troph (based on the full data set), as well as the confidence limits. Even though the max-min limits cannot be used for testing statistically significant differences between EEIs they may be used for giving reasonable certainty that the 'true' GM-troph is included.

The test of the different average approaches undertaken here is only based on 11 different substances comprising seven different TMoA. To verify the general value of the outcome, a higher number of substances covering a larger number of TMoA should be tested.

It is recommended to use EC_{50}(chronic) values when possible but as only acute data will be available in most cases, the use of best estimate assessment factors are recommended to extrapolate from acute to chronic values. Even though there is a need for research in this area, an acute to chronic ratio of 10 between $HC50_{EC50}$(acute) and $HC50_{EC50}$(chronic) is recommended as a starting point.

Because of the comparative framework of LCIA seeking best estimates, it is recommended only to use test results from laboratory tests, fulfilling certain standard conditions, e.g. standard organism and restrictions on test duration and endpoints as described in Appendix B, when estimating the $HC50_{EC50}$ value. These standard conditions are described here for acute tests, but detailed criteria for choice of chronic data still need to be developed.

The ability of a geometric mean to represent the toxicity (including chronic toxicity) of very toxic substances and very sensitive species has not been dealt with yet, and further research is needed. However, it may be anticipated, on the basis of the results from the tests performed here of different average approaches on 11 substances (including very toxic pesticides, e.g. terbutylazine), that the GM-troph with its max-min limits at least to some degree accounts for very toxic substances if representative toxicity data are available.

As mentioned, test on a wider range of substances should be performed to further verify the GM-troph approach and its ability to represent substances that are very toxic to specific species. Also further research on detailed criteria for choice of chronic test data should be included as well as studies on best estimate assessment factors for acute to chronic extrapolation.

Acknowledgement

This paper is highly influenced by discussions that have been going on in the OMNIITOX community since late 2002, especially in the ecotoxicity task force. The authors therefore like to give special thanks to Sverker Molander and Jérôme Payet for fruitful discussions and input. Also thanks to Bo Nyström who participated in the work at an early stage. The report on which this paper is based was reviewed by two external experts in connection with the Lausanne Review Workshop arranged by the UNEP-SETAC Life Cycle Initiative, 1 and 2 December 2003, Lausanne, Switzerland. Thanks to the two external experts Peter Chapman and Nico van Straalen for constructive review comments. Also thanks to Ole Kusk for discussions and input on algae test. Finally, the authors gratefully acknowledge the financial support of the Danish Ministry of Science, Technology and Innovation given to KEMI (Centre for Chemicals in Industrial Production).

References

Aldenberg T, Jaworska J, Traas TP (2002): Normal Species Sensitivity Distributions and Probabilistic Ecological Risk Assessment. Chapter 5 in: Species Sensitivity Distribution in Ecotoxicology. Posthuma L., Suter II G.W. and Traas T.P. (eds.), pp. 49-102. Lewis, Boca Raton, FL, USA

Bliss CI (1935): The calculation of the dosage-mortality curve. Ann. Appl. Biol. 22, 134-167

Cairns JJr, Niederlehner BR, Smith EP (1995): Ecosystem Effects: Functional End Points. Chapter 19 in: Fundamentals of Aquatic Toxicology. Rand, G.M. (ed.), pp. 589-607. Taylor & Francis, Philadelphia, USA

Calow P (1998): General Principles and Overview. Chapter 1 in: Handbook of Ecotoxicology. Calow P (ed.), pp. 1-5. Blackwell Science, Oxford, Great Britain

Campbell RC (1974): Statistics for Biologists. Second edition. Cambridge University Press, Cambridge, Great Britain

Chapman PF, Crane M, Wiles JA, Noppert F, McIndoe EC (1996): Asking the Right Questions: Ecotoxicology and Statistics. SETAC, Belgium. The report of a workshop held in Royal Holloway University of London, Egham, Surrey, United Kingdom, 26-27 April 1995

Chapman PM, Wang F, Janssen CR, Goulet RR, Kamunde CN (2003): Conducting ecological risk assessments of inorganic metals and metalloids: current status. Human Ecol. Risk Assess. 9, 641-697

