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Simple estimation of effect factors for toxicity used for screening LCA

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Nordic Environmental Co-operation

The Nordic Environmental Action Plan 2005-2008 forms the framework for the Nordic countries' environmental co-operation both within the Nordic region and in relation to the adjacent areas, the Arctic, the EU and other international forums. The programme aims for results that will consolidate the position of the Nordic region as the leader in the environmental field. One of the overall goals is to create a healthier living environment for the Nordic people.

Nordic co-operation

Nordic co-operation, one of the oldest and most wide-ranging regional partnerships in the world, involves Denmark, Finland, Iceland, Norway, Sweden, the Faroe Islands, Greenland and Åland. Co-operation reinforces the sense of Nordic community while respecting national differences and similarities, makes it possible to uphold Nordic interests in the world at large and promotes positive relations between neighbouring peoples.

Co-operation was formalised in 1952 when *the Nordic Council* was set up as a forum for parliamentarians and governments. The Helsinki Treaty of 1962 has formed the framework for Nordic partnership ever since. The *Nordic Council of Ministers* was set up in 1971 as the formal forum for co-operation between the governments of the Nordic countries and the political leadership of the autonomous areas, i.e. the Faroe Islands, Greenland and Åland.

Content

Preface

This report summarizes the results from the project: “Simple estimation of effect factors for toxicity used for screening LCA”.

The Institute for Product Development has been project manager.

The main result of this project is the software “Effect Factor Calculator”, which is a software developed in the database program Microsoft Access. This report explains the methodology and premises used for the development. It also serves as a manual on how to use the program and the calculated results.

The carrying out of the project has been supported by:

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Critical review has been performed by:

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Summary and conclusions

Almost any Life Cycle Assessment (LCA)-study will include assessment of a number of chemical substances.

It is often difficult and time consuming to get access to relevant data for chemical substances and it often takes the knowledge of a specialist to interpret these data and to calculate effect factors as it is done in the EDIP Method. Due to this, the effects of the emission of chemical substances are likely to be omitted from many LCAs.

The overall purpose of this project is to facilitate the integration of the assessment of chemical substances in Life Cycle Assessment. This is put into practice by the following tasks:

- Establish a database with data on human toxicity and ecotoxicity for chemical substances derived from risk-phrases.
- Establish a software that can calculate effect factors according to the EDIP Methodology from these data.
- It is furthermore the purpose to apply this model to calculate effect factors for substances present on official - and advisory lists.

To perform calculations of effect factors for a chemical substance the following data is needed:

- Data on human toxicity and ecotoxicity to estimate the level of possible toxic effects
- Physical/chemical data to estimate the fate of the substance, when it is emitted to the environment

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

Four lists were identified, where substances have been assigned risk-phrases according to the EU legislation:

- The EU list of dangerous chemical substances based on the EC Directive 67/548/EEC on dangerous substances (including the 28th adaptation)
- N-Class Database
- The 29th Adaptation to the EU list mentioned above

- The Advisory list for self classification of dangerous substances elaborated by the Danish Environmental Agency (Miljøstyrelsen)

The total outcome from these lists sum up to 27.322 substances with unique CAS numbers and more than 2/3 of the datasets originate from the Danish "Advisory list for self classification of dangerous substances". The values behind this list have been estimated by means of computer models, so-called QSAR models (Quantitative Structure-Activity Relationship). In the database that has been established with this project the origin of each dataset can be identified.

Behind each risk-phrase is a set of criteria specifying when a substance should be assigned the respective risk-phrase. In order to systematically extract this information the criteria for each Risk-phrase have been evaluated and the risk-phrases "containing" relevant information have been selected.

For risk-phrases where the criteria are made up by an interval, the midpoint value is used for the calculation, and the error is within a factor of approx. 10. The effect factors derived from such risk-phrases thus can be categorised as a fairly good estimation.

For risk-phrases where the criteria is defined by a toxicity value lower than a specific threshold value, it has not been judged correct to use the midpoint value between the threshold value and zero. Some substances have toxicity values that are several orders of magnitude below the threshold value. It is therefore assumed that the logarithmic mean is more representative, as it reflects the wide span (over several decades) of these values.

If a substance appears on one of the lists, but is not assigned any risk-phrase related to acute toxicity, it should be expected that the toxicity of this substance is lower than the lowest level of toxicity that would require a classification due to human toxicity or ecotoxicity. But this is not the case for all substances.

It is however possible to distinguish between two kinds of "No classification":

- Substances that are not classified and where sufficient **data is available** to support this.
- Substances that are not classified and where **no data is available** or available data is insufficient to support this. What the list expresses about this group of substances is merely something like: "There is not sufficient data to require a classification".

In spite of the above mentioned uncertainties a toxicity level corresponding to the lowest level of toxicity value that requires a classification, is chosen for a best estimate. This value is thus a maximum value.

The origin and the quality of the applied toxicity data is attached to each set of calculated effect factors as and indication of the uncertainty.

In order to estimate the potential effect of a chemical substance to the environment it is not sufficient to know about the toxic properties. It is also necessary to uncover the fate of the substance when it is emitted to the environment. To do this a set of physical/chemical data have been extracted from the EPIWIN software. Some values are genuine experimental data while others are estimated based on the chemical structure of the respective substance or by a property/property estimation technique. These parameters are stored in the software and the origin of the data is also specified. Values for all relevant parameters have been extracted for 28.033 substances with unique CAS numbers.

A software in the shape of a Microsoft Access file has been developed and effect factors for 23.029 substances have been calculated.

Effect factors calculated by the conventional method for 120 substances were compared to effect factors calculated by the risk-phrase method. This comparison (though insufficient) provides an indication of how good an estimate the risk-phrase method can generate.

Though this comparison is based on a limited number of substances it indicates that effect factors calculated by the risk-phrase method represent a fairly good estimate - especially when you consider that effect factors have been generated for more than 23.000 substances compared to those approx. 200 that have had effect factors calculated from individual data collected from the literature

Evaluating the deviations it should be taken into consideration that the values calculated by the conventional method not necessarily are “true values”. Effect factors calculated by the EDIP method from individual data may also deviate depending on the quality of the toxicity – and physical/chemical data found and employed.

By means of this tool you can calculate effect factors in three ways:

- Calculation that requires only an input of CAS-numbers. (Available for 23.029 substances).
- Calculation that requires an input of CAS-numbers and risk-phrases. (Available for 28.033 substances).
- Calculation based entirely or partly on input of individual data provided by the user.

The effect factors calculated from toxicity values derived from the risk-phrases will inevitable be connected with some uncertainty. The uncertainty will differ depending on the risk-phrase applied, and the origin of the underlying data. To each set of effect factors calculated is attached some “Comments on data quality”, that serves to characterize the quality of the underlying toxicity data.

By using the effect factors calculated on the basis of toxicity information derived from risk-phrases it is outmost import to be aware of the premises for each set of calculated effect factors as they are expressed in the attached “Comments on data quality”.

Sammenfatning og konklusion

Næsten enhver Livscyklus Vurdering (LCA) vil omfatte vurdering af et antal kemiske stoffer.

Det er ofte vanskeligt og tidskrævende at få adgang til relevante data for kemiske stoffer, og det kræver en specialists kompetence at fortolke disse data og beregne effekt faktorer, som det er beskrevet i UMIP metoden. Derfor er der en tendens til at effekterne af de kemiske stoffer udelades fra mange Livscyklus Vurderinger.

Det overordnede formål med dette projekt er at lette integrationen af vurderingen af kemiske stoffer i Livscyklus Vurderinger. Dette er omsat til praksis gennem følgende delopgaver:

- Etablering af en database med human toksikologiske – og økotoksikologiske data udledt af risikosætninger.
- Etablere et beregningsprogram, som kan beregne effekt faktorer i henhold til UMIP metoden ud fra disse data.
- Det er desuden formålet at beregne effekt faktorer for kemiske stoffer, som er opført på officielle – og vejledende lister over farlige stoffer.

For at kunne beregne effekt faktorer for kemiske stoffer er der behov for følgende data:

- Data om human toksicitet og økotoksicitet til at vurdere niveauet af mulige toksiske effekter
- Fysisk/kemiske data til at vurdere den skæbne et kemisk stof vil få, når det udledes til miljøet

Tilgangen i dette projekt er baseret på antagelsen om at relevante data for toksicitet kan udledes fra de risikosætninger, som tildeles kemiske stoffer på officielle - og vejledende lister, og at denne information kan transformeres til ét tal, som kan repræsentere et niveau for toksiciteten.

Fire lister, hvor kemiske stoffer er tildelt risikosætninger i henhold til EU's lovgivning, er identificeret:

- EU listen over farlige stoffer baseret på EC Directive 67/548/EEC on dangerous substances (including the 28th adaptation)
- N-Class Database
- Den 29. tilpasning af ovennævnte EU liste
- Vejledende liste til selvklassificering af farlige stoffer fra den danske Miljøstyrelse

Indholdet af disse lister udgør 27.322 kemiske stoffer med entydige CAS-numre, og mere end 2/3 af disse stammer fra den ” Vejledende liste til selvklassificering af farlige stoffer”. Værdierne på denne liste er tilvejebragt ved hjælp af computer baserede modeller ud fra stoffernes struktur. Det er såkaldte QSAR modeller (Quantitative Structure-Activity Relationship). I den i dette projekt etablerede database er oprindelse af hvert data sæt angivet.

Bag hver risikosætning ligger et sæt kriterier, som specificerer hvornår et stof skal tildeles den respektive risikosætning. Kriterierne for hver enkel risikosætning er gennemgået, og risikosætninger som ”indeholdt” relevant information er udvalgt.

For risikosætninger hvor kriterierne udgøres af et interval er middelværdien valgt som grundlag for beregningen, og usikkerheden ligger indenfor en faktor 10. Effekt faktorer beregnet ud fra kemiske stoffer med disse risikosætninger kan således betegnes som et rimeligt godt estimat.

For risikosætninger hvor kriterierne er defineret ud fra en toksikologisk værdi, som er lavere end en bestemt grænseværdi, er det vurderet at det ikke ville være korrekt at anvende middelværdien mellem grænseværdien og nul. Nogle kemiske stoffer har toksicitet værdier, som ligger flere størrelsesordener under grænseværdien. Det er derfor antaget, at den logaritmiske middelværdi vil være mere repræsentativ, da den bedre reflekterer det store spænd (flere dekader), der er mellem disse værdier.

Hvis et stof optræder på en af disse lister, men ikke er tildelt en risikosætning relevant for akut toksicitet, skulle man forvente, at toksiciteten for dette stof er lavere end den laveste værdi, som ville kræve en klassifikation for human toksicitet eller økotoksicitet. Men dette er ikke sikkert for alle stoffer.

Det er imidlertid muligt at skelne mellem to slags ”ikke klassificeret”:

- Kemiske stoffer som ikke er klassificeret og hvor der er tilstrækkeligt **tilgængelige data** til at understøtte dette.
- Kemiske stoffer som ikke er klassificeret og hvor **der ikke er tilgængelige data** til at understøtte dette eller hvor tilgængelige data er utilstrækkelige. Sagt på en anden måde: Der er ikke tilstrækkelige data til at myndighederne kan kræve en klassifikation.

På trods af ovennævnte usikkerheder vælges et toksicitets niveau svarende til den laveste toksicitets værdi, som kræver klassifikation, som det bedste estimat. Denne værdi repræsenterer således en maksimal værdi.

Oprindelsen og kvaliteten af de anvendte data for toksicitet er vedhæftet hvert enkelt sæt af beregnede effekt faktorer, som en indikation af usikkerheden.

For at kunne estimere effekten af et kemisk stof i miljøet er det ikke tilstrækkeligt kun at kende de toksikologiske egenskaber. Det er også nødvendigt at afdække et givet stofs skæbne, når det udledes til miljøet. For at kunne dette, er et sæt fysisk/kemiske data ekstraheret ud fra EPIWIN programmet. Nogle data herfra er gode eksperimentelle værdier, mens andre er estimeret på grundlag af stoffets kemiske struktur. De ekstraherede værdier er lagret i det udviklede program, med angivelse af de enkelte datas oprindelse. Værdier for alle relevante fysisk/kemiske parametre er ekstraheret for 28.033 kemiske stoffer med entydige CAS-numre.

Et program i form af en Microsoft Access fil er udviklet og effekt faktorer for 23.029 stoffer er beregnet.

Effekt faktorer beregnet på konventionel vis for 120 stoffer blev sammenlignet med effekt faktorer beregnet med risikosætningsmetoden. Denne sammenligning (selv om den er utilstrækkelig) giver en indikation af hvor gode estimater, der kan genereres med risikosætningsmetoden.

Skønt den sammenligning er baseret på et begrænset antal kemiske stoffer indikerer den at effekt faktorer beregnet med risikosætningsmetoden er et rimeligt godt estimat – specielt når det tages i betragtning, at effekt faktorer har kunnet beregnes for mere end 23.000 stoffer i forhold til de ca. 200 stoffer, der er beregnet effekt faktorer for baseret på individuelle data hentet fra den toksikologiske litteratur.

Ved evalueringen af afvigelserne skal man være opmærksom på, at de værdier som beregnes på konventionel vis ikke nødvendigvis er ”sande værdier” Effekt faktorer beregnet ud fra UMIP metoden på grundlag af individuelle data kan også variere afhængig af kvaliteten af de data (toksikologiske – og fysisk/kemiske -), som var tilgængelige.

Med dette værktøj er det muligt at beregne effekt faktorer på tre måder:

- Beregning som kun kræver input af et CAS-nummer. (Tilgænglig for 23.029 stoffer).
- Beregning som kræver input af et CAS-nummer og risikosætninger. (Tilgænglig for 28.033 stoffer).
- Beregning baseret helt eller delvis på input af individuelle data leveret af brugeren.

Effekt faktorer beregnet på grundlag toksikologiske data udledt af risikosætninger vil uvægerligt være forbundet med en vis usikkerhed. Usikkerheden vil variere afhængig af den anvendte risikosætning og oprindelsen af de underliggende data. Med hvert sæt af beregnede effekt faktorer følger et sæt ”Kommentarer om data kvaliteten”, som tjener til at karakterisere kvaliteten af de bagvedliggende toksikologiske data.

Ved anvendelsen af effekt faktorer beregnet på grundlag toksicitets data udledt fra risikosætninger er det meget vigtigt at være opmærksom

på det grundlag, der er for hvert enkelt sæt af beregnende effekt faktorer, som det er udtrykt i de medfølgende ”Kommentarer om data kvaliteten”.

Review statement

The reviewed project has dealt with several problematic aspects of life-cycle impact assessment (LCIA) of potentially toxic substances that has been contributing to practitioner avoidance of this impact category. These aspects are related to both model complexity and data availability.

The obstacles related to ***data availability*** for reaching a truly operational model were approached by two means. As one means of gaining information the project relies on *risk-phrases* (R-phrases) assigned to chemical substances as a result of classification and labelling work in accordance with the European chemicals legislation where the R-phrases occur both at labels and in Material Safety Data Sheets. The R-phrases are used first for identifying more than 20000 chemical substances by unique CAS-numbers and then for deriving toxicity values for human and ecotoxicity in the absence of available measured values following a simple set of rules. The other means for finding information has been an extensive use of the US EPA *property estimation software* called EPIWIN that based on both measured and calculated chemical substance property data, provides data necessary for the computation of effect factors. The effect factors have been computed according to the Danish EDIP-method.

