OMNIITOX: LCA Methodology

Bringing Science and Pragmatism together

A Tiered Approach for Modelling Toxicological Impacts in LCA

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Abstract

Goal, Scope and Background. The EU 5th framework project OMNIITOX will develop models calculating characterisation factors for assessing the potential toxic impacts of chemicals within the framework of LCA. These models will become accessible through a web-based information system. The key objective of the OMNIITOX project is to increase the coverage of substances by such models. In order to reach this objective, simpler models which need less but available data, will have to be developed while maintaining scientific quality.

Methods. Experience within the OMNIITOX project has taught that data availability and quality are crucial issues for calculating characterisation factors. Data availability determines whether calculating characterisation factors is possible at all, whereas data quality determines to what extent the resulting characterisation factors are reliable. Today, there is insufficient knowledge and/or resources to have high data availability as well as high data quality and high model quality at the same time.

Results. The OMNIITOX project is developing two inter-related models in order to be able to provide LCA impact assessment characterisation factors for toxic releases for as broad a range of chemicals as possible: 1) A base model representing a state-of-the-art multimedia model and 2) a simple model derived from the base model using statistical tools.

Discussion. A preliminary decision tree for using the OMNIITOX information system (IS) is presented. The decision tree aims to illustrate how the OMNIITOX IS can assist an LCA practitioner in finding or deriving characterisation factors for use in life cycle impact assessment of toxic releases.

Conclusions and Outlook. Data availability and quality are crucial issues when calculating characterisation factors for the toxicity impact categories. The OMNIITOX project is developing a tiered model approach for this. It is foreseen that a first version of the base model will be ready in late summer of 2004, whereas a first version of the simple base model is expected a few months later.

Keywords: Ecotoxicity; human toxicity; LCIA; life cycle impact assessment; modelling; multimedia modelling; OMNIITOX; substance data; substance properties; toxicity assessment

1 Goal, Scope and Background

OMNIITOX is an EU 5th research framework project aiming at the enhancement of models and information tools necessary for decision-making regarding potentially hazardous compounds. Life cycle assessment (LCA) and (environmental) risk assessment ((E)RA) practitioners can benefit from the OMNIITOX research and development. LCA and (E)RA use different starting points for their assessments. Recent studies have revealed inconsistencies between results from the two methods (Saouter and Feijtel 2000, Saouter et al. 2002). These differences need to be understood, explained and eventually avoided if they appear unnecessary. The work within OMNIITOX deals with this issue, amongst other things.

Based on the results of these studies and after consultation of various industry partners, the following problem definition was defined for the OMNIITOX project: "Given the limited availability of data for chemical properties available, the OMNIITOX-project aims at defining simplified operational models for characterisation of toxic impacts for a large number of substances [...]."

In other words, the OMNIITOX model framework must be able to increase the coverage of substances and, for that, simpler models demanding less, but available data (compared to current methods) need to be included. Simplification is thus not an aim in itself but the means for increasing substance coverage. In achieving this aim, a balance has to be found between progressing science and improving practice (practice, being the availability of substance data and the amount of resources a user can reasonably allocate to data collection, etc.). OMNIITOX is thus striving for a practically feasible and yet scientifically defendable tool to calculate characterisation factors for toxicological impacts, potentially for 'all' chemicals taking into account the limited availability of data. This article reports on the *plans* of the OMNIITOX project for developing the models complying with these aims, which are currently being implemented.

2 Methods: Lessons learned

Before developing the models, an analysis and comparison of existing models was made first (cf. Koning and Guinée 2004; see also Dreyer et al. 2003). As part of this analysis and comparison work, characterisation factors were calculated for 162 chemicals occurring in four industry case studies: 1) a case study on three detergent alternatives (regular powder; compact powder; compact liquid; 60 chemicals; Pant et al. 2004); 2) on two light-weight bus body alternatives (aluminium and composite alternative; 35 chemicals); 3) on chlorinated paraffins and alternatives in metal working fluids (21 chemicals; Christensen and Olsen 2004); and 4) on three cosmetic products (shower gel; eau de toilette; face cream) (46 chemicals).