D'Agostino, RB (1986): Tests for normal distribution. In: Goodness-of-Fit Techniques. D'Agostino, R.B., Stephens, M.A., (eds.), pp. 367-419. Marcel Dekker, New York, USA

EC (2003a): Environmental Risk Assessment. Chapter 3 (Part II) in: Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances, Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Institute for Health and Consumer Protection. European Commission. ECB, JRC, Ispra, Italy

EC (2003b): Proposal for a Regulation of the European Parliament and of the Council concerning the Registration, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency and amending Directive 1999/45/EC and Regulation (EC) {on Persistent Organic Pollutants}. COM (2003) 644, Brussels, 29 October 2003

EEC (1967): Approximation of laws, regulations and administrative provision relating to the classification, packaging and labelling of dangerous substances (Council Directive 1967/548/EEC, June 27)

ECOTOX (2003): ECOTOXicology Database system. US EPA: http://www.epa.gov/ecotox/

Forbes VE, Calow P (2002a): Species Sensitivity Distribution Revisited: A Critical Appraisal. Human and Ecological Risk Assessment 8 (3) 473-492

Forbes VE, Calow P (2002b): Extrapolating in Ecological Risk Assessment: Balancing Pragmatism and Precaution in Chemical Controls Legislation. BioScience 52 (3) 249-257.

Goedkoop M, Spriensma R (2001a): The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Report. Third edition. Pré Consultants, Amersfoort, The Netherlands http://www.pre.nl

Goedkoop M, Spriensma R (2001b): The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Annex. Third edition. Pré Consultants, Amersfoort, The Netherlands http://www.pre.nl

Hauschild M, Pennington D (2002): Indicators for Ecotoxicity in Life-Cycle Impact Assessment. Chapter 6 in: Life-cycle Impact Assessment: Striving Towards Best Practice, Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds.), pp. 149-176. SETAC-Europe, Brussels, Belgium

Hauschild M, Wenzel H, Damborg A, Tørsløv J (1998): Ecotoxicity as a criterion in the environmental assessment of products. Chapter 6 in: Environmental Assessment of Products: Volume 2: Scientific background, London, Hauschild M, Wenzel H (eds.), pp. 203-314. Chapman & Hall, London, Great Britain

Huijbregts M, Thissen U, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AM J, Wegener Sleeswijk A, Reijnders L (2000): Priority assessment of toxic substances in life cycle assessment. Part I: Calculation of toxicity potentials for 181 substances with the nested multi-media fate, exposure and effects model USES-LCA. Chemosphere 41 (2000) 541-573

ISO (2000): ISO 14042: Environmental management – Life cycle assessment – Life cycle impact assessment. International Organisation for Standardisation, Geneva, Switzerland

Kusk O (2003): Personal communication with Ole Kusk, Environment and Resources, Technical University of Denmark

IUCLID (2000): European Chemical Bureau: IUCLID CD-ROM Year 2000 edition. Public data on high volume chemicals. ISBN 92-828-8641-7

Larsen HF, Hauschild M (2004a): Evaluation of ecotoxicity effect indicators for use in LCIA. *Submitted to Int J LCA*

Larsen HF, Hansen MS, Hauschild M (2004b): Including chemical-related impact categories in LCA on printed matter – does it matter? *Submitted to Journal of Cleaner Production*

Larsen HF, Payet J, Molander S, Hauschild M (2004c): Implementation of the OMNIITOX Base Model. Contribution to work package 8 of the OMNIITOX project as part A of appropriate deliverable D41. Part VIII – Implementation of the ecotoxicological effects module. EC Project contract G1RD-CT-2001-00501 http://www.omniitox.net/

Lewis MA (1998): Freshwater Primary Producers. Chapter 3 in: Handbook of Ecotoxicology. Calow P. (ed.), pp. 28-50. Blackwell Science, Oxford, Great Britain

Mayfield CI (1998): Microbial Systems. Chapter 2 in: Handbook of Ecotoxicology. Calow P (ed.), pp. 9-27. Blackwell Science, Oxford, Great Britain