Some of the ***model complexity*** aspects addressed in the project is related to the simplification of the data treatment given by the use of R-phrases and to a computer implementation of the EDIP method in a Microsoft Access database that gives an inexperienced user the possibility to have effect factors based on R-phrases and EPIWIN-data with the sole input of a CAS-number. This part of the project represents a significant step forward for a more frequent assessment of toxicants within LCA that open up for further work making the results available for ordinary LCA practitioners and users of effect/characterization factors. The software provided also provides the user with the possibility for a manual input of toxicity values and/or fate related data in order to compute effect factors. This option does however put requirements on the user in terms of some expertise in toxicology and/or knowledge of the EDIP-method.

The overall performance of the R-phrase/EPIWIN approach has been assessed by a comparison with existing effect factors, calculated according to the EDIP-method but using measured data. The result of the assessment is encouraging, and given the very limited information contained in R-phrases and the low quality of the EPIWIN derived data the outcome is promising for many of the types of effect factors covered in the assessment. However, the deviations that are revealed in the comparison are of a magnitude that indicates that a further development of meth-

ods for LCIA is required. Thus the approach employed has some less favourable sides. The resulting uncertainty is large, but given that the alternative is to have no effect factors at all, this is judged acceptable, especially given the presentation of information on the uncertainty of the toxicity data applied in the software.

Göteborg and Lyngby, December 2004

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1 Introduction

1.1 Background

Life Cycle Assessment (LCA) is one approach to evaluate the environmental impacts of chemical substances. Another approach is the Risk Assessment (RA) [15]. The relationship between these two sets of methodologies is covered by Flemström et. al. [16]. The most decisive difference between the two approaches is related to goal and scope.

The results of an LCA is linked to the “functional unit” and the purpose is often to compare environmental impacts from “Product A” to the alternative “Product B” in the form of e.g. competitors product, next – or previous generation product or a new product concept. The results in terms of environmental impact categories are expresses as the marginal environmental impact from the manufacturing, use and disposal of one product. The total number of the produced product is thus not considered.

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

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

The LCA methodology also includes the possibility to encompass site specific considerations, but it is rarely used. The reason for this among others is that many products are manufactured and marketed globally and geographic scenarios are comprehensive and difficult to predict.

Life Cycle Impact Assessment (LCIA) is the specific part of an LCA where the potential environmental impact is evaluated by classification and characterisation of identified raw materials and emissions associated with the product life cycle.

This issue has been covered by the Omniitox project [13] that addressed the five main issues:

1. Comparison of LCIA and (E)RA
2. Comparing LCIA methods
3. Extending the scope of LCIA methods
4. Developing the OMNIITOX Information System
5. Use of LCA for regulatory assessment of chemicals

Several methods for the classification and characterization of toxic substances have been identified as a result of this project [14]. Seven different methods have been described and the effort needed to perform the analyses has been evaluated in terms of competence and data (quality, quantity, availability and data gaps). The focus in the OMNIITOX project has been on the development of the methodology. A result of this is the "OMNIITOX Base model", which is a more data demanding, more sophisticated model that can be applied to substances with relatively wide data availability. This characterisation model is developed as a result of the study of the seven different methods. A less data demanding model called the "simplified base model" has also been developed based on the comprehensive "base model". This model should produce compatible characterization factors for screening purposes.

Another relevant activity is going on in the UNEP/SETAC Life Cycle initiative [17] where the issue of LCIA of chemical substances is covered by the Task Force "Toxicity Impact (TF LCIA 3)". In this context it is planned to compare characterisation factors for a number of chemical substances calculated by different LCIA methods – among other the EDIP Methodology. The calculation tools developed in the present project will be applied for this task.

The present project deals with the EDIP-characterization methodology for toxic substances. EDIP is the abbreviation for Environmental Design of Industrial Products. The focus is on this method and addresses the issue of data availability and the facilitation of the application by LCA practitioners.

1.2 Need of the project results

Almost any LCA-study will include assessment from a number of chemical substances.

In the EDIP method [1 & 2] the LCIA is expressed in terms of the "Effect factors" for each chemical substance. To perform calculations of these effect factors you need:

- Data on human toxicity and ecotoxicity
- Physical/chemical data

These data are often difficult to get access to and it often takes the knowledge of a specialist to interpret these data and to calculate effect factors. Thus there is a need to establish a database with toxicological- and physical/chemical data for chemical substances that can form the basis for the calculation of the effect factors.

The status is now that it takes a skilled person one man-day to collect data and calculate a set of effect factors for one chemical substance [11] in accordance with the EDIP Methodology [1 & 2]. At the Department of Manufacturing Engineering and Management (IPL) at the Technical University of Denmark so far effect factors have been calculated for approx. 200 substances [11].

Since effect factors have only been calculated for this small fraction of chemicals and it is a heavy burden to collect data and calculate new effect factors, the effects of the emission of chemical substances are likely to be omitted from many LCAs. There is thus a substantial need to facilitate the calculation of effect factors for chemical substances.

1.3 Basic idea of the project

An obvious shortcut to extract human toxicity- and ecotoxicity data that are better than no data would be to develop a simple model connecting the rules for Classification and Labelling of Dangerous Substances [3] and the calculation of effect factors used in LCIA. All chemical substances and preparations marketed in the European Union must have assigned risk-phrases and symbols corresponding to their potential hazard to man and the environment [3 & 4].

Information about labelling and classification will be easy accessible from the health and safety datasheets that will be available by those company that applies the chemical substances or from their suppliers.

It will thus be possible to calculate effect factors based on the classification on the List of dangerous substances [4] in cases, where you do not have the sufficient resources to calculate these effect factors “the hard way”. Such effect factors based on less accurate data will be far better than “no data”, and make it possible to many LCA-practitioners that are not skilled in toxicology, to include chemical substances in their LCA

1.4 Purpose

The purpose of this project is

- To establish a database with data on human toxicity and ecotoxicity for chemical substances derived from risk-phrases.
- To establish a software that can calculate effect factors according to the EDIP Methodology [1 & 2] from these data. (As a spin-off from this project the software can also calculate effect factor from individual data provided by the user.)

The only difference to the EDIP method is that the toxicity data used is derived from risk-phrases as explained in section 2.2. The fate modelling should be performed strictly in accordance with the EDIP method.
It is furthermore the purpose to apply this model to calculate effect factors for substances present on official - and advisory lists (see next chapter).

1.5 Target Group

The target group is the general LCA practitioners who do not necessary posses any more than a basic knowledge of toxicity. It is also presupposed that the user has a basic knowledge of the EDIP Methodology [1 & 2].

2 Establishing a toxicity database

2.1 Identification of relevant lists

This task is to identify lists of substances that have been assigned Risk-phrases according to the EU legislation [3]. Four lists have been identified and they are shown in table 1. To be able to work with these substances in computer models it is necessary to use CAS numbers as an unambiguous identification of each chemical substance. Chemical Abstract Service registry number serves as an international identification number for a well-defined chemical substance.

Table 1 Lists of substances with Risk-phrases

	Total number of substances	Total number of substances with unique CAS numbers	Number of substances added to the database
The EU list of dangerous chemical substances based on the EC Directive 67/548/EEC on dangerous substances (including the 28th adaptation) [4]	3.769	2.820	2.820
N-Class Database [10]	7.416	7.027	4.371
The 29th Adaptation the EU list mentioned above [6]	130	130	8
The Advisory list for self classification of dangerous substances elaborated by the Danish Environmental Agency (Miljøstyrelsen) [5].	20.624	20.622	20.123
Total			**27.322**

Having identified relevant lists the next step is to extract each chemical substance from these lists that have a unique CAS number. The extracted datasets are stored in a database. The number of substances having unique CAS numbers is shown in the column “Total number of substances with unique CAS numbers” in the table 1. This number is smaller than the total number because some chemical substances do not have a CAS number or because a CAS number appears several times on a list.

The EU-list [4] is considered to be the most authoritative and to contain the most reliable data, and the CAS numbers extracted from this list is added firstly to the database. Data from the N-Class database [10] is considered the second most reliable data, and CAS numbers extracted from this list is added next if they do not already appear on the EU-list. The number of relevant substances appears from the column to the right: “Number of substances added to the database.

Data from the 29th Adaptation [6] only contains a few substances that do not already appear on one of the two lists mentioned above. The last list is the Danish "Advisory list for self classification of dangerous substances" [5]. The values from this list are considered the most unreliable as they have been estimated by means of computer models, so-called QSAR models (Quantitative Structure-Activity Relationship). Data from this list have only been added to the database if they do not appear on any of the three other lists.

The total outcome from these lists sum up to 27.322 substances and more than 2/3 of the datasets originate from the Danish "Advisory list for self classification of dangerous substances" [5]. In the database that has been established with this project the origin of each dataset can be identified.

It has been evaluated if the criteria used for the Nordic Eco-labelling (Svanen) could be used in this context. The criteria and the appending list were not found useful in this context as it includes only a small number of substances (30). Approximately half of these substances already appear on the above mentioned lists.

2.2 Selection of relevant toxicity data from risk-phrases

The approach of this project is based on the assumption that relevant toxicity data can be extracted from the risk-phrases that have been assigned to the chemical substances on the above mentioned lists, and that this information can be transformed into one figure representing the level of toxicity. Behind each risk-phrase is a set of criteria [3] specifying when a substance should be assigned the respective risk-phrase. If e.g. a substance is assigned the risk-phrase R25 (Toxic if swallowed) it means that it has an LD_{50} between 25 – and 250 mg/kg body weight. The next step is to transform this interval into one figure. For substances having the risk-phrase R25 the representative level of toxicity can be set to the midpoint value (LD_{50} = 112,5 mg/kg body weight). Toxicity information can also be derived from some other risk-phrases as explained in the following.

In order to systematically extract this information the criteria [3] for each Risk-phrase have been evaluated and the risk-phrases "containing" relevant information have been selected, and the ones that have not been found useful have been left out. Appendix 1 contains a complete reference to all the risk-phrases and the reasons for why the have been chosen or left out.

The main reasons for leaving out risk-phrases are:

- The risk-phrase relates to fire and explosion risk etc.
- The risk-phrase only contains "supplementary toxicity information" like:
    - Sensitisation
    - Eye irritation
    - CMR substances (only a qualitative statement)
    - Bees, Flora, Fauna (Not implemented yet)

The "supplementary toxicity information" refers to toxicity information which is not applicable to the EDIP methodology – like sensitisation and eye irritation. Other risk-phrases only express a qualitative statement – like those referring to the CMR properties (R45, R48 etc.). As the EDIP methodology requires a quantitative toxicity value these risk-phrases will not be of any use in this context.

Substances that were assigned risk-phrases relating to skin toxicity (R21, R24 and R27) only very few (19) did not have a risk-phrase relating to oral toxicity. This is why these risk-phrases have not been found useful.

The risk phrases that are employed for calculation of effect factors have been listed in table 2.

Table 2 Risk-phrases containing relevant toxicological information

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

In table 2 the values applied for the calculation of effect factors are shown in the column "Representative toxicity level employed for calculation of effect factors". For risk-phrases that have criteria set up in terms

of an interval the midpoint value is chosen for a good estimate. For risk-phrases where the criteria is defined by a toxicity value lower than a specific threshold value the "Representative toxicity level" is estimated in a different way as explained in section 2.2.2.

Though some substances are not assigned any of the risk-phrases listed in table 2, it might be possible to extract some useful information of relevance for these substances. This issue will be dealt with in section 2.2.3 and 2.2.4.

According to the toxicity information that can be extracted from the risk-phrases they can be divided in four categories:

2.2.1 Category 1 - Substances with risk-phrase criteria based on an intervals

For risk-phrases where the criteria are made up by an interval, the midpoint value is used for the calculation, and the error is within a factor of approx. 10. The effect factors derived from such risk-phrases thus can be categorised as a fairly good estimation. This applies for the risk-phrases R20, R22, R23, R25, R51 and R52.

2.2.2 Category 2 - Substances with risk-phrase criteria based on threshold values

For risk-phrases where the criteria is defined by a toxicity value lower than a specific threshold value, it has not been judged correct to use the midpoint value between the threshold value and zero. Some substances have toxicity values that are several orders of magnitude below the threshold value. It is therefore assumed that a representative ("true") value is closer to zero than half of the threshold value.

In order to "estimate" a representative value two different datasets have been analyzed.

One is a list of 357 substances from the N-Class database with $L(E)C_{50}$ values below 1 mg/liter water (1.000 mg/ m^3 water). These values are based on "data" [10], which means that there are sufficient toxicity data on the substance to support the classification. Almost 90% of these substances have $L(E)C_{50}$ between 10 and 1.000 mg/ m^3 water.

The other dataset is a list of 49 substances assigned R50 (Very toxic to aquatic organisms), which was taken from those pesticides that are approved for use in outdoor agriculture in Denmark [7].

Mean values from these data are shown below

Table 3 Mean values for some chemical substances with L(E)C50 values below 1000 mg/ m3 water

L(E)C50 mg/m^3 water	Number of substances	Mean value	Mean value based on logarithmic mean
Dataset from N-Class	357	285	67
Dataset for pesticides	49	140	21

There is no objective way to select among these different mean values nor to say that the chemical substances constituting these datasets are representative. However it is assumed that the logarithmic mean is more representative, as it reflects the wide span (over several decades) of these values. As the 357 substances from the N-Class database are expected to be more representative than the 49 pesticides the representative value of 67 mg/ m^3 water is chosen, well knowing this is an arbitrary choice.

Rounding up this value it is therefore assumed that 10% (100 mg/ m^3 water) of the threshold value would make a good estimate for a representative value for this category. The effect factors derived from these risk-phrases are thus set to 10% of the threshold value, this value can however be categorised as a less reliable estimation. This applies for the risk-phrases R26, R28 and R50.

2.2.3 Category 3 - Substances not assigned risk-phrases relevant to human toxicity

If a substance appears on one of the lists, but is not assigned any risk-phrase related to acute human toxicity, it should be expected that it has an LD_{50} higher than 2.000 mg/kg body and or an LC_{50}.higher than 20.000 mg/m^3 air/4 hr; which are the lower level of the interval for the risk-phrases R22 and R20 respectively. However this is not the case. There will be data for many substances supporting this expectation, but definitely not all. Data on oral toxicity will occur more frequently than data on inhalation toxicity [12]. However it is assumed reasonable for this purpose to conclude that these substances will have an LD_{50} above 2.000 mg/kg body weight, and to use this value to calculate effect factors as maximum values, bearing in mind the uncertainty. This will be specified in the notes that are attached to each set of calculated effect factors.

This group of substances covers substances that have not been assigned any of the risk-phrases R20, R22, R23, R25, R26 or R28.

2.2.4 Category 4 - Substances not assigned risk-phrases relevant to ecotoxicity

If a substance appears on one of the lists, but is not assigned any risk-phrase related to ecotoxicity, it cannot automatically be concluded that it

has an LC_{50} / EC_{50} / IC_{50} higher than 100.000 mg/m^3 water. However it is possible to distinguish between two kinds of “No classification”:

- Substances that are not classified as "Dangerous for the environment" (N) and where sufficient **data is available** to support this.
- Substances that are not classified as "Dangerous for the environment" (N) and where **no data is available** or available data is insufficient to support this.

The quality assignment is taken from the N-Class database [10].

For substances that have their “No Classification” based on sufficient data it can be concluded that LC_{50} / EC_{50} / IC_{50} is higher than 100.000 mg/m^3 water

By the calculation of effect factors for substances that have their “No Classification” based on no data or insufficient data an LC_{50} / EC_{50} / IC_{50} of 100.000 mg/m^3 water is also applied for lack of better estimates. The effect factors calculated on the basis of these values will make up a very uncertain estimate. This will be specified in the notes that are attached to each set of calculated effect factors.