The characterisation factors were calculated applying four different existing LCIA models:

- EDIP97 (Hauschild and Wenzel 1998)
- USES-LCA (Huijbregts et al 2000a. 2000b)
- CalTOX 4.0 beta (http://eetd.lbl.gov/ied/era/)
- IMPACT 2002 (Pennington et al. submitted, adopted in Jolliet et al. 2003)

Three of these four models provided compilations of pre-calculated characterisation factors; only IMPACT 2002, which was still under development at the time of the comparison, could not provide such a compilation. It was first checked for which chemicals of the case study inventories characterisation factors were already available in the existing compilations of USES-LCA, EDIP and CalTOX 4.0. It appeared that USES-LCA could provide characterisation factors for 12% and EDIP and CalTOX 4.0 both for 26% of the chemicals of the case study inventories. Note that the case studies excluded considerations associated with transport and energy supply, hence focused primarily on the specific chemicals of the different case studies.

Subsequently, new characterisation factors were calculated using a consistent, albeit simplified, data set – termed the Minimum Requirement List (MRL). This exercise had the purpose to increase inter-comparability of characterisation factors and to determine whether the existing methods could be run on such a minimal set of data.

The MRL is a minimal list of data with respect to calculating characterisation factors with existing models and with respect to what may be expected to be readily available for many chemicals (**Table 1**). However, the quality of the factors calculated with this minimal data set as well as the relevance of some of the parameters to all chemicals and models are often debatable (cf. Koning and Guinée 2004).

For the new calculations based on the MRL, it appeared that a sufficient data set for calculating CFs could be found for approximately 90% of the industry case study chemicals for EDIP97; for USES-LCA this figure amounted to 70%, and to approximately 50–55% for CalTOX 4.0 and IMPACT 2002. Note that the four methods significantly differ in the emission compartments covered and number of category indicator results produced.

Table 1: Minimum requirement list (MRL)

Property	Unit
Acidity dissociation constant	Dimensionless
Basicity dissociation constant	Dimensionless
Degradation rate constant with OH-radicals	$m^3.molec^{-1}.d^{-1}$
Half-life by hydrolysis in water	Days
Henry's Law constant	$Pa.m^3/mol$
Melting point	K
Molecular weight	g/mol
Octanol-water partition coefficient	Dimensionless
Particle - gas partition coefficient	m^3/ug
Steady state partition coefficient between water and sediments	l/kg
Steady state partition coefficient between water and soil	l/kg
Vapour pressure	Pa
Water solubility	kg/m^3
Acute inhalation toxicity to rodent	mg/l
Acute oral toxicity to rodent	mg/kg
Acute lethal toxicity to freshwater fish	mg/l
Acute toxicity to invertebrates	mg/l
Algal growth inhibition expressed in growth rate reduction	mg/l
Algal growth inhibition expressed in biomass reduction	mg/l
Mutagenicity based on salmonella or E.coli bacteria	Dimensionless
Ready biodegradability expressed in $\%O_2$ uptake	Dimensionless
Ready biodegradability expressed in %DOC removal	Dimensionless
Ready biodegradability expressed in $\%CO_2$ production	Dimensionless
Ready biodegradability	Dimensionless
Inherent biodegradability	Dimensionless

It is clear from these figures that the simple model EDIP97 is capable of covering significantly more chemicals than the other three models that are based on multimedia modelling approaches. Although it is tempting, it cannot be further concluded from these figures that one of the three multimedia models (USES-LCA, CalTOX 4.0 and IMPACT 2002) is more capable of covering chemicals using the MRL than the other. This is due to the fact that different people have calculated the characterisation factors for each of these methods, the models are essentially based on similar fundamental principles, and that these people may have had different views on which data are acceptable and made different efforts to getting further data for running the models.

Characterisation factors based on the MRL are likely to be highly uncertain. For example, the MRL doesn't contain information on all substance properties needed for the calculation of characterisation factors with USES-LCA. To be more specific, there was no information available on chronic human toxicity (Acceptable Daily Intakes), chronic ecotoxicity (Maximum Permissible Addition), and biodegradation (half lives). These substance properties had to be esti-

mated from the (basic) data given in the MRL. The estimation methods used are scientifically questionable, rough at best. Moreover, the data collected for the MRL properties may be erroneous (e.g. because of typing, interpretation or other errors) and/or uncertain. Therefore the calculated characterisation factors are also debatable and should be used with extreme caution, if at all beyond the purpose for which they were developed. As a consequence, the list of data requirements for the OMNIITOX models has been slightly enlarged including more complete and robust effect data (see below). Additionally, more robust estimation methods for property values will become important in the further development of the OMNIITOX models.