Newman MC, Dixon P M (1996): Ecologically Meaningful Estimates of Lethal Effect in Individuals. Chapter 8 in: Ecotoxicology - A Hierarchical Treatment, Newman, MC, Jagoe, CH (eds.), pp. 225-253. Lewis, Boca Raton, FL, USA

Newman MC, Ownby DR, Mézin LCA, Powell DC, Christensen TRL, Lerberg SB, Anderson B-A, Padma TV (2002): Species Sensitivity Distributiions in Ecological Risk Assessment: Distributional Assumptions, Alternate Bootstrap Techniques, and Estimation of Adequate Number of Species. Chapter 7 in: Species Sensitivity Distributions in Ecotoxicology. Posthuma L, Suter II G.W. and Traas TP (eds.), pp. 119-132. Lewis, Boca Raton, FL, USA

OECD (1998): Detailed Review Paper on Aquatic Testing Methods for Pesticides and Industrial Chemicals. Part 1: Report and Part 2: Annexes. Series on Testing and Assessment No. 11. OECD, Paris, France

OECD (2003): Manual for investigations of HPV chemicals. Chapter 2: SIDS, the SIDS plan and the SIDSA dossier. OECD Existing Chemicals Programme http://www.oecd.org

Payet J, Jolliet O (2003): Comparative assessment of the toxic impact of metals on aquatic ecosystems: The AMI method. In: Life-Cycle Assessment of Metals: Issues and research directions. Alain Dubreuil (ed). SETAC, Pensacola, FL, USA

Payet J, Larsen HF (2004): Endpoint Modelling for the Life Cycle Impact Assessment on Ecosystems. *In prep.*

Payet J, Pennington D, Hauschild M, Jolliet O (2003). Comparative Assessment of toxic Impact on Aquatic Ecosystems: The AMI method (Assessment of the Mean Impact). *Submitted to Environ. Toxicol. Chem.*

Pennington D, Payet J, Hauschild M (2004). Aquatic ecotoxicological indicators in life-cycle assessment. Environ. Toxicol. Chem. 23 (7) 1796-1807

Pest. Man (1996): The Pesticide Manual. 11.ed. Book. ISBN 1 901396 11 8. The British Crop Protection Council, 49 Downing Street Farnham, Surrey GU9 7PH, UK

Pratt JR, Cairns JJr (1996): Ecotoxicology and the Redundancy Problem: Understanding Effects on Community Structure and Function. Chapter 12 in: Ecotoxicology - A Hierarchical Treatment. Newman MC, Jagoe CH (eds.), pp. 347-370. Lewis, Boca Raton, FL, USA

RIVM (1999): Appendix A in: Environmental Risk Limits in The Netherlands. Part III Data. Könemann H (ed.). Report No. 601640 001. RIVM, Bilthoven, The Netherlands

Russom CL, Bradbury SP, Broderius SJ, Hammermeister DE, Drummond RA (1997): Predicting modes of toxic action from chemical structure: Acute toxicity in the fathead minnow (*Pimephales promelas*). Environmental Toxicology and Chemistry 16 (5) 948-967

Sand-Jensen K (2000): Økologi og biodiversitet. Overordnede mønstre for individer, bestande og økosystemer. Gads forlag, København, Danmark.

Stephens MA (1986): Tests based on EDF statistics. In: Goodness-of-Fit Techniques. D'Agostino, R.B., Stephens, M.A. (eds.), pp. 97-193. Marcel Dekker, New York, USA

Solbé JF, De LG (1998): Freshwater Fish. Chapter 5 in: Handbook of Ecotoxicology. Calow P. (ed.), pp. 66-82. Blackwell Science, Oxford, Great Britain

Udo de Haes HA, Lindeijer E (2002): The conceptual Structure of Life-Cycle Impact Assessment. Chapter 8 in: Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich E, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington D, Potting J, Steen B (eds.): Life-cycle Impact Assessment: Striving Towards Best Practice, pp. 209-225. SETAC-Europe, Brussels