This group of substances covers substances that have not been assigned any of the risk-phrases R50, R51 or R52.

2.2.5 Origin of the risk-phrases

One dimension of the quality is what sort of information that can be derived from the risk-phrases on the assumption that the risk-phrase assignment is based on “true” data. Another dimension is the quality of the data on which the risk-phrase assignment is based.

The risk-phrases applied in this context originate from 4 different sources as specified in the table 1. The three first lists [4, 10 & 6] are official lists based on evaluation of available human toxicity – and ecotoxicity data. Risk-phrases from these lists can be characterised as being of high quality. The assignments of “No classification” differ in quality as it is mentioned in the previous two sections.

The Advisory List [5] is based on data estimated on the basis of computer models - so called QSAR models (Quantitative Structure-Activity Relationship), and thus introduces another uncertainty.

The origins of the risk-phrases are shown in table 4.

Table 4 Distribution of the origin for the risk-phrases.

Human toxicity risk phrases	Official lists	QSAR
R20 or R22	34%	46%
R23 or R25	13%	0%
R26 or R28	10%	0%
No classification but no statement	47%	54%

Ecotoxicity risk phrases	Official lists	QSAR
R51	22%	17%
R52	3%	6%
R50	32%	20%
No Clasisfication and sufficient data	16%	58%
No Clasisfication but insufficint data or no information	28%	

Total number of substances	7199	20123

By using the effect factors calculated on the basis of toxicity information derived from risk-phrases it is outmost import to be aware of the premises for each set of calculated effect factors as they are expressed in the attached notes. This issue will be dealt with in more detail in section 6.2.

2.3 Assessment factors

Assessment factors are applied in the EDIP Methodology [1 & 2] in order to compensate the quality and the relevance of the toxicity data available.

For human toxicity the values derived are based on LD_{50} or LC_{50} and for such data the EDIP methodology sets a high assessment factor of 100.000. [2, page 390].

For ecotoxicity the EDIP Methodology operates with one assessment factor for chronic ecotoxicity and another for acute ecotoxicity:

- For chronic ecotoxicity the assessment factor is set to 100 as the values extracted from the risk-phrases fall in the category “Data for acute ecotoxicity (EC_{50}) available for at least one species from each of the classes fish, crustacea and algae” [2, page 253].
- For acute ecotoxicity the assessment factor is set to 10 as the values extracted from the risk-phrases fall in the category “Data for acute ecotoxicity (EC_{50}) available for at least one species from each of the classes fish, crustacea and algae” [2, page 256].

It is thus the same data that is applied to calculate effect factors for acute – and chronic ecotoxicity. The only difference is the assessment factor. Assessment factors will be discussed in more detail in chapter 5.

3 Establishing a database with physical / chemical data

In order to estimate the potential effect of a chemical substance to the environment it is not sufficient to know about the toxic properties. It is also necessary to uncover the fate of the substance when it is emitted to the environment. To do this a set of physical/chemical data is required to predict the fate of a given chemical substance in the environment. These parameters are:

- Atmospheric half life (Half life air OH reaction (days) 12 hrs day, 1,5E6 OH/cm3), AHL
- Henry's Law Constant, H
- The octanol water partitioning coefficient, K_{OW}
- Biodegradability factor, BIO
- Coefficient of adsorption for substances in soil expressed for organic fraction of soil, K_{OC}
- Bio Concentration Factor, BCF

From these data you can perform a fate modelling and calculate effect factors for human toxicity and ecotoxicity in accordance with the EDIP Methodology [1 & 2]. This is explained in detail in the next chapter.

The above parameters have been extracted from the EPIWIN software [9]. Some values are genuine experimental data while others are estimated based on the chemical structure of the respective substance or by a property/property estimation technique. These parameters are stored in the software and the origin of the data is also specified.

Values for all the above mentioned parameters have been extracted for 28.033 substances with unique CAS numbers. 23.029 of these substances are also present on the list containing risk-phrases (section 2.1).

4 Tools for calculation of effect factors from risk-phrases

4.1 Development

The basis for calculating effect factors has now been established in the shape of three types of data:

- Database connecting CAS-numbers and substance names to risk-phrase numbers.
- Database with human toxicity – and ecotoxicity data estimated on the basis of risk-phrases.
- Database with physical/chemical data extracted from the EPIWIN database [9]

By means of these three components it is possible to calculate effect factors as illustrated in figure 1 below. The calculation is performed in a Microsoft Access database file, as described in detail in the next chapter.

Figure 1 Database Structure

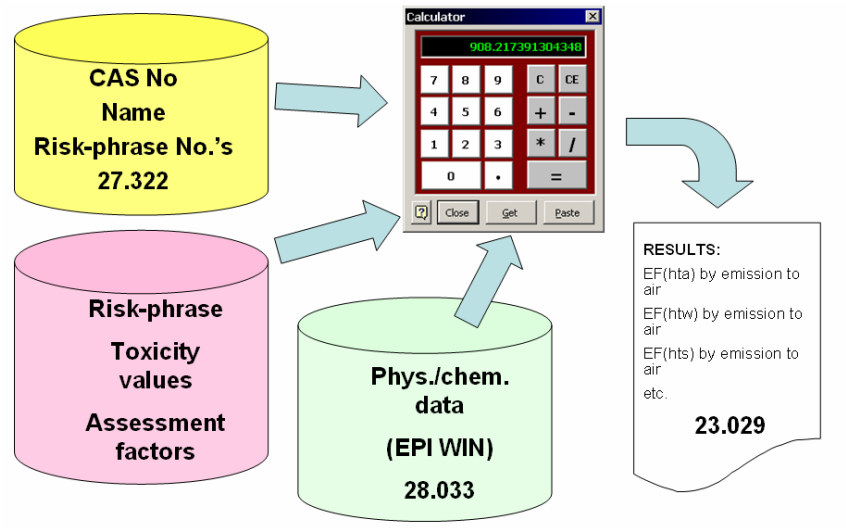


Figure 1 outlines the way the calculation has been performed using risk-phrases as the source of toxicity data. It is also possible to calculate effect factors based entirely (or partly) on individual data, as it is described in more detail in the section 6.1.3.

In both applications the calculation is executed strictly according to the EDIP method [1 & 2]. The calculation method is documented in the Appendix 2.

4.2 Testing of the calculation model

As mentioned in section 1.2 effect factors have so far been calculated for approx. 200 chemical substances. Approx. 120 of these appear among the 23.029 substances for which effect factors have been calculated from the risk-phrases. Effect factors calculated by the Department of Manufacturing Engineering and Management (IPL) for these 120 substances were compared to effect factors calculated by the risk-phrase method. This comparison (though insufficient) can provide an indication of how good an estimate the risk-phrase method can generate.

Some essential figures from this comparison are shown in table 5 and table 6.

Table 5

Comparing effect factors for human toxicity calculated by IPL (Reference value) with effect factors calculated by the risk-phrase method (Risk-value). The figures are the number of substances where the ratio [Reference value / Risk-value] is between 0,1 and 10 or both values are zero.

Effect Factors for human toxicity	Risk Phrase assigned	No Risk Phrase assigned
EF(hta)_air	45%	56%
EF(htw)_air	69%	56%
EF(hts)_air	67%	62%
EF(hta)_water	78%	75%
EF(htw)_water	44%	38%
EF(hts)_water	92%	79%
EF(hta)_soil	78%	75%
EF(htw)_soil	94%	78%
EF(hts)_soil	42%	57%

Table 6

Comparing effect factors for ecotoxicity calculated by IPL (Reference value) with effect factors calculated by the risk-phrase method (Risk-value). The figures are the number of substances where the ratio [Reference value / Risk-value] is between 0,1 and 10 or both values are zero.

Effect Factors for ecotoxicity	Risk Phrase assigned	No Risk Phrase assigned
EF(etwc)_air	70%	64%
EF(etsc)_air	71%	66%
EF(etwa)_water	44%	27%
EF(etwc)_water	35%	24%
EF(etsc)_water	87%	91%
EF(etwc)_soil	86%	91%
EF(etsc)_soil	25%	26%

In table 5 the column “Risk-phrase assigned” refers to the fraction of the substances that have at least one risk-phrase relevant to human toxicity assigned (R20, R22, R23, R25, R26 and/or R28). The column “No Risk-phrase assigned” refers to the fraction of the substances that do not have any of these risk-phrases assigned. For these substances a value for LD_{50} of 2.000 mg/kg body weight has been set (see section 2.2.3) to represent a maximum value.

In table 6 the column “Risk-phrase assigned” refers to the fraction of the substances that have at least one risk-phrase relevant to ecotoxicity assigned (R50, R51 and/or R52). The column “No Risk-phrase assigned” refers to the fraction of the substances that do not have any of these risk-phrases assigned. For these substances a value for LC_{50} / EC_{50} / IC_{50} of 100.000 mg/m^3 water has been set (see section 2.2.4) to represent a maximum value.

From the table 5 and table 6 it can be seen that:

- The match of substances that have not been assigned a risk-phrase (categories 3 and 4) is not much worse than the match for those with a risk-phrase assigned (categories 1 and 2).
- The matches differ for each effect factor, but generally it can be concluded that the matches are quite good, bearing in mind the uncertainties that are usually involved in this kind of calculations.

In order to give an impression of the deviation two different examples are shown below. They represent a very good match (figure 2) and a less convincing match (figure 3). The lines indicate the interval, where the ratio [Reference value / Risk-value] is between 0,1 and 10 . Please notice that zero values are not shown in these diagrams.

Figure 2

Comparison of results from calculating an effect factor for human toxicity. The lines indicate the interval, where the ratio [Factors calculated from risk-phrases / Factors calculated by IPL] is between 0,1 and 10 . Zero values are not shown.

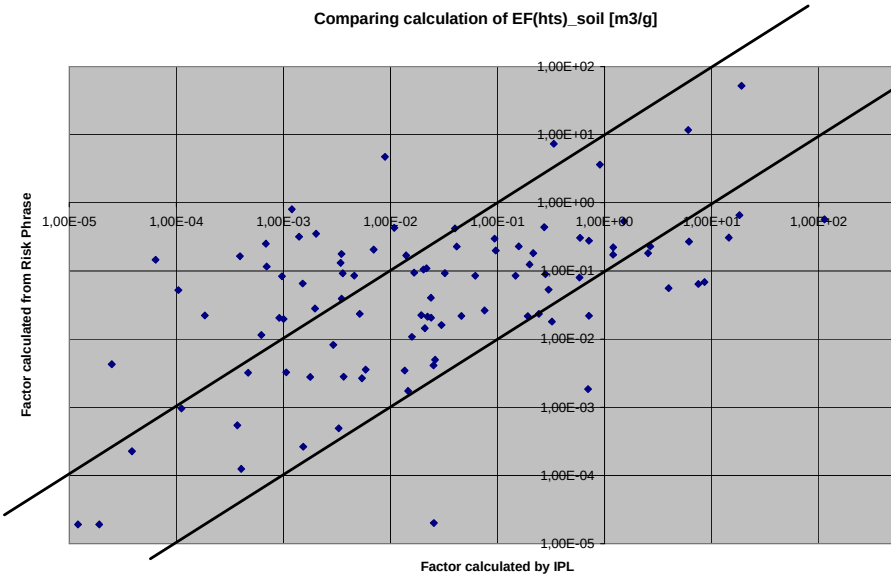
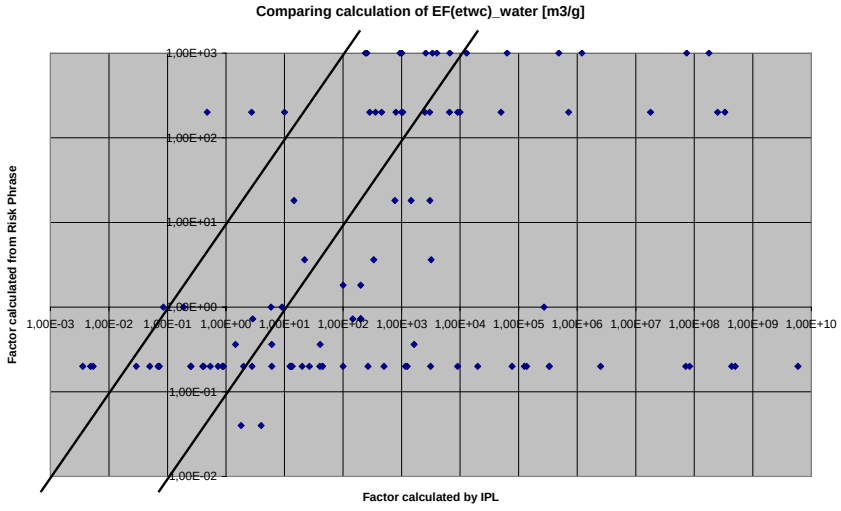


Figure 3

Comparison of results from calculating an effect factor for ecotoxicity. The lines indicate the interval, where the ratio [Factors calculated from risk-phrases / Factors calculated by IPL] is between 0,1 and 10 . Zero values are not shown.



Figures from this comparison of all effect factors are given in the Appendix 3, and comparisons in the form of XY-plots are given in Appendix 4.

From figure 3 and from other XY-plots in Appendix 4 it can be seen that the risk-phrase method gives a discrete output (step-wise in stead of continuous). It is obvious that the applied toxicity data are discrete as they all origin from a few risk-phrases. This indicates that the fate-related physical/chemical data extracted from EPIWIN [9] are to some extent discrete too. Though quite surprising, this phenomenon has not been studied in any further detail, as it is considered to be peripheral to this project.

Evaluating the deviations it should be taken into consideration that those values that have been presented here as reference not necessarily are “the true values”. Effect factors calculated by the EDIP method from individual data may also deviate depending on the quality of the toxicity – and physical/chemical data you may find and employ.

Though this comparison is based on a limited number of substances it indicates that effect factors calculated by the risk-phrase method represent a fairly good estimate - especially when you consider that effect factors have been generated for more than 23.000 substances compared to those approx. 200 that have had effect factors calculated from individual data collected from the literature. Furthermore each set of calculated effect factors are supplied with a set of “Comments on data quality” indicating the quality of the underlying toxicity data. This is dealt with in further detail in section 6.2.

5 Discussion

This chapter discuss the uncertainty related to the effect factors that can be calculated by the described method using risk-phrases. In order to understand the aspects of the uncertainty it is necessary to understand the nature of the effect factors and what they imply.

The effect factors express the toxicity potentials of a specific chemical substance. The effect factors (or equivalency factors) that are calculated according to the EDIP methodology has the unit m^3/g. E.g. the effect factor $EF(htw)_{air}$ for acetic acid is

$3.3\ 10^{-6}$ m^3water/g. This expresses the toxicity potential in m^3water into which 1 g of acetic acid (emitted to air) should be diluted for its concentration to be so low that no toxicological effects to humans are expected. In this case it is predicted on the basis of the physical / chemical data that a certain fraction of the acetic acid emitted to air will be transferred to the water compartment and constitute a human toxicity potential here.

It thus appears that the higher the value of the effect factor the higher is the toxicity potential. For more details about the effect factors is referred to the original literature [1 & 2].

By using the effect factors calculated by the risk-phrase method the LCA practitioner might ask the question:

> *What is the uncertainty the calculated values and how could they jeopardise the seriousness of my conclusions?*

It is not possible to give a precise answer. In the following it is however the ambition to uncover the nature of the uncertainty and how to cope with it.