3 REACH

The aim of the OMNIITOX project imposes that the OMNIITOX models should better comply with the most likely available data. Due to the availability constraint and the fact that OMNIITOX is a project funded by the EU Research Framework Program, the MRL was based on the ongoing chemical-related policy negotiations at the EU level: the EU chemical's assessment regulation that is often referred to as REACH.

REACH is an acronym standing for Registration (chemicals produced or imported in volumes more than 1 t/year need to be registered), Evaluation (registration dossiers for chemicals produced > 100 t/year will be evaluated[1]) and Authorisation (substances of high concern will need to authorised for each use[2]); of CHemicals (for a more extensive explanation, see CEC (2003)). The REACH regulation is still under development. A draft of the REACH regulation – 'White Paper, Strategy for a future chemicals policy' (CEC 2001) – was presented on the internet in May 2003 and all stakeholders were given the opportunity to comment on the proposal. Based on the comments received, a final draft of REACH is currently under preparation by the European Commission and will soon be presented to the Parliament and Council.

[1] Amongst others to check for conformity with requirements and to assess possible testing proposals. The latter is mainly in order to avoid unnecessary animal testing.

[2] This applies to so-called CMR (Carcinogenic, Mutagenic or toxic to Reproduction) and PBT (Persistent, Bio-accumulative and Toxic) substances as well as substances with endocrine disrupting properties.

Among other developments, the registration dossier of a chemical will contain information on the identity and substance properties that are also part of the OMNIITOX MRL.[3] It is anticipated that the new REACH legislation will be in force by 2006. The industry will then have several years to collect missing data for their substances. The allowed amount of time depends on the annual production volume of a substance (**Table 2**). REACH data are thus expected to become available between 2007 and 2015. Taking into account earlier experience with data provision for EU legislation purposes, one should be prepared for an even longer time perspective. This means that REACH data may not be available for quite a long time.

4 Result: The OMNIITOX model framework

In order to comply with the OMNIITOX problem definition and based on the assumption that REACH should reflect a practical level of minimum data requirements, OMNIITOX will develop a base model (BM) and a simple base model (SBM) for LCIA characterisation (in the context of toxicological effects).

The models will link to the data expected to become available through REACH, among other data sources. As the REACH system may remain under negotiation for a while, potentially even leading to substantial changes towards the present status, a starting point for these OMNIITOX models needed to be fixed. The preliminary starting point is now fixed to a deminimus set, largely based on one of the counter proposals submitted by The European Chemical Industry Council (CEFIC: http://www.cefic.be/) as a reaction to the Commission's proposal. A small number of indispensable properties were added to this particular stakeholder negotiating position for facilitating modelling, resulting in an adapted MRL (**Table 3**). Apart from these added substance properties, it is expected that the substance properties given in Table 3 will become available since industry has already accepted them in the ongoing negotiations.

The base model will be a state-of-the-art multimedia model, and serve as a reference point for further simplifications and

[3] Note that the REACH registration dossier is primarily intended for assessing chemicals from a regulatory perspective, hence its suitability in the context of relative comparison assessments such as LCA will be considered with caution.

Table 2: Proposed data requirements in EU-chemical legislation according to different production volume classes

Production volume class	Tonnage	Data requirement	Number of substances (estimated)	Data expected to be available from industry in (yr)
Low (LPV)	0–1	None[a]	Unknown yet	–
Low (LPV)	1–10	Unknown yet	19700	2015
Mid (MPV)	10–100	Annex VIIA	4700	2015
High (HPV)	100–1000	Annex VIII level 1	3000	2010
High (HPV)	1000–	Annex VIII level 2	2600	2007

[a]Chemicals manufactured or imported in tonnages below 1 ton/year/producer will not be subject to registration.