US EPA (2000): Data collection and development on high production volume (HPV) chemicals. Federal Register 65 (248) 81686-81698 http://www.epa.gov/chemrtk/

Versteeg DJ, Belanger SE, Carr GJ (1999): Understanding single-species and model ecosystem sensitivity. Data-based comparison. Environ. Toxicol. Chem. 18, 1329-1346

Whittaker RH (1975): Communities and Ecosystems. Second edition. Macmillan, New York, USA

Glossary

AF	Assessment Factor
EC_{50}	Effect Concentration (50% of test organism affected)
EDIP	Environmental Design of Industrial Products
EEI	Ecotoxicity Effect Indicator
GM	Geometric Mean
HC50	Hazardous Concentration for 50% of included species

LC_{50}	Lethal concentration (50% of test organism dead)
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
LOEC	Lowest Observed Effect Concentration
$LowEC_{50}$	Lowest EC_{50}
NEC	No Effect Concentration
NOEC	No Observed Effect Concentration
OECD	Organisation for Economic Co-operation and Development
OMNIITOX	Operational Models aNd Information tools for Industrial applications of eco/TOXicological impact assessments
PAF	Potentially Affected Fraction of species
PNEC	Predicted No Effect Concentration
PVF	Potentially Vanished Fraction of species
QSAR	Quantitative Structure Activity Relationship
SSD	Species Sensitivity Distribution
TGD	Technical Guidance Document
TMoA	Toxic Mode of Action

Appendix A. Environmental compartments

For an EEI a distinction is typically made between at least the two compartments water and soil as in the EDIP method (Hauschild et al. 1998) and the Eco-indicator 99 method (Goedkoop and Spriensma 2001a, 2001b). In other LCIA methods like USES-LCA (Huijbregts 2000) a more detailed distinction is made. Water is thus divided into freshwater and saltwater which is further divided into a pelagic and a sediment part. In risk assessment a distinction is typically also made between the aquatic compartment (pelagic) and the sediment (benthic) as described in the TGD (EC 2003a). From an ecological point of view the pelagic and the benthic (sediment) compartment are quite different with different types of organisms but in most cases with high interaction.

In order not to create bias in the effect indicator by mixing up two quite different habitats/compartments (e.g. due to lack of sediment data in many cases), it is recommended to distinguish between the pelagic and the sediment compartment. Tests on benthic or sediment dwelling organism should be included in a separate sediment compartment. Same basic estimation principle as for the freshwater pelagic compartment may be used, and lack of toxicity data could as a starting point be solved by use of the equilibrium partitioning method (EC 2003a). Also for the marine compartment, at least separated in a pelagic and a sediment compartment, and the soil (terrestrial) compartment, the same approach may be used, but based on saltwater organism and soil organism respectively. However, the inclusion of the marine and soil compartment needs further research, if the average PAF approach (i.e. GM-troph) is going to be applied, and this lies outside the scope of this paper.

Appendix B. Ecotoxicity tests

Appendix B.1. Overall performance criteria

Calow (1998) defines five performance criteria for ecotoxicity tests:

- Relevance, ecological realism
- Reproducibility
- Reliability
- Robustness
- Repeatability/sensitivity

In LCIA, we are integrating impacts over time and space, so, in that sense, we are far from ecological realism of the potential effect of the integrated emissions we estimate. This restriction, dictated by the nature of the life cycle or product system, and the fact that the LCA is focused on a functional unit rather than full output from the processes, points in the direction of not putting highest priority on ecological relevance. The fact that EEI is to be used in the comparative framework of LCIA, i.e. for comparison of emitted substances, puts the focus on reproducibility, robustness and repeatability/sensitivity.

What we are dealing with in LCIA is anticipatory tests (as opposed to assessment tests) where reproducibility is important (Calow 1998). On the other hand if we are dealing with site specific LCIA, we will approach the relevance of using assessment tests because ecological realism may become more important.