The uncertainty consists of 4 elements:

- The EDIP methodology itself
- The applied toxicity data
- The applied physical / chemical data
- The application of the calculated effect factors in the specific LCA

The uncertainty of the EDIP methodology deals with the question of to what extent this methodology reflect the situation in “the real world”. It is not considered to be the scope of this project to deal with this issue, though it is relevant to bare this uncertainty in mind. This and similar issues are covered by the OMNIITOX project [13 & 14].

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

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

The assessment factor is dependent on the quality and the relevance of the available toxicity data as it is demonstrated in the table 7 below.

Table 7

Determination of assessment factors based on the quality and the relevance of available toxicity data. Taken from [2].

Criterion	Assessment factor
Extrapolation from LC_{50} or LD_{50} from animal experiments	10^5
Extrapolation from LC_{L0} or LD_{L0} from animal experiments	$5 \cdot 10^4$
Extrapolation from LOAEL from short-term animal experiments	10^4
Extrapolation from LC_{L0} or LD_{L0} from acute human studies	$5 \cdot 10^3$
Extrapolation from NOAEL from short-term experiments (less than a year) **or** extrapolation from LOAEL from chronic experiments (lasting a year or more)	10^3
Extrapolation from validated long-term animal experiments (lasting more than a year) **or** extrapolation from LOAEL in human studies **or** extrapolation from the lowest irritant concentration on inhalation in humans	10^2
Extrapolation from NOAEL found in validated long-term studies in humans.	10

Human toxicity data applied by the risk-phrase method is entirely based on LD_{50} or LC_{50} values from animal experiments and the assessment factor is thus 100.000. Though the difference in the assessment factors to some extent reflects the nature of the respective toxicity data it should be emphasized that the estimation of chronic effects in humans made on the basis of experience from short-term exposure in animals is highly uncertain [2]. This means that using the risk-phrase method is imposing the highest degree of uncertainty within the EDIP method. This uncertainty might probably for many substances be higher than e.g. the uncertainty of selecting a representative value for LD_{50} in the interval between 200 and 2000 mg / kg bodyweight as it is the case for R22. The uncertainty of the representative toxicity data derived from the risk-phrases also imply uncertainties as it is described in detail in section 2.2.

By the calculation of effect factors for ecotoxicity the *"Predicted No Effect Concentration"* (PNEC) is the value that needs to be derived. PNEC is the concentration of a substance in the environment expected

not to cause ecotoxicological effects. The PNEC is determined from the equation:

PNEC=Lowest available toxicity data found / Assessment Factor

The assessment factor is dependent on the quality and the relevance of the available toxicity data in the same way as described for human toxicity above (table 7). However due to the nature of ecotoxicity the assessment factors are generally lower. They vary from 10 to 1000 for chronic effects and from 10to 100 for acute effects [2]. Furthermore as the criteria for the risk-phrases relevant to ecotoxicity are based on ecotoxicity data of higher quality and relevance the applied assessment factors are considerably lower than for human toxicity. This indicates that the calculated assessment factors for ecotoxicity are less uncertain than those for human toxicity.

The physical / chemical data used by the risk-phrase method are extracted from the EPIWIN software [9]. The physical / chemical data applied by the calculation of effect factors performed by IPL (see section 4.2) also originate from the EPIWIN software. It can thus be concluded that the uncertainty related to these data are negligible. This is also confirmed by a few random checks that were done in connection to the testing of calculation model as described in section 4.2.

It can thus be concluded that the highest degree of uncertainty by the calculation of effect factors is related to the toxicity data. The uncertainty is higher for human toxicity than for ecotoxicity. This conclusion is considered to be true for both the risk-phrase method and the method based on individual data [11].

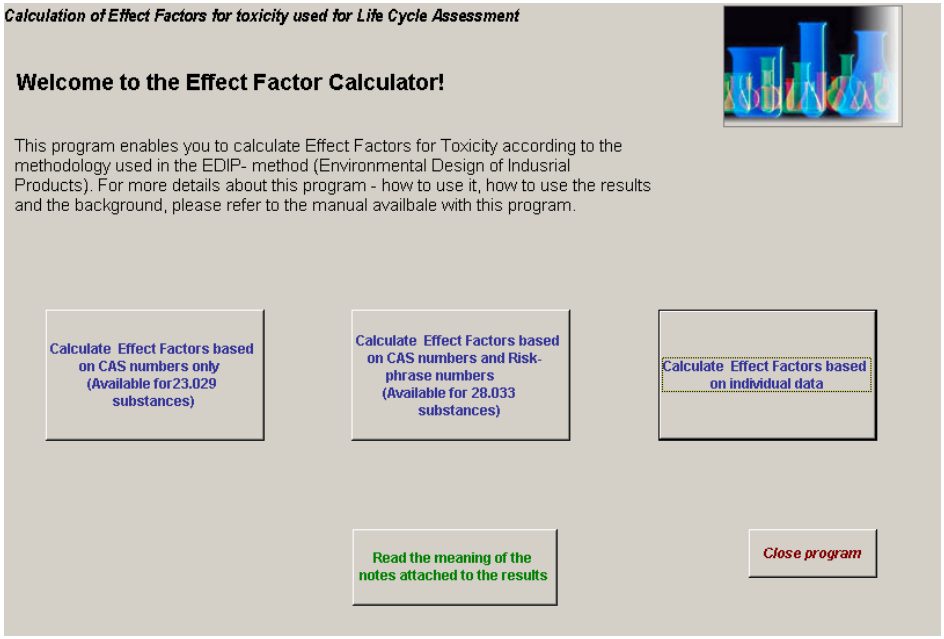
The last element of uncertainty is the application of the calculated effect factors in each specific LCA. Whether the uncertainty of a calculated effect factor is acceptable or not depends very much on the context in which it is applied. Each set of calculated effect factors is accompanied by some “Comments on data quality”, that serves to characterize the quality of the toxicity data.

These comments should be studied carefully and taken into consideration when assessing the results of the LCA in question and the importance of an uncertainty should be uncovered by the sensitivity analysis. If you need to narrow the interval of uncertainty it is recommended to search for specific toxicity data for the particular substances and recalculate the effect factor by using model 2 as it is described in section 6.1.

6 How to use

6.1 How to calculate

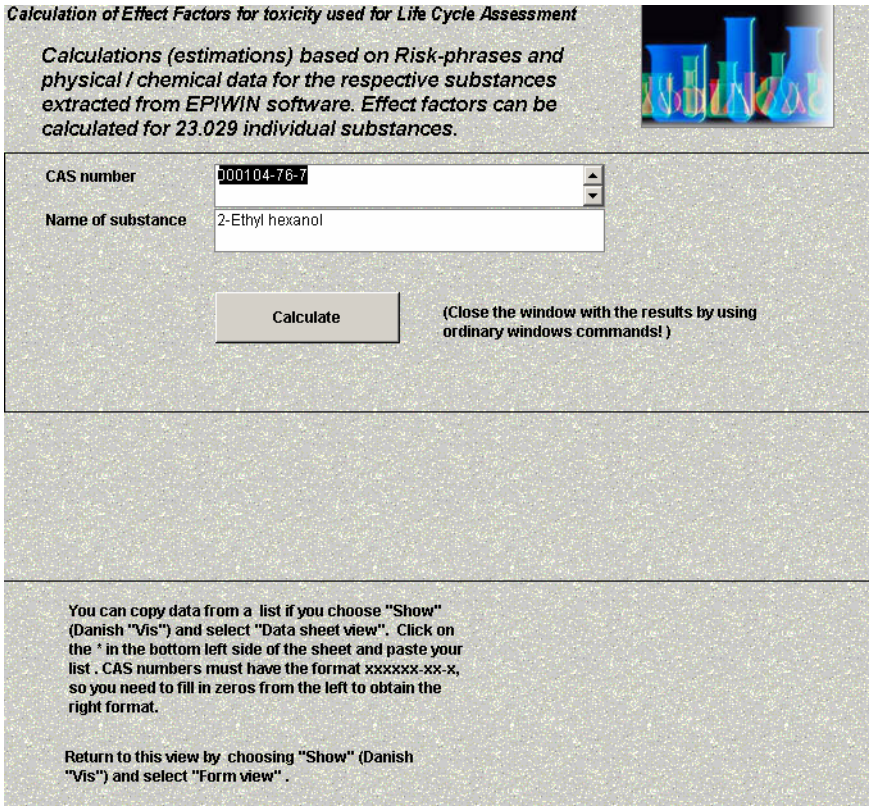
The Effect Factor Calculator can be started by opening the file Eff_factor.mdb. To operate this calculator you need the database programme MS Access 2000 or a later version, and you must have a status on the applied computer that allows you to execute macros and the file should NOT have the attribute “Read only” (Danish: “Skriveskyttet”). When you open the file this screen will appear and allow you to calculate effect factors based on risk-phrases or individually supplied data:



Which method to use for calculation depends on the amount of effort you want to invest and the ambitions you have in terms of quality of the calculated effect factors.

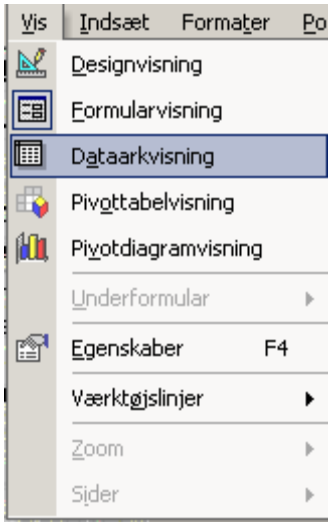
6.1.1 Calculation using only CAS-numbers

The easiest way to perform the calculation is to apply the button to the left. You get this screen:

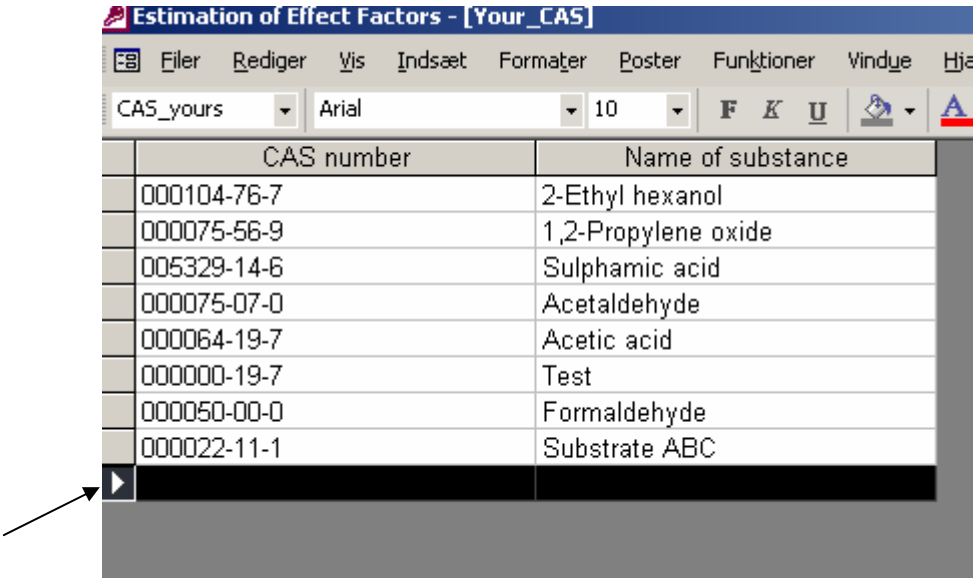


The only thing you need to do is to enter a CAS-number and a name (optional). This calculation (estimation) is based on Risk-phrases and physical / chemical data for the respective substances extracted from the EPIWIN software [9]. Please notice that CAS numbers must have the format 000000-00-0, so you need to fill in zeros from the left to obtain the right format.

If you want to enter a large number of substances you can change the view by choosing "Show" (Danish: "Vis") and select "Data sheet view" (Danish: Dataarkvisning).

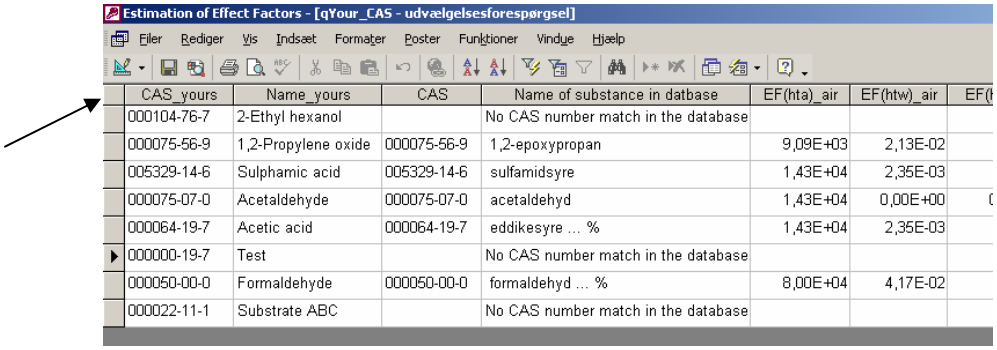


and you get this screen:



By clicking to the left of the last (empty) line you can enter a large number of data sets in two columns format. Return to the previous window by choosing "Show" (Danish: "Vis") and select "Form view" (Danish: Formularvisning).

Press the “Calculate” button to perform the calculations and you will get this view:



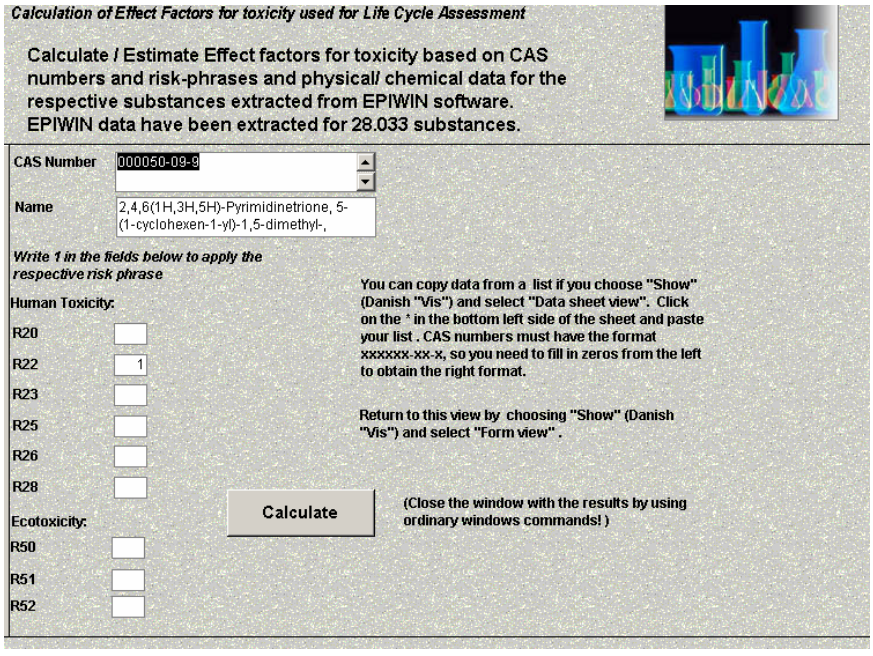
CAS_yours	Name_yours	CAS	Name of substance in datbase	EF(hta)_air	EF(htw)_air	EF(
000104-76-7	2-Ethyl hexanol		No CAS number match in the database			
000075-56-9	1,2-Propylene oxide	000075-56-9	1,2-epoxypropan	9,09E+03	2,13E-02	
005329-14-6	Sulphamic acid	005329-14-6	sulfamidsyre	1,43E+04	2,35E-03	
000075-07-0	Acetaldehyde	000075-07-0	acetaldehyd	1,43E+04	0,00E+00	
000064-19-7	Acetic acid	000064-19-7	eddikesyre ... %	1,43E+04	2,35E-03	
000000-19-7	Test		No CAS number match in the database			
000050-00-0	Formaldehyde	000050-00-0	formaldehyd ... %	8,00E+04	4,17E-02	
000022-11-1	Substrate ABC		No CAS number match in the database			

The data can be copied by clicking the square in the upper left side of the window and choose Edit, Copy. Close the window to return to the previous window.