Table 3: Adapted minimum requirement list (MRL) of chemical properties taking into account CEFIC suggestions in the ongoing REACH negotiations

Property	Parameter measured	Unit
Physico-chemical properties		
Melting-point	MELTING T	°K or °C
Boiling-point	BOILING T	°K or °C
Vapour pressure	Vapour pressure in Pascal at specified temperature	Pa
Water solubility	Solubility in water at specified temperature	kg/m^3
Partition coefficient(s)	K_{ow}/ P_{ow} or 10 (log P)	–
Biotic degradation	% Degradation at a certain time depending on OECD guideline used	% at time=t2 (validated by % at time=t1)
	BODt (Biological oxygen demand after time=t)	g (BOD)/g (compound)
Abiotic degradation	COD (Chemical Oxygen Demand)	g (COD)/g (compound)
	Half-life period, t½	days
Absorption/desorption screening test	K_d and K_{oc} (measured for soil)	cm^3/g
Toxicological properties		
Acute toxicity; two routes	LD_{50} for rodent (oral)	mg/kg bw/d
	LC_{50} for rodent (inhalation)	mg/l
	LD_{50} for rodent (dermal)	mg/ kg bw/d
Sub-chronic 28 day test (expected, not yet in industry counter proposal C !!)	NOAEL (oral)	mg/kg bw/d
	NOAEL (inhalation)	mg/l
	NOAEL (dermal)	mg/kg bw/d
Ecotoxicological properties		
Acute toxicity for fish	LC_{50}	mg/l
	EC_{50} and NOEC	mg/l
Acute toxicity for daphnia	$L(E)C_{50}$	mg/l
Growth inhibition on algae	EC_{50}	mg/l
Bacterial inhibition	% inhibition (measured as reduced oxygen consumption)	% inhibition

$LC(D)_{50}$ = the median lethal concentration/dose, i.e. the concentration/dose of substance that is estimated to be lethal to 50% of the test organisms; EC_{50} = effective concentration, i.e. the concentration that effects 50% of a test population after a specific exposure time on a designated criterion (e.g. growth rate); $L(E)C_{50}$ = LC_{50} or EC_{50}; NOEC = no observed effect concentration; NOAEL = no observed adverse effect level

extensions. The simple base model will have the purpose of covering more chemicals than the BM with fewer input properties and more readily available data for these properties. If empirical data for some properties are lacking for a given chemical, these may be supplied by using specific estimation methods such as Quantitative Structure Activity Relationships (QSAR) or other estimation methods.[4]

4.1 Base model (BM)

The OMNIITOX base model will provide a state-of-the-art multimedia approach for estimating characterisation factors specifically developed in the context of life cycle assessment. The model will draw, among other things, on the scientific contributions of Huijbregts et al. (2000a, 2000b), Hertwich (1999), and methods as adopted in Pennington et al. (submitted).

The substance classes for which the model will primarily be valid are hydrophobic and slightly hydrophylic organics. Amphiphilic and dissociating organic chemicals and inorganic substances, such as metal containing compounds, can be modelled in a generic way (based on Huijbregts et al. 2000a, 2000b).

In terms of geography, a generic continent representing Western Europe will be covered. The calculations can be done using generic release scenarios within this European zone. This European zone is nested in a global zone to allow for the assessment of emissions outside of the European zone and for chemicals that are transported outside this European zone. The set-up will be chosen in such a way that a higher spatial resolution within and outside Europe (e.g. at country or watershed level) is possible.

The minimum data required to run the model are a function of the chemical class and partitioning tendencies in the environment. It is intended to run on the data described in Table 3 as a deminimus basis. To ensure high quality, data are selected in principle using a hierarchy of four proposed levels:

1. Peer reviewed data
2. Data expected to become available through REACH
3. Other non-reviewed measured data sources
4. QSARs and simplistic rules-of-thumb

For some substance properties a distinction between category 3 & 4 is not relevant as some QSAR's can be very robust, e.g. narcosis effects.

[4] It is expected that any chemical can be covered in this way, and that there will be no need to also develop a stand-alone selection method (see Larsen et al. (2004) for a discussion of selection methods).