As our goal is to treat all chemicals equally, we should aim at choosing a set of tests reflecting the sensitivity of representative 'standard' organism from at least three trophic levels. This should be done in a way where the knowledge of today is taken into account, trying to avoid bias due to differences in sensitivity of haphazard test organism included. For most of the chemicals to be modelled by the EEI, we only have access to three acute data values, i.e. $E(L)C_{50}$ values for fish, daphnia and algae, as defined by for example the proposal for a new EU legislation on chemicals, i.e. REACH, EC (2003b) and the OECD work on investigations of high production volume chemicals (OECD 2003). Inclusion of non-standardised test result values in the calculation of the effect indicators, in those cases where it is possible, will increase variance and most probably create bias because the type and availability of such data is very variable among chemicals.

Furthermore, as illustrated by Newman and Dixon (1996), when comparing the predominant dose or concentration response methods (time endpoint methods) with time response methods (time to death, TTD methods), exposure time and covariance from factors like sex, bodyweight and genotype can have significant influence on the acute lethal EC_{50} determined in a laboratory test. These results strengthen the arguments for only using results from standardised tests when seeking best estimate in a comparative framework based on few available data.

There are thus good reasons to aim at basing the effect indicator exclusively on results from use of standardised test guidelines and standardised test organisms. However, we recognize that this kind of information in many cases is not directly available from the data sources typically used, e.g. ECOTOX (2003), and many test data which could be very useable (if reliable) are not produced under conditions strictly following a standardised test guideline. Therefore, besides the standard test guidelines, focus in the following sections will also be on test species and some other of the key test criteria to be used when choosing relevant data input.

Appendix B.2. Specific demands on ecotoxicity tests

If we look at standard freshwater laboratory tests, single species tests are dominating and the results are to a large extent used for regulatory purposes (e.g. water quality criteria) as reflected in the EU legislation on chemicals, i.e. Annex V of 67/548/EEC (EEC 1967) and in USA for example the 'Chemical Right-to-Know Initiative' on high production volume chemicals (US EPA 2000). A lot of work on standardisation, evaluation etc. on single species laboratory tests has therefore been done, and ecotoxicity test data comes almost exclusively from this source.

Below, is a short assessment and recommendation on which key test criteria (i.e. endpoint, species and test duration) to focus upon when choosing acute data for primary producers, primary consumers and secondary consumers, to be included in the estimation of the EEI. For further evaluation of acute tests and key test conditions including recommendations on standard test guidelines, see Larsen et al. (2004c).

Appendix B.2.1. Primary producers

Among standard laboratory tests with primary producers, tests with freshwater algae are dominating. Even though vascular plants play an important role in a freshwater ecosystem (e.g. as food and shelter), only a few standardised methods exist (Lewis 1998) and due to the limited amount of test results, the sensitivity of these species is not as well understood as the sensitivity of algae. So, for freshwater primary producers other than algae, standard tests either do not exist or the number of test results is very limited. It is therefore assessed that inclusion of non-algae test results may create bias in the calculation of the average toxicity of chemicals due to lack of data for the main part. Therefore, it is recommended, that the test results on primary producers to be included in the calculation of the EEI only includes algae.

Lewis (1998) compiles existing standard test guidelines for algae. Almost all of these and a few more are assessed in the OECD Detailed Review Paper (DRP) on aquatic testing methods (OECD 1998). On this basis, six standard algae test methods are chosen and compiled in Larsen et al. (2004c).

The endpoints used for algae tests include inhibition of growth and photosynthesis. Growth inhibition can either be measured as reduction in biomass production or as a reduction in growth rate. No scientific consensus exists on which to choose so both biomass and growth rate are acceptable (Lewis 1998). However, according to Kusk (2003) the use of growth rate is dominating today. One of the reasons for this is that reduction in growth rate is relatively independent of the test time (as long as the growth is exponential) as compared to reduction in biomass which is dependent on the final biomass at the end of the test period (Kusk 2003). Effects on photosynthetic activity seem to be less sensitive to toxic exposure than inhibition of growth in most cases (Lewis 1998). It is therefore recommended to use test results based on inhibition of growth, i.e. either biomass or growth rate, as data input in the calculation of average toxicity to algae.