Effect factors for 23.029 substances have been calculated and are presented in the MS Excel file *"Factor_23029.xls"*, which is available with this publication.

6.1.2 Calculation by means of CAS-numbers and risk-phrases

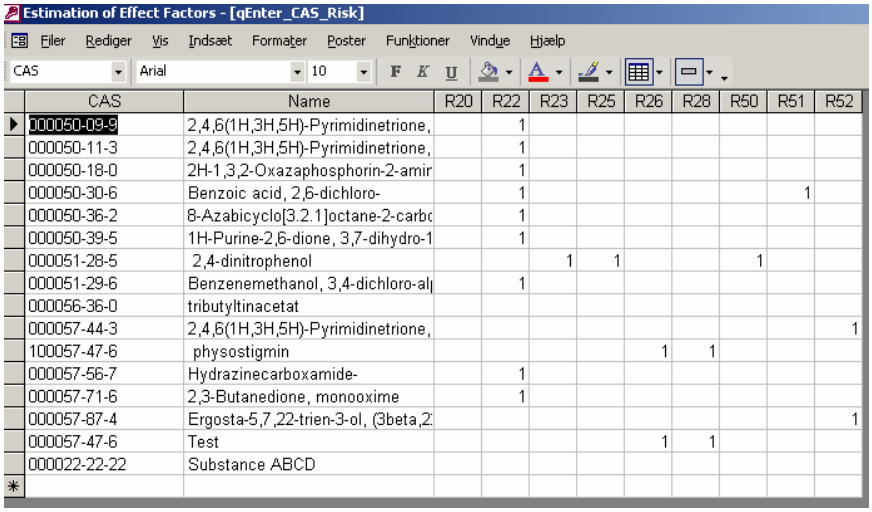
If you did not find the relevant substances by using the method in section 6.1.1 you can apply the button in the middle. You get this screen:



All you need to enter here beside the CAS-number are the risk-phrases. If you choose not to enter any risk-phrase relevant to human toxicity and/or ecotoxicity you can still perform the calculation. This means that you assume that the substance has a human toxicity lower than the criteria for the risk-phrase R20/22 and an ecotoxicity lower than the criteria for R52.

"Lower" in this context means higher in terms of value of LD_{50}, LC_{50} etc. The calculated results thus represent maximum values.

Entering of a large number of substances can be done as described above in section 6.1.1.:

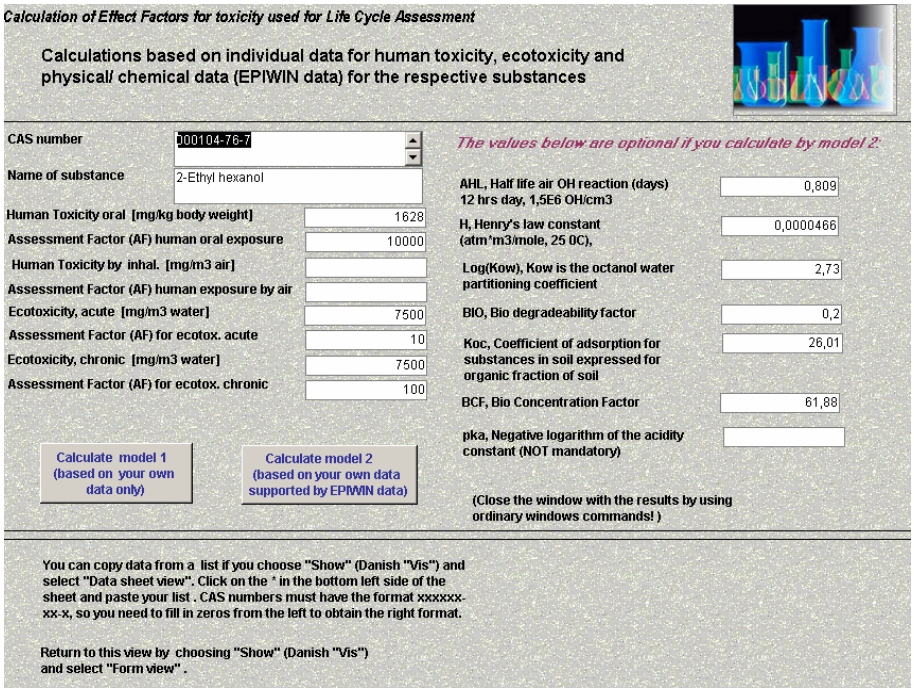


CAS	Name	R20	R22	R23	R25	R26	R28	R50	R51	R52
000050-09-9	2,4,6(1H,3H,5H)-Pyrimidinetrione,		1							
000050-11-3	2,4,6(1H,3H,5H)-Pyrimidinetrione,		1							
000050-18-0	2H-1,3,2-Oxazaphosphorin-2-amir		1							
000050-30-6	Benzoic acid, 2,6-dichloro-		1						1	
000050-36-2	8-Azabicyclo[3.2.1]octane-2-carbc		1							
000050-39-5	1H-Purine-2,6-dione, 3,7-dihydro-1		1							
000051-28-5	2,4-dinitrophenol			1	1			1		
000051-29-6	Benzenemethanol, 3,4-dichloro-al		1							
000056-36-0	tributyltinacetat									
000057-44-3	2,4,6(1H,3H,5H)-Pyrimidinetrione,									1
100057-47-6	physostigmin					1	1			
000057-56-7	Hydrazinecarboxamide-		1							
000057-71-6	2,3-Butanedione, monooxime		1							
000057-87-4	Ergosta-5,7,22-trien-3-ol, (3beta,2									1
000057-47-6	Test					1	1			
000022-22-22	Substance ABCD									

Return to the previous window by choosing "Show" (Danish: "Vis") and select "Form view" (Danish: Formularvisning). Press the "Calculate" button to perform the calculations to see the results.

6.1.3 Calculation by means of individual data

If you did not find any relevant substances by using the methods mentioned above, or you want to calculate effect factors based on your own data, you can click the button to the right and supply your individual data to the calculator. You get this view:



Please notice that the application of this part of the tool requires some skills in toxicology and the way emissions of chemical substances are assessed in the EDIP Methodology [1 & 2].

If you are able to supply all the data specified above you can calculate effect factors by clicking the button “Calculate model 1”. Data for the left column can be found in the toxicological literature. Data for the physical / chemical data can be found in the literature or be estimated by means of the EPIWIN software [9]. If you are only in possession of the toxicity data and none (or just a few) of the physical / chemical data you can use the button “Calculate model 2”. In this case the calculator will apply the respective physical/chemical data for the specified substance (CAS-number) from the database with 28.033 substances described in chapter 3.

The estimation of assessment factors should be performed according to the EDIP Methodology [2, pages 390, 253 and 250].

This screen also opens up for entering larger numbers of data sets as described above. Be sure to apply the same number of columns and notice that columns designed to receive numeric value only will accept numeric entries.

The calculation based entirely on individual data (model 1) can also be performed by the MS Excel file *“Effect_Factor_Calculator.xls”*, which is available with this publication.

6.2 How to use the results

The effect factors calculated from toxicity values derived from the risk-phrases will inevitable be connected with some uncertainty. The uncertainty will differ depending on the risk-phrase applied, and the origin of that phrase. To each set of effect factors calculated is attached some "Comments on data quality", that serves to characterize the quality of the toxicity data. A list of all the notes used to characterize the data applied for the calculation of each data set is shown in Appendix 5. You can obtain this list by pressing the button "Read the meaning of the notes attached to the results", which is available from the main menu screen that appears when you open the file, as described in the beginning of this chapter.

It is highly recommended to study these comments carefully and be aware of their premises as it appears from section 2.2 and chapter 5.

14) Koning, A. de et.al (2002), Inventory and classification of LCA characterisation methods for assessing toxic releases, Contribution to Work-package 7 of the OMNII-TOX Project as part A of appropriate deliverable D11. To be downloaded from http://www.omniitox.net/ or http://omniitox.imi.chalmers.se/OfficialMirror/ .
15) Technical Guidance Document 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 of the Council concerning the placing of biocidal products on the market. EUR 20418 EN/1, European Communities, 2003, http://ecb.jrc.it/home.php?CONTENU=/Technical-Guidance-Document/sommaire.php
16) Flemström, K., R. Carlson & M. Erixon, 2004, Relationships between Life Cycle Assessment and Risk Assessment – Potentials and Obstacles, Naturvårdsverket, Report 5379.
17) The UNEP/SETAC The Life Cycle Initiative, Task Force on Toxicity impacts (TF LCIA 3) http://www.uneptie.org/pc/sustain/lcinitiative/home.htm

R18	In use, may form flammable/explosive vapour-air mixture.	Risk-phrase criteria not relevant to toxicity or ecotocicity
R19	May form explosive peroxides.	Risk-phrase criteria not relevant to toxicity or ecotocicity
R20	Harmful by inhalation.	Risk-phrase criteria relevant to human toxicity
R21	Harmful in contact with skin.	Risk-phrase refers to dermal toxicity and is not used. Of 27.322 substances that were assigned risk-phrases relating to skin toxicity (R21, R24 and R27) only very few (19) did not have a risk-phrase relating to oral toxicity.
R22	Harmful if swallowed.	Risk-phrase criteria relevant to human toxicity
R23	Toxic by inhalation.	Risk-phrase criteria relevant to human toxicity
R24	Toxic in contact with skin.	Risk-phrase refers to dermal toxicity and is not used. Of 27.322 substances that were assigned risk-phrases relating to skin toxicity (R21, R24 and R27) only very few (19) did not have a risk-phrase relating to oral toxicity.
R25	Toxic if swallowed.	Risk-phrase criteria relevant to human toxicity
R26	Very toxic by inhalation.	Risk-phrase criteria relevant to human toxicity
R27	Very toxic in contact with skin.	Risk-phrase refers to dermal toxicity and is not used. Of 27.322 substances that were assigned risk-phrases relating to skin toxicity (R21, R24 and R27) only very few (19) did not have a risk-phrase relating to oral toxicity.
R28	Very toxic if swallowed.	Risk-phrase criteria relevant to human toxicity
R29	Contact with water liberates toxic gas.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R30	Can become highly flammable in use.	Risk-phrase criteria not relevant to toxicity or ecotocicity

R31	Contact with acids liberates toxic gas.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R32	Contact with acids liberates very toxic gas.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R33	Danger of cumulative effects.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R34	Causes burns.	Risk-phrase criteria refers to burning and irritation of skin and is not used.
R35	Causes severe burns.	Risk-phrase criteria refers to burning and irritation of skin and is not used.
R36	Irritating to eyes.	Risk-phrase criteria refers to burning and irritation of skin and is not used.
R37	Irritating to respiratory system.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R38	Irritating to skin.	Risk-phrase criteria refers to burning and irritation of skin and is not used.
R39	Danger of very serious irreversible effects.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R40	Limited evidence of carcinogenic effects.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R41	Risk of serious damage to eyes.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R42	May cause sensitisation by inhalation.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not

		used.
R43	May cause sensitisation by skin contact.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R44	Risk of explosion if heated under confinement.	Risk-phrase criteria not relevant to toxicity or ecotocicity
R45	May cause cancer.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R46	May cause heritable genetic damage.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R47	Not Active	Risk-phrase is not active
R48	Danger of serious damage to health by prolonged exposure.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R49	May cause cancer by inhalation.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R50	Very toxic to aquatic organisms.	Risk-phrase criteria relevant to ecotoxicity
R51	Toxic to aquatic organisms.	Risk-phrase criteria relevant to ecotoxicity
R52	Harmful to aquatic organisms.	Risk-phrase criteria relevant to ecotoxicity
R53	May cause long-term adverse effects in the aquatic environment.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.

R54	Toxic to flora.	Risk-phrase does not refer to quantitative (eco)toxicity criteria and is not used.(Criteria have not been specified). Of 27322 substances no substances were asigned this risk-phrase.
R55	Toxic to fauna.	Risk-phrase does not refer to quantitative (eco)toxicity criteria and is not used.(Criteria have not been specified). Of 27322 substances no substances were asigned this risk-phrase.
R56	Toxic to soil organisms.	Risk-phrase does not refer to quantitative (eco)toxicity criteria and is not used.(Criteria have not been specified). Of 27322 substances no substances were asigned this risk-phrase.
R57	Toxic to bees.	Risk-phrase does not refer to quantitative (eco)toxicity criteria and is not used.(Criteria have not been specified). Of 27322 substances no substances were asigned this risk-phrase.
R58	May cause long-term adverse effects in the environment.	Risk-phrase does not refer to quantitative (eco)toxicity criteria and is not used.(Criteria have not been specified). Of 27322 substances two substances were asigned this risk-phrase.
R59	Dangerous for the ozone layer.	Risk-phrase criteria not relevant to toxicity or ecotocicity
R60	May impair fertility.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R61	May cause harm to the unborn child.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.

R62	Possible risk of impaired fertility.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R63	Possible risk of harm to the unborn child.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.
R64	May cause harm to breast-fed babies.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R65	Harmful: may cause lung damage if swallowed.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R66	Repeated exposure may cause skin dryness or cracking.	Risk-phrase criteria refers to burning and irritation of skin and is not used.
R67	Vapours may cause drowsiness and dizziness.	Risk-phrase criteria refers to supplementary (eco)toxicity information that is not quantified and is not used.
R68	Possible risk of irreversible effects.	Risk-phrase criteria refers to supplementary toxicity information and this phrase is used in co-existence with risk-phrases referring to quantitative criteria.