The Base Model's technique for calculating time-integrated (or cumulative) concentrations associated with the release of a unit mass of chemical into the environment relies on a straightforward, non-homogenous matrix solution to solve the simultaneous, linear (or pseudo-linear) first order, ordinary differential equations for an n-compartment system at steady-state. The BM framework is entirely formulated using matrix algebra. Thus, apart from the well-established fate matrix, also the human exposure and the effect modules are established in a matrix format. This yields some significant advantages compared to traditional model frameworks; updating or extending the model (e.g. by new compartments, exposure pathways or effect types) is facilitated by simply adding rows or columns to the fate, exposure or effect matrices. Interpretability of intermediate and final results (e.g. identification of the dominating pathway) is significantly improved. Model comparability is enhanced by clearly defined intermediate results. This framework in principle also serves as a flexible model library, capable of hosting several models while model equations can easily be exchanged.

Seven principal media are represented, each of which is further sub-divided into compartments:

1. Fresh water
2. Fresh water sediment
3. Marine water
4. Marine sediment
5. Soil, including different use types (natural soil, agricultural soil)
6. Air
7. Vegetation

Replacing the traditional concept of a dose, the intake fraction (iF) will be adopted to express exposure of humans (as described in Bennett et al. 2002). An iF is the fraction of mass of a chemical released into the environment that is ultimately taken in by the human population as a result of food contamination, inhalation, and dermal exposure. Direct (inhalation), as well as indirect (ingestion of food products) pathways, will be implemented in the BM, as described in Pennington et al. (submitted). Departing from a traditional subsistence-based exposure scenario (food and water locally supplied and containing local contaminant levels), the BM will incorporate a production-based approach (accounting for contaminants imported from different regions via food supplies and the spatial relationship to the emission source of food production/water supply) (Bachmann et al. 2004, Pennington et al. submitted).

For human health effects, a distinction will be made between cancer and non-cancer effects. For assessing both cancer and non-cancer effects, the base model will adopt the concepts of Crettaz and colleagues (Crettaz et al. 2002, Pennington et al. 2002) – a benchmark approach for addressing human health effects in comparative assessments such as LCA and based on the risk assessment proposals of the US EPA. The approach is based on the maximum likelihood estimate of the effect dose inducing a 10% risk over background, denoted the ED_{10}. Distinctions are retained between responses to inhalation and oral exposures. With respect to ecotoxicological effects, an effect based average indicator will be adopted instead of a no-effect based (i.e. PNEC) type as typically used within traditional regulatory risk assessment approaches due to the lack of consistency across such regulatory thresholds.

4.2 Simple base model (SBM)

The simple base model (SBM) will be able to cover a much higher number of substances than the base model (BM) as it will be based on less, but more widely available, input parameters (substance properties) than the BM. Although the SBM will consequently be much simpler than the BM, the aim is to have commensurable (i.e. having the same metric) and comparable values between the SBM characterisation factors and the BM characterisation factors. This is desirable in order to consistently obtain aggregate category indicator values from the different models and to allow LCA practitioners to cover all chemicals in the inventory. Therefore, the SBM will be derived from the BM using statistical tools (cf. Van de Meent et al. 2002). SBM characterisation factors are conjectured to have a much higher uncertainty in many cases than the characterisation factors calculated with the BM. The added uncertainties of the SBM compared to the BM will therefore be quantified.

Feasibility studies examining ways of deriving a SBM from a BM using regression models and other statistical tools have been performed, seeking inspiration from other chemical ranking and scoring systems and making surveys of the availability of different chemical properties in commonly accessible databases. In absence of the final OMNIITOX base model, the USES-LCA model (Huijbregts 2000a, 2000b) with its data set on 181 substances was used to learn to understand the possible role of regression models for a simplified model on the basis of a (future) base model. Prior to carrying out the regression analyses, however, a number of theoretical analyses of the mathematical structure of the USES-LCA model was undertaken. These give clues towards the model specification in the regression model: which variables to include, and which transformations (logarithms, squares, etc.) to perform.

After a combination of theoretical analyses, statistical analyses and trial-and-error, it appeared possible to deduce regression models that account for a substantial amount of variance (often 70–90%) of the logarithm of the characterisation factors for aquatic and terrestrial ecotoxicity and human toxicity for different emission compartments (air, water and soil) on the basis of two or three input variables from the original USES-LCA dataset. These variables are: a measure of toxicity (the maximum tolerable concentration for ecotoxicity or the acceptable daily intake and/or the tolerable concentration in air for human toxicity), a measure of persistence (the degradation half life, most often for the emission compartment), and sometimes the Henry's coefficient. Predictions from such a simplified model can be accompanied by an estimated uncertainty of the prediction. Preliminary results of this, and similar statistical analyses, have been reported, for example, by Olsen et al. (2003).