Algae tests on growth rate are multi-generation tests and they are therefore in principle chronic (or long term) tests. However, proliferation is typically due to mitosis (no sexual reproduction) and EC_{50} values are within generic risk assessment, according to the TGD (EC 2003a), considered as acute values (or short term values) whereas NOEC values from the same test are used as chronic values or long term values. For the EEI we recommend using the EC_{50} as both an acute value and as a chronic value.

The most frequently used algae species in standard laboratory tests are the two green algae *Raphidocelis subcapitata* (former name *Selenastrum capricornutum*) and *Scenedesmus subspicatus* but also blue-green algae and diatoms are used. The sensitivity of the different algae species may vary more or less depending on the chemical tested. In some cases more than a factor 100 or even more than a factor 1000 is found between species, especially for pesticides and some metals. Unfortunately, the response to chemicals is unpredictable (Lewis 1998). A way to deal with this variation is to include test results on different species if available. The recommended species include: *Raphidocelis subcapitata*, *Scenedesmus subspicatus*, *Scenedesmus quadricauda*, *Chlorella vulgaris*, *Anabaena flos-aqua*, *Microcystis aeruginosa*, *Navicula seminulum* and *Navicula pelliculosa*.

Typical test duration for standard algae test is 72 – 96 hours chosen to obtain exponential growth during the test period. This is also the duration of test methods aiming at estimating EC_{50} for growth inhibition (Lewis 1998). The TGD (EC 2003a) states that it is generally accepted that EC_{50} values from test duration of 72 hours or longer may be considered as results from a short term test. Of all standard tests, as compiled in Larsen et al. (2004c), only the FIFRA test has a duration above 96 hours, viz. 120 hours. It is therefore recommended that a test duration of 72 hours – 120 hours is used for the EEI.

Appendix B.2.2. Primary consumers

Invertebrates play a very important role as part of the primary consumers in the aquatic ecosystem. In standard laboratory tests the crustaceans (phylum Arthropoda) are dominating, especially the genus *Daphnia* with the species *D. magna* and *D. pulex* accounting for the major part of the test results on invertebrates. As is the case for algae, these kinds of tests are to a large extent used for regulatory purposes. The organisms used for laboratory tests on primary consumers almost exclusively belong to the invertebrates.

As described in the OECD Detailed Review Paper (DRP) (OECD 1998) on aquatic testing methods on herbivores (and omnivores), i.e. primary consumers, a lot of non-standardised methods making use of a wide range of non-standardised organisms are published. These are all invertebrates and the dominating taxonomic phyla include Arthropoda (Crustacea, Insecta), Protozoans (e.g. *Paramecium*), Rotifera (e.g. *Brachionus*), Cnidarians (*Hydra*), Platyhelminthes (*Dugesia*) and Mollusca. For acute tests, only six species with matching standard test guidelines are given the rating A (or AA) in the OECD DRP (OECD 1998) meaning that these tests are international standards, or international draft standards or national standards that have been subject to national (or international) ring-testing. These species with adjacent test methods are compiled in Larsen et al. (2004c). The six species, which are recommended for the EEI, are: *Daphnia magna*, *Daphnia pulex*, *Daphnia sp.*, *Ceriodaphnia dubia*, *Neomysis mercedis* and *Brachionus calyciflorus*.

The endpoint typically used in acute test on invertebrates is mortality or immobility (*Daphnia*). Immobility is used in test on *Daphnia* because it is very difficult to determine when the organism is actually dead. For the EEI, an EC_{50} value based on mortality or immobility is recommended.

For the test duration it is recommended to use 24-96 hours (48 hours preferred) for the genuses *Daphnia* and *Ceriodaphnia*. For *Neomysis* a test duration of 96 hours is recommended and for *Brachionus* 24 hours.

Appendix B.2.3. Secondary consumers

Fish play a very important role as part of the secondary (and tertiary) consumers in the aquatic ecosystem. In standard laboratory tests on carnivores, tests on fish belonging to the superorder Teleostei (‘bony fishes’) are dominating, especially species like rainbow trout (*Onchorhynchus mykiss*) and bluegill sunfish (*Lepomis macrochirus*) are used. As is the case for algae and invertebrates, these kinds of tests are to a large extent used for regulatory purposes.