Appendix 2

Documentation of the applied calculation method

Symbol	Parameter	Unit	Formula or Input	Reference
CAS No	CAS Number	-	Input from the user	
Name	Substance Name	-	Given from the CAS number	
Toxicity data				
HTo	Human Tox oral, Lowest relevant and reliable human toxicity data found, oral admin.	mg / kg body weight	**Risk-phrase method:** Value extracted from the risk-phrase **Individual method:** Data input from the user	
HTa	Lowest relevant and reliable human toxicity data found, inhalation admin.	mg/m^3	**Risk-phrase method:** Value extracted from the risk-phrase **Individual method:** Data input from the user	
ETa	Data for ecotoxicity acute	mg / m^3 water	**Risk-phrase method:** Value extracted from the risk-phrase **Individual method:** Data input from the user	
ETc	Data for ecotoxicity chronic	mg / m^3 water	**Risk-phrase method:** Value extracted from the risk-phrase **Individual method:** Data input from the user	

AFho	Assessment factor for oral exposure, human	-	**Risk-phrase method:** 100.000 **Individual method:** Input from the user based on the EDIP methodology	[2], p 390
AFha	Assessment factor for exposure by air, human	-	**Risk-phrase method:** 100.000 **Individual method:** Input from the user based on the EDIP methodology	[2], p 390
AFeta	Assessment factor for ecotoxicity acute	-	**Risk-phrase method:** 10 **Individual method:** Input from the user based on the EDIP methodology	[2], p 256
AFetc	Assessment factor for ecotoxicity chronic	-	**Risk-phrase method:** 100 **Individual method:** Input from the user based on the EDIP methodology	[2], p 253
Parameters				
AHL	Atmospheric half life	days (12 hour day)	**Risk-phrase method:** Value extracted from EPIWIN **Individual method:** Value extracted from EPIWIN or Data input from the user	
H	Henry's Law Constant	atm*m^3/mol	**Risk-phrase method:** Value extracted from EPIWIN **Individual method:** Value extracted from EPIWIN or Data input from the user	
LK_{ow} (Log K_{ow})	Log K_{ow}. K_{ow} is the octanol water partitioning coefficient (KOW = POW)	-	**Risk-phrase method:** Value extracted from EPIWIN **Individual method:** Value extracted from EPIWIN or Data input from the user	

BIO	BIO degradeability factor	-	**Risk-phrase method:** If the "Linear Biodegradation Probability" is <5 BIO is set to 1 otherwise it is set to 0,2 **Individual method:** Value estimated as for the risk-phrase method or Data input from the user	
K_{oc}	Coefficient of adsorption for substances in soil expressed for organic fraction of soil	-	**Risk-phrase method:** Value extracted from EPIWIN **Individual method:** Value extracted from EPIWIN or Data input from the user	
BCF	Bio Concentration Factor	kg water / kg fish	**Risk-phrase method:** Value extracted from EPIWIN **Individual method:** Value extracted from EPIWIN or Data input from the user	
Constants				
a	Ratio of distribution between water and soil (Global default value)	-	0,2	[1], p 284
$f_{a\ (via\ air)}$	That part of the emission which contribute to toxicity via air	-	1	[1], p 285
$f_{wa\ (via\ soil)}$	That part of the emission which contribute to acute ecotoxicity in water	-	0	[1], p 267
$f_{wa\ (via\ air)}$	That part of the emission which contribute to acute ecotoxicity in water	-	0	[1], p 265
I_a	Intake factor for air	-	1	[2], p 367
T_a	Transfer factor from air	-	1	[2], p 367
$T_{s,d}$	Transfer factor from soil, direct	-	1	[2], p 367

I_w	Intake factor for water	kg fish / kg body weight / day	0,000371	[2], p 367
$I_{s,p}$	Intake factor for soil via plants	kg plant / kg body weight / day	0,0093	[2], p 367
$I_{s,d}$	Intake factor for soil, direct	kg soil / kg body weight / day	0,00000286	[2], p 367
$I_{s,b}$	Intake factor for soil, via beef	kg beef / kg body weight / day	0,00153	[2], p 367
$I_{s,m}$	Intake factor for soil, via milk	kg milk / kg body weight / day	0,0132	[2], p 367
f_{oc}	Relative content of organic carbon (g/g)	kg/kg	0,02	[2], p 374
d^*	Density of soil	kg/l	1,5	[2], p 373
f_w^*	Water content of soil	l/l	0,4	[2], p 373
CF	Factor to convert from g to mg (or m3 to liter)	mg/g	1000	-
W_h	Bodyweight of an average person	kg	70	[2], p 391
V_h	Volume inhaled daily	m^3	20	[2], p 391
$f_{wa\ (via\ water)}$	That part of the emission which contribute to acute ecotoxicity in water	-	1	[1], p 266
BI_s	Daily ingestion of soil for cattle	kg	0,41	[2], p 381

BI_p	Daily ingestion of plants for cattle	kg	16,9	[2], p 381
Determination of fractions				
$f_{w\ (via\ air)}$	That part of the emission which contribute to toxicity via surface water	-	=IF(AHL>1;a;0)	[1], p 285
$f_{s\ (via\ air)}$	That part of the emission which contribute to toxicity via soil	-	=IF(AHL>1;1-a;0)	[1], p 285
$f_{w\ (via\ water)}$	That part of the emission which contribute to toxicity via surface water	-	=IF(H>0,001;IF(AHL>1;a;0);1)	[1], p 286
$f_{a\ (via\ water)}$	That part of the emission which contribute to toxicity via air	-	=IF(H>0,001;1;0)	[1], p 286
$f_{s\ (via\ water)}$	That part of the emission which contribute to toxicity via soil	-	=IF(H>0,001;IF(AHL>1;1-a;0);0)	[1], p 286
$f_{w\ (via\ soil)}$	That part of the emission which contribute to toxicity via surface water	-	=IF(H>0,001;IF(AHL>1;a;0);0)	[1], p 287
$f_{a\ (via\ soil)}$	That part of the emission which contribute to toxicity via air	-	=IF(H>0,001;1;0)	[1], p 287
$f_{s\ (via\ soil)}$	That part of the emission which contribute to toxicity via soil	-	=IF(H>0,001;IF(AHL>1;1-a;0);1)	[1], p 287
$f_{wa\ (via\ air)}$	That part of the emission which contribute to acute ecotoxicity in water	-	=0	[1], p 265
$f_{wc\ (via\ air)}$	That part of the emission which contribute to chronic ecotoxicity in water	-	=IF(AHL>1;a;0)	[1], p 265
$f_{sc\ (via\ air)}$	That part of the emission which contribute to chronic ecotoxicity in soil	-	=IF(AHL>1;1-a;0)	[1], p 265
$f_{wa\ (via\ water)}$	That part of the emission which contribute to acute ecotoxicity in water	-	=1	[1], p 266

$f_{wc\ (via\ water)}$	That part of the emission which contribute to chronic ecotoxicity in water	-	=IF(H>0,001;IF(AHL>1;a;0);1)	[1], p 266
$f_{sc\ (via\ water)}$	That part of the emission which contribute to chronic ecotoxicity in soil	-	=IF(H>0,001;IF(AHL>1;1-a;0);0)	[1], p 266
$f_{wa\ (via\ soil)}$	That part of the emission which contribute to acute ecotoxicity in water	-	=0	[1], p 267
$f_{wc\ (via\ soil)}$	That part of the emission which contribute to chronic ecotoxicity in water	-	=IF(H>0,001;IF(AHL>1;a;0);0)	[1], p 267
$f_{sc\ (via\ soil)}$	That part of the emission which contribute to chronic ecotoxicity in soil	-	=IF(H>0,001;IF(AHL>1;1-a;0);1)	[1], p 267
Determination of intermediate values				
K_d	Coefficient of adsorption in soil	-	=foc*Koc	[2], p 374
B_b	Biotransfer factor from soil and food to meat in cattle		=POTENS(10;LKow-7,6)	[2], p 381
B_m	Biotransfer factor from soil and food to milk in cattle		=POTENS(10;LKow-8,1)	[2], p 383
$T_{s,p}$	Transfer factor from soil, plants	-	=SCF/(Kd+(fw/d))	[2], p 367
$T_{s,b}$	Transfer factor from soil, beef		=BIp*Bb*SCF/(Kd+fw/d)+BIs*Bb	[2], p 381
$T_{s,m}$	Transfer factor from soil, milk		=BIp*Bm*SCF/(Kd+fw/d)+BIs*Bm	[2], p 383
I_s*T_s	Total from soil		=SUM(Isp*Tsp+Isd*Tsd+Isb*Tsb+Ism*Tsm)	-
SCF	Stem Concentration Factor	-	=(0,82+POTENS(10;0,95*LKow-2,05))*0,748*POTENS(EKSP(1);-(LKow-1,78)*(LKow-1,78)/2,44)	[2], p 374
T_w	Transfer factor from water (= BCF)	-	=BCF	[1], p289

Determination of reference doses etc.				
HRD	Human Reference Dose	mg / kg body weight / day	=HTo/AFho	[1], p 295
HRC	Human Reference Concentration (HRC kan beregnes fra HRD se side 390 i Sci Back..)	mg/m^3 air	=IF(HTa>0;HTa/AFha;HRD*Wh/Vh)	[1], p 294
$PNEC_{wa}$	The highest concentration assessed not produce acute ecotoxic effects in the water compartment	g / m^3 water	=ETa/AFeta/CF	[1], p 271
$PNEC_{wc}$	The highest concentration assessed not produce chronic ecotoxic effects in the water compartment	g / m^3 water	=ETc/AFetc/CF	[1], p 269
$PNEC_{sc}$	The highest concentration assessed not produce chronic ecotoxic effects in the soil compartment	g / m^3 water	=(Kd+0,27)*d*PNECwc	[1], p 272
HTF_a	Human Toxicity Factor for exposure via air	m^3 air/g	=1/HRC*CF	[1], p 294
HTF_w	Human Toxicity Factor for exposure via surface water	kg body weight / mg	=1/HRD	[1], p 294
HTF_s	Human Toxicity Factor for exposure via soil	kg body weight / mg	=1/HRD	[1], p 294
ETF_{wa}	Ecotoxicity Factor for acute effects in water	m^3 water/g	=1/PNECwa	[1], p 268
ETF_{wc}	Ecotoxicity Factor for chronic effects in water	m^3 water/g	=1/PNECwc	[1], p 268
ETF_{sc}	Ecotoxicity Factor for chronic effects in soil	m^3 soil/g	=1/PNECsc	[1], p 268

Human Toxicity			
EF(hta) by emission to air	m^3 air/g	=faa*Ia*Ta*HTFa	[1], p 296
EF(htw) by emission to air	m^3 water/g	=fwa*Iw*Tw*HTFw*BIO	[1], p 296
EF(hts) by emission to air	m^3 soil/g	=fsa*IsTs*HTFs*BIO/d	[1], p 296
EF(hta) by emission to water	m^3 air/g	=faw*Ia*Ta*HTFa	[1], p 296
EF(htw) by emission to water	m^3 water/g	=fww*Iw*Tw*HTFw*BIO	[1], p 296
EF(hts) by emission to water	m^3 soil/g	=fsw*IsTs*HTFs*BIO	[1], p 296
EF(hta) by emission to soil	m^3 air/g	=fas*Ia*Ta*HTFa	[1], p 296
EF(htw) by emission to soil	m^3 water/g	=fws*Iw*Tw*HTFw*BIO	[1], p 296
EF(hts) by emission to soil	m^3 soil/g	=fss*IsTs*HTFs*BIO/d	[1], p 296
Ecotoxicity			
EF(etwc) by emission to air	m^3 water/g	=fwca*BIO*ETFwc	[1], p 275
EF(etsc) by emission to air	m^3 soil/g	=fsca*BIO*ETFsc	[1], p 275
EF(etwc) by emission to water	m^3 water/g	=fwcw*BIO*ETFwc	[1], p 275
EF(etwa) by emission to water	m^3 water/g	=fwaw*ETFwa	[1], p 275
EF(etsc) by emission to water	m^3 soil/g	=fscw*BIO*ETFsc	[1], p 275
EF(etwc) by emission to soil	m^3 water/g	=fwcs*BIO*ETFwc	[1], p 275
EF(etsc) by emission to soil	m^3 soil/g	=fscs*BIO*ETFsc	[1], p 275

Appendix 3

Comparing effect factors for human toxicity calculated by IPL respectively by the risk-phrase method

Effect Factor Risk phrase assigned	EF(hta)_air	EF(htw)_air	EF(hts)_air	EF(hta)_water	EF(htw)_water	EF(hts)_water	EF(hta)_soil	EF(htw)_soil	EF(hts)_soil
Number of substances	51	51	51	50	50	50	50	50	50
Risk-value is too low	67%	24%	27%	6%	52%	6%	6%	6%	58%
Risk-value is too high	33%	22%	18%	18%	48%	4%	18%	4%	42%
Both values are zero	0%	55%	55%	76%	0%	90%	76%	90%	0%
Risk-value is zero	0%	16%	16%	2%	14%	2%	2%	2%	14%
Reference-value / Risk-value is between 0,1 and 10	45%	14%	12%	2%	44%	2%	2%	4%	42%
Reference-value / Risk-value is between (0,01 - 0,1) and (10 - 100)	43%	10%	8%	2%	20%	4%	2%	2%	28%
Reference-value / Risk-value is between (0,001 - 00,1) and (100 - 1000)	8%	4%	10%	2%	14%	0%	2%	0%	14%
Reference-value / Risk-value is lower than 0,001 or higher than 1000	4%	2%	0%	16%	8%	2%	16%	2%	2%

Effect Factor No Risk phrase assigned	EF(hta)_air	EF(htw)_air	EF(hts)_air	EF(hta)_water	EF(htw)_water	EF(hts)_water	EF(hta)_soil	EF(htw)_soil	EF(hts)_soil
Number of substances	68	68	68	68	68	68	68	68	68
Risk-value is too low	32%	32%	28%	13%	47%	10%	13%	19%	43%
Risk-value is too high	66%	25%	29%	32%	44%	19%	32%	10%	49%
Both values are zero	1%	43%	43%	54%	9%	71%	54%	71%	9%
Risk-value is zero	0%	15%	15%	4%	12%	7%	4%	7%	12%
Reference-value / Risk-value is between 0,1 and 10	54%	13%	19%	21%	29%	9%	21%	7%	49%
Reference-value / Risk-value is between (0,01 - 0,1) and (10 - 100)	21%	12%	13%	9%	25%	4%	9%	9%	16%
Reference-value / Risk-value is between (0,001 - 00,1) and (100 - 1000)	15%	12%	9%	3%	16%	7%	3%	4%	10%
Reference-value / Risk-value is lower than 0,001 or higher than 1000	9%	6%	1%	9%	9%	1%	9%	1%	4%

Risk-value is the value calculated by means of the risk-phrase method
Reference-value is the value calculated by IPL

Comparing effect factors for ecotoxicity calculated by IPL respectively by the risk-phrase method