Having learned from the feasibility studies, a simple base model is currently being developed according to the following steps:

- Perform analytical preparatory work giving clues as to which variables to include, and which transformations (logarithms, squares, etc.) to perform.
- Apply specific regression tools identifying key properties (cf. Wold et al. 2001) and combine insights from this with results of the data availability study selecting key parameters.

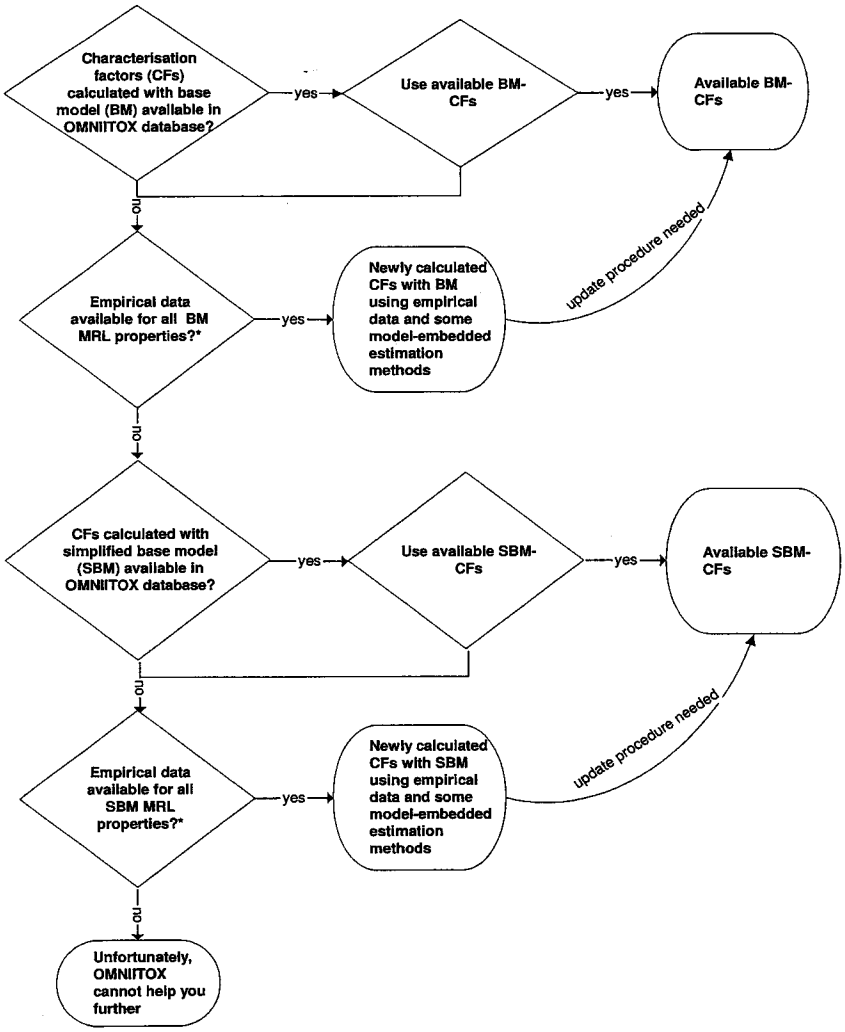
- Apply the regression framework to derive predictive equations for characterisation factors with uncertainty estimates.
- Apply common sense and environmental knowledge to make the SBM expressions mechanistically understandable through adjusting coefficients to match with expert knowledge.

For each category indicator and initial emission compartment (e.g. Human Toxicity Potential for emission to air, Human Toxicity Potential for emission to water, etc.), a linear equation will be derived in this way for estimating characterisation factors for at least the ordinary hydrophobic organic substances.

5 Discussion: Preliminary decision tree for using the OMNIITOX information system

A preliminary decision tree for using the OMNIITOX information system (IS) is proposed; see **Fig. 1**. The decision tree aims at illustrating how the OMNIITOX IS can assist an LCA practitioner in finding or