According to the OECD Detailed Review Paper (DRP) on aquatic testing methods (OECD 1998), only tests on carnivores fish have been published and these test are dominating the group of non-herbivores consumers. So, besides test on fish only a few carnivore species from each of the phyla Protozoans (e.g. *Paramecium*), Arthropoda (Insecta), Platyhelminthes (*Dugesia*) and the taxon Amphibia are represented. For acute tests, only 14 species with matching standard test guidelines are given the rating A (or AA) as both overall score and on standardisation in the OECD DRP (OECD 1998). These are all fish tests and compiled together with adjacent test methods in Larsen et al. (2004c). The 14 species, which are recommended for the EEI, are: *Ambassis macleayi, Carassius auratus auratus, Cyprinus carpio carpio, Danio rerio (Brachydanio rerio), Ictalurus punctatus, Lepomis cyanellus, Lepomis macrochirus, Leuciscus idus, Melanotaenia splendida inornata, Onchorhynchus kisutch, Onchorhynchus mykiss (Salmo gairdneri), Oryzias latipes, Pimephales promelas, Poecilia reticulate* and *Salvelnius fontinalis*.

The endpoint typically used in acute test on fish is mortality. For the EEI, an LC_{50} value is recommended.

For the test durations it is recommended to use 96 - 336 hours (96 hours preferred) for the EEI. A test duration of 96 hours (short term acute test, not including feeding) is used in all recommended standard tests (i.e. given the rating A (or AA), see above) except for two (OECD 1998). In these two tests, which are long term acute tests (feeding included), the measure of an acute effect (end point LC_{50}) is included and the exposure period is short (i.e. acute) as compared to the life span of the organisms (OECD 1998, Solbé 1998).

Appendix: Publications, posters and oral presentations

Publications in international journals (included in Ph.D. thesis):

Larsen HF, Birkved M, Hauschild M, Pennington D, Guinée J (2004). Evaluation of Selection Methods for Toxicological Impacts in LCA. Recommendations for OMNIITOX. *Int J LCA 9(5), 307-319.*

Larsen HF, Hauschild M (2004). Selection Methods in LCIA: Comparison of Chemical Ranking and Scoring Methods for use as Selection Methods. *Submitted to Int J LCA.*

Larsen HF, Hansen MS, Hauschild M (2004). Including chemical-related impact categories in LCA on printed matter – does it matter? *Submitted to Journal of Cleaner Production.*

Larsen HF, Hauschild M (2004). Evaluation of ecotoxicity effect indicators for use in LCIA. *Submitted to Int J LCA.*

Larsen HF, Hauschild M (2004). GM-troph – A low data demand ecotoxicity effect indicator for use in LCIA. *Submitted to Int J LCA.*

Publications in international journals (not included in Ph.D. thesis):

Olsen, SI, Christensen FM, Hauschild M, Pedersen F, Larsen HF, Tørsløv J (2001). Life cycle impact assessment and risk assessment – a methodological comparison. *Environmental Impact Assessment Review 21(2001), 385-404.*

Peer reviewed reports:

Larsen HF, Hansen MS, Hauschild M (2004). Ecolabelling of printed matter. Part II: Life cycle assessment of model sheet fed offset printed matter. Environmental Project No. XXX. (final draft April 2004). Danish Environmental Protection Agency. Final draft preliminary available at: http://ipltest.kpd.ipt.dtu.dk/ipl/upload/lcv/127_2.pdf

Larsen HF, Payet J, Molander S, Hauschild M (2004). Implementation of the OMNIITOX Base Model. Contribution to work package 8 of the OMNIITOX project as part A of appropriate deliverable D41. Part VIII – Implementation of the ecotoxicological effects module. EC Project contract G1RD-CT-2001-00501. http://www.omniitox.net/

Reports:

Johnsen N, Bøg C, Poll C, Larsen HF (2004). Ecolabelling of printed matter. Part I. Environmental Project No. XXX. (final draft April 2004). Danish Environmental Protection Agency.