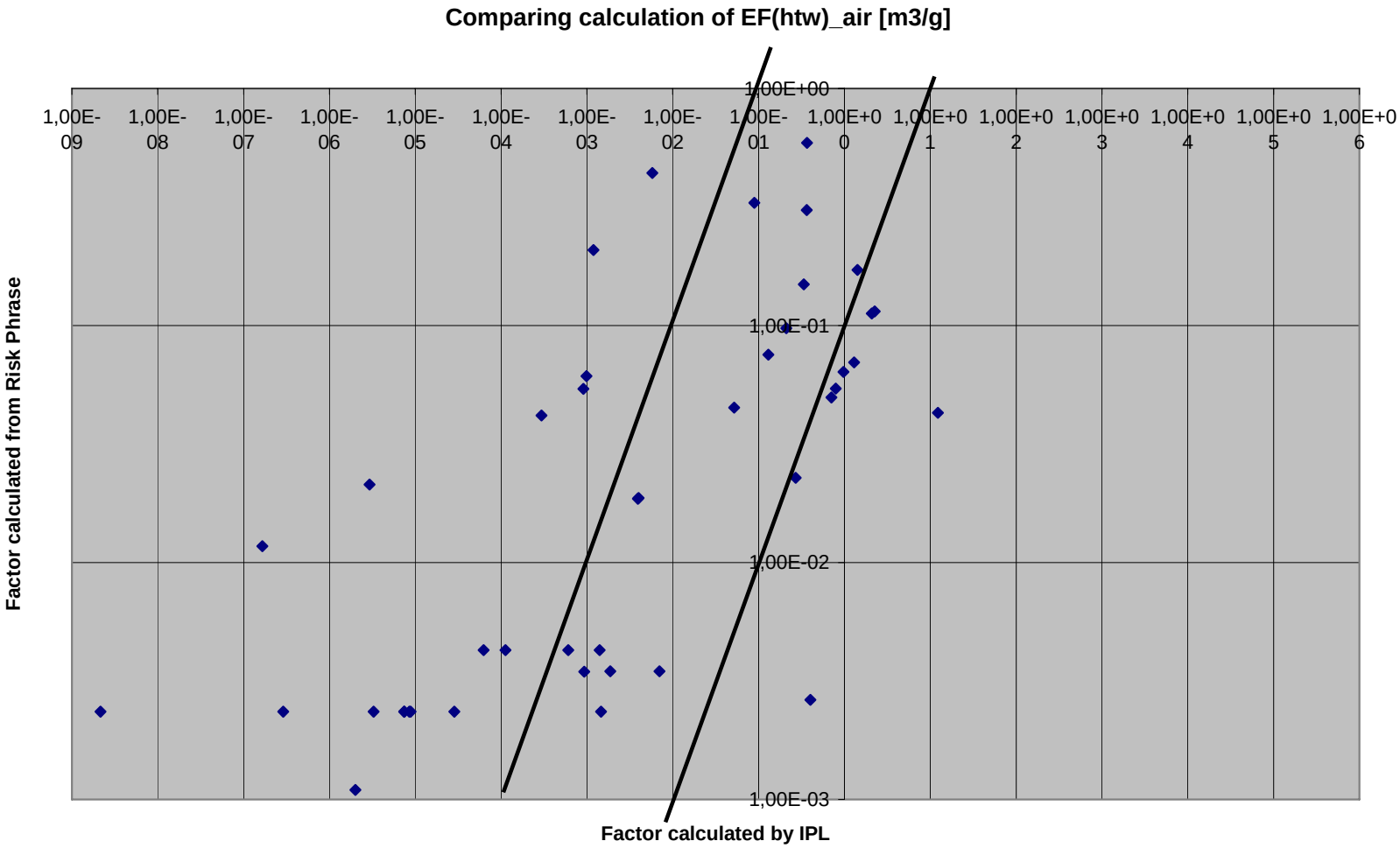
Effect Factor Risk phrase assigned	EF(etwc)_air	EF(etsc)_air	EF(etwa)_water	EF(etwc)_water	EF(etsc)_water	EF(etwc)_soil	EF(etsc)_soil
Number of substances	63	63	63	63	63	63	63
Risk-value is too low	35%	32%	78%	84%	11%	14%	83%
Risk-value is too high	5%	8%	21%	11%	6%	3%	16%
Both values are zero	60%	60%	2%	5%	83%	83%	2%
Risk-value is zero	6%	6%	0%	6%	3%	3%	6%
Reference-value / Risk-value is between 0,1 and 10	10%	11%	43%	30%	5%	3%	24%
Reference-value / Risk-value is between (0,01 - 0,1) and (10 - 100)	11%	14%	38%	27%	5%	2%	22%
Reference-value / Risk-value is between (0,001 - 00,1) and (100 - 1000)	11%	5%	6%	19%	3%	10%	25%
Reference-value / Risk-value is lower than 0,001 or higher than 1000	2%	3%	11%	13%	2%	0%	21%

Effect Factor No Risk phrase assigned	EF(etwc)_air	EF(etsc)_air	EF(etwa)_water	EF(etwc)_water	EF(etsc)_water	EF(etwc)_soil	EF(etsc)_soil
Number of substances	70	70	70	70	70	70	70
Risk-value is too low	40%	39%	89%	86%	7%	7%	84%
Risk-value is too high	9%	10%	11%	13%	1%	1%	14%
Both values are zero	51%	51%	0%	1%	91%	91%	1%
Risk-value is zero	17%	17%	0%	14%	3%	3%	14%
Reference-value / Risk-value is between 0,1 and 10	13%	14%	27%	23%	0%	0%	24%
Reference-value / Risk-value is between (0,01 - 0,1) and (10 - 100)	14%	10%	24%	24%	3%	4%	17%
Reference-value / Risk-value is between (0,001 - 00,1) and (100 - 1000)	1%	3%	17%	7%	1%	0%	11%
Reference-value / Risk-value is lower than 0,001 or higher than 1000	3%	4%	31%	30%	1%	1%	31%

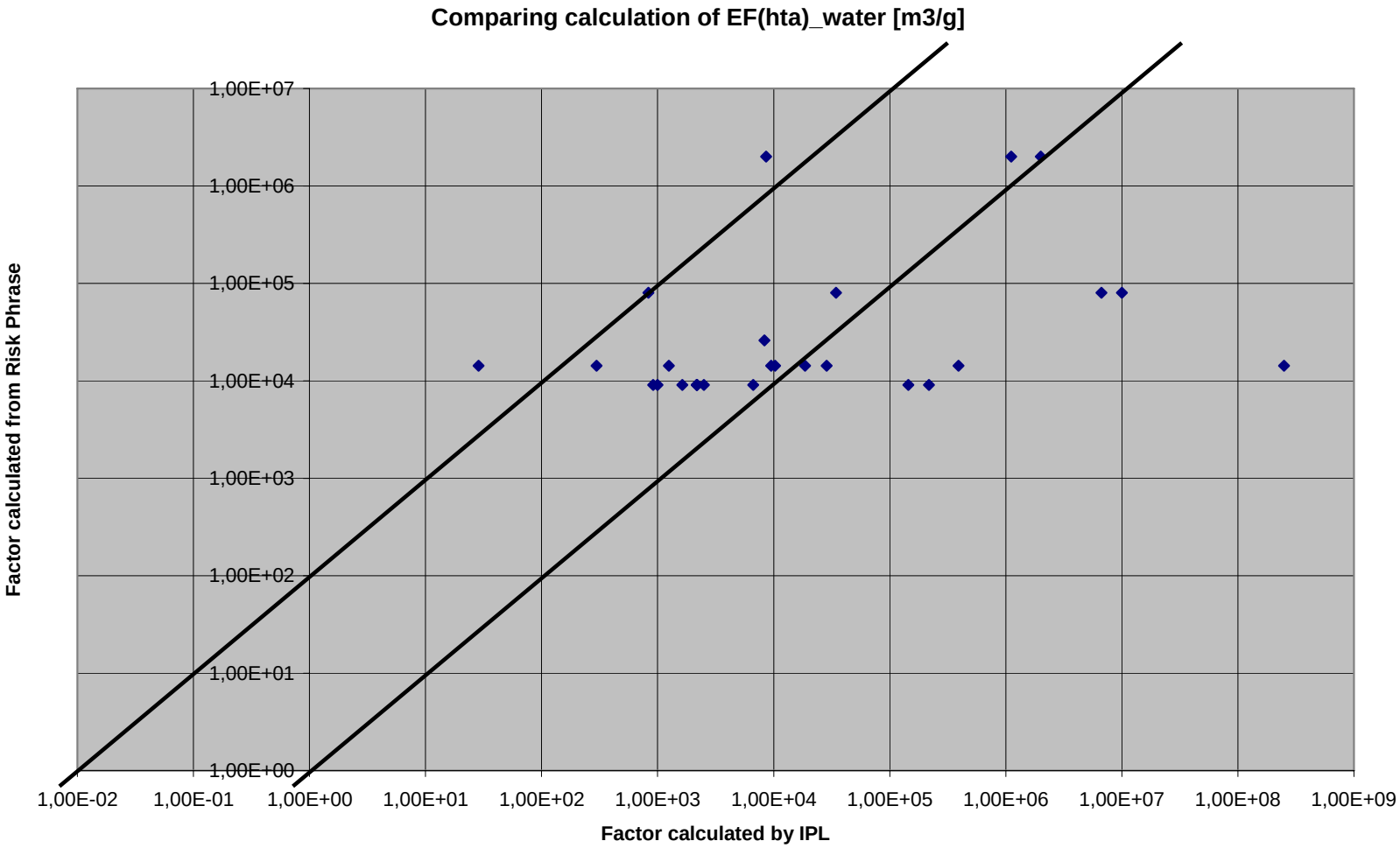
Risk-value is the value calculated by means of the risk-phrase method
Reference-value is the value calculated by IPL

Appendix 4

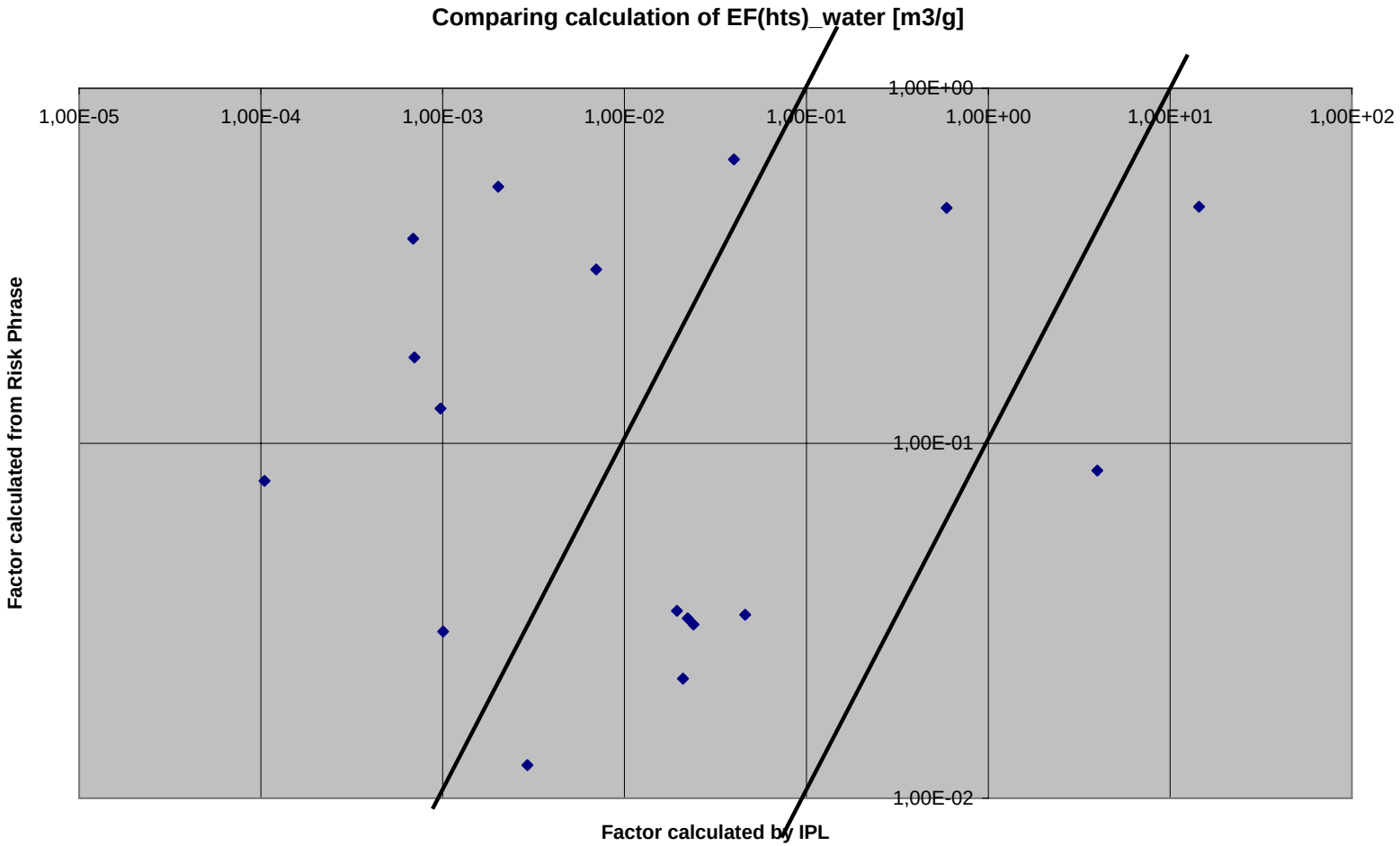
Comparing effect factors for human toxicity calculated by IPL respectively by the risk-phrase method, XY-plots



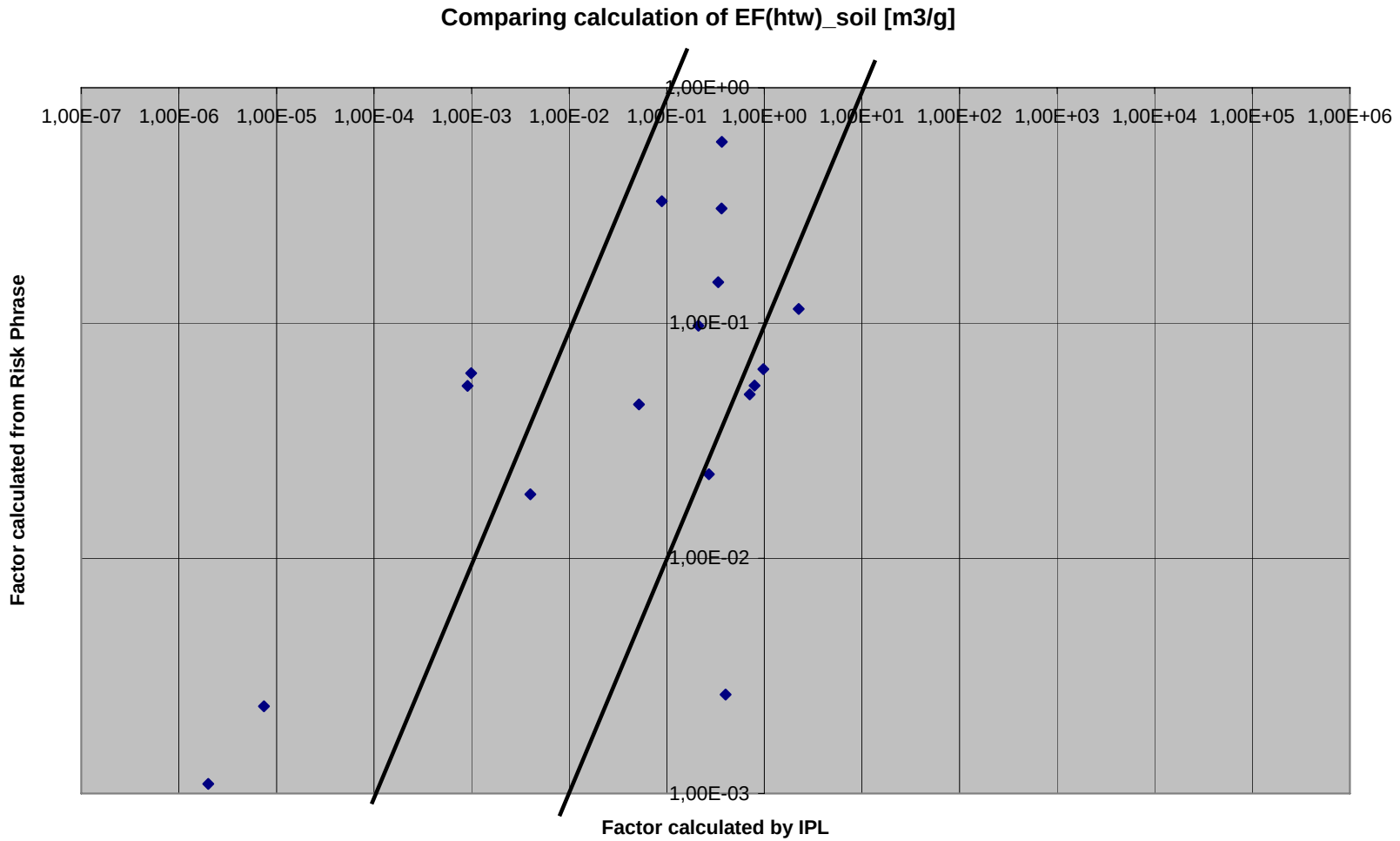
Please notice that zero values are not shown in this diagram!