Larsen HF, Birkved M, Hauschild M, Pennington D, Guinée J (2002b). Inventory of LCIA selection methods for assessing toxic releases. Methods and typology report part B. Contribution to Work-package 7 of the OMNIITOX Project as part B of appropriate deliverable D11. EC Project contract G1RD-CT-2001-00501. http://www.omniitox.net/

Posters:

Larsen HF, Hansen MS, Hauschild M (2004). Including chemical-related impact categories in in LCA on printed matter – does it matter? Poster presented at the 14th annual meeting of SETAC-Europe, 18-22 April 2004 in Prague, Czech Republic. Abstract No.: TUPO12/017.

Birkved M, Strandensen M, Larsen HF, Olsen SI, Hauschild M, Bachmann TM (2004). Calculation of site specific characterisation factors for metal ecotoxicity using decoupled multi species fate and exposure modelling. Poster presented at the 14th annual meeting of SETAC-Europe, 18-22 April 2004 in Prague, Czech Republic. Abstract No.: TUPO12/005.

Larsen HF, Birkved M, Hauschild M (2003). Evaluation of selection methods for use in Life Cycle Impact Assessment. Poster presented at the 13th annual meeting of SETAC-Europe, 26 April – 1 May 2003 in Hamburg, Germany. Abstract No.: WEP/231.

Larsen HF (2003). Work package 7 : Comparing LCIA methods: Selection methods. Presented at the OMNIITOX Mid-term review meeting with the European Commission. 23-01-2003. Brussels. Belgium.

Larsen HF, Hansen J, Laursen S, Knudsen HH, Ledakowicz JS, Machnowski W (2001). Environmental profiles on chemicals (EPC): A substitution tool i.a. used in the textile industry. Poster presented at the 11th annual meeting of SETAC-Europe, 6-10 May 2001 in Madrid, Spain. Abstract No.: M/FF252.

Oral presentations:

Larsen HF, Hansen MS, Hauschild M (2004). Including chemical-related impact categories in LCA on printed matter – does it matter? Presented at Dansk Kemiingeniør Konference 2004, DK2-2004 (Danish Chemical Engineers Conference). Department of Chemical Engineering. Technical University of Denmark. 26-05-2004. Lyngby, Denmark. Extended abstract.

Larsen HF, Payet J, Molander S (2004). Ecotoxicity effect indicator for use in the OMNIITOX base model. Presented at the 14th annual meeting of SETAC-Europe, 18-22 April 2004 in Prague, Czech Republic. Abstract No.: TH5AM1/05.

Larsen HF (2003). Life Cycle Impact Assessment (LCIA) with focus on chemicals. Presented at the workshop and seminar: Exploring Possibilities for Increased Baltic Co-operation within the Field of Environmental Education. Øresund Environment Educational Institutions in the Baltic area. 30-05-2003. Copenhagen, Denmark.

Larsen HF, Birkved M, Hauschild M. (2002). LCIA selection methods for assessing toxic releases. Presented at the 12th annual meeting of SETAC-Europe, 12-16 May 2002 in Vienna, Austria. Abstract No.: 34-04.

Larsen HF (2001). Miljøoptimering af afvaskning ved tryk med vandfortyndbar flexotrykfarve. Præsenteret på ” Konference for tekniske ledere” EMBALLAGEINDUSTRIEN , 12/9-2001. Svendborg. (Evaluation of best available technology when using water dilutable flexographic printing inks – focus on cleaning.

Presented at the “Conference for technical leaders” arranged by the Danish Packaging Industry. 12-09-2003, Svendborg, Denmark).

Larsen HF (2001). Livscyklusvurdering af kemikalier. Præsenteret på ”Workshop om Grafisk Produktdatabase” . Grafisk Arbejdsgiverforening (GA). 13/11-2001. Odense. (Life cycle assessment including chemicals. Presented at the worhshop: ”Product database for the printing industry”. Arranged by the Graphics Association of Denmark (GA). 13-11-2001. Odense, Denmark.

Miscellaneous

External expert at 3 diploma examines at Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland. March 2003.

Reviewer for Journal of Industrial Ecology (2003-)