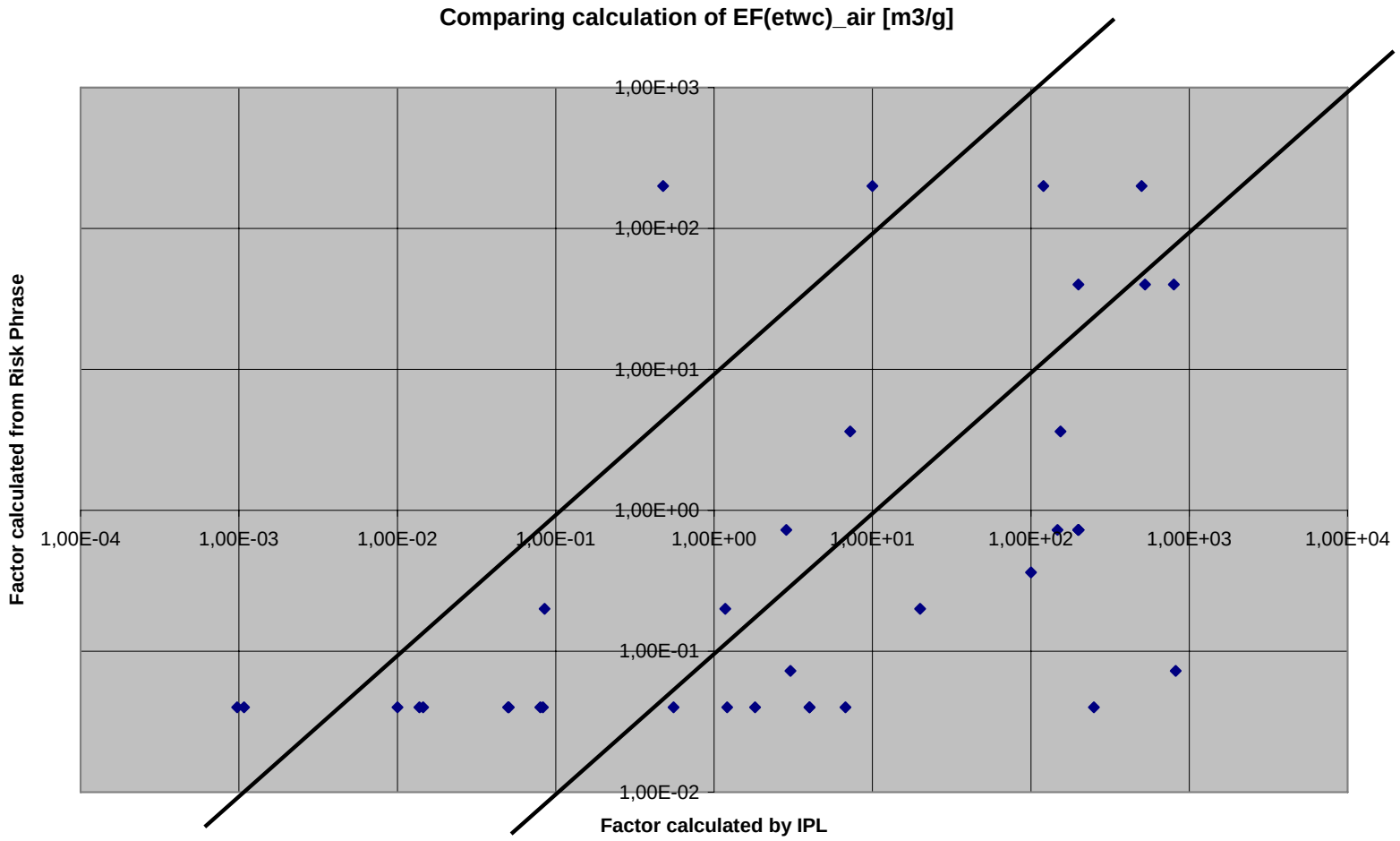
Please notice that zero values are not shown in this diagram!



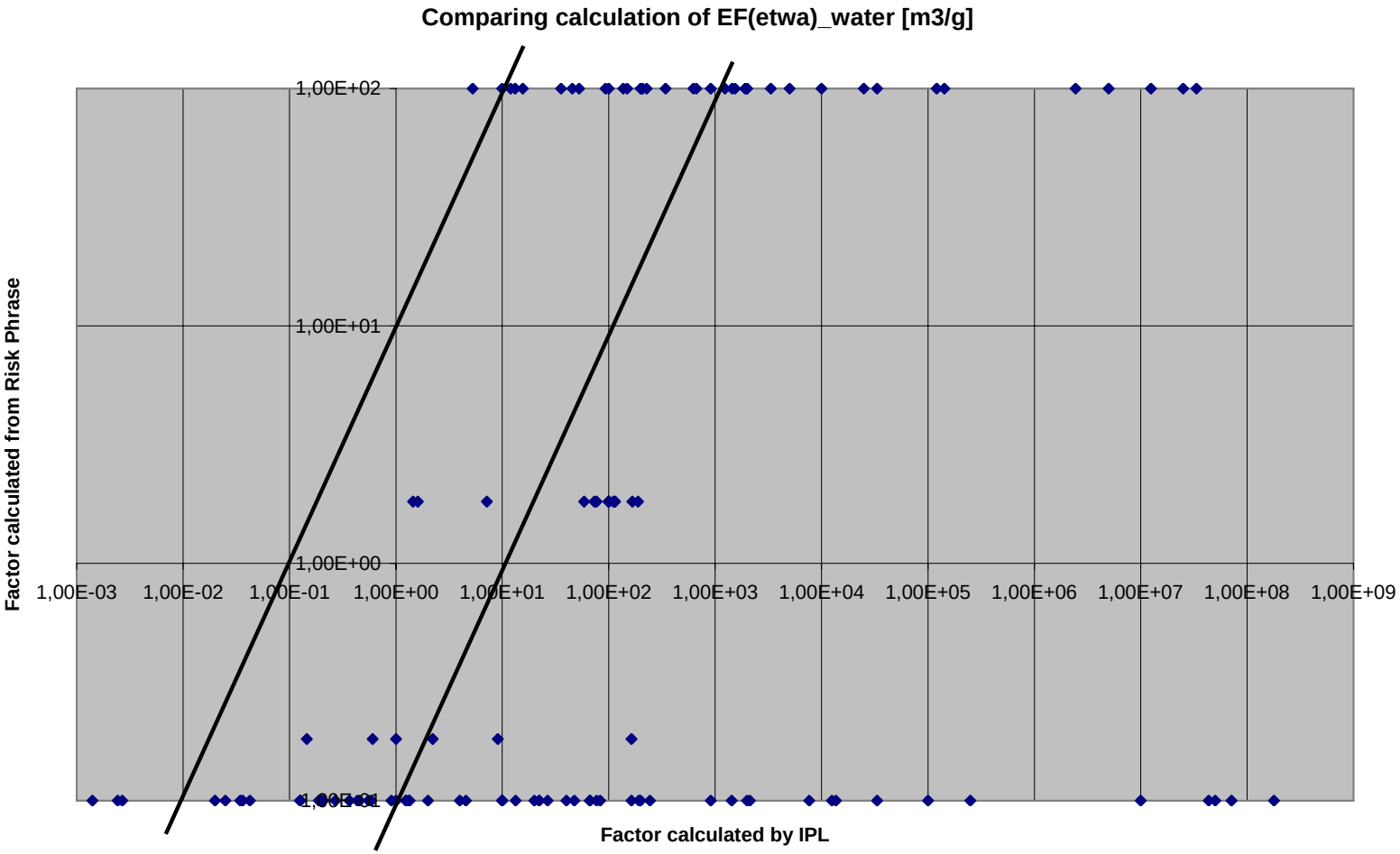
Please notice that zero values are not shown in this diagram!



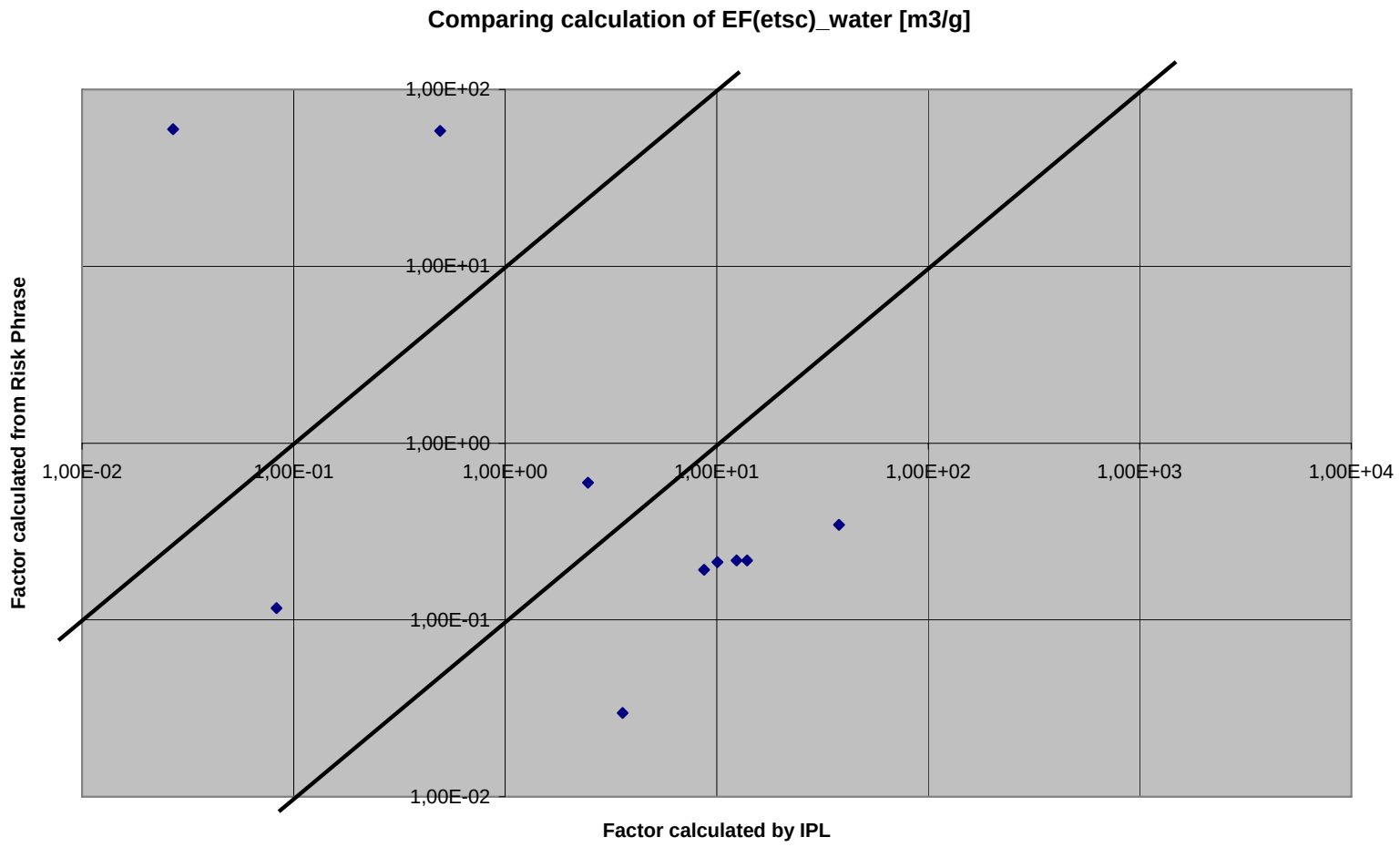
Please notice that zero values are not shown in this diagram!



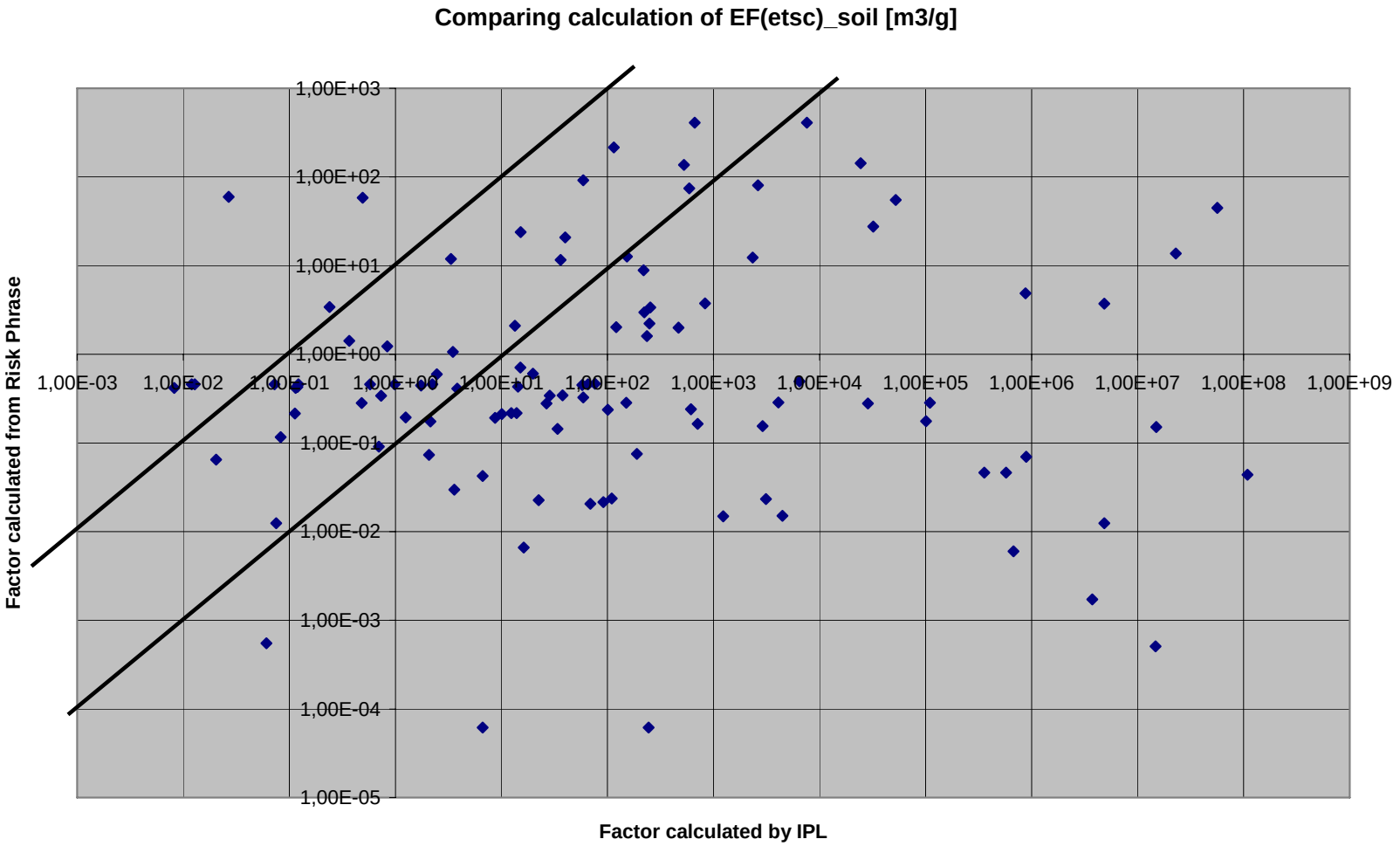
Please notice that zero values are not shown in this diagram!



Please notice that zero values are not shown in this diagram!



Please notice that zero values are not shown in this diagram!



Please notice that zero values are not shown in this diagram!

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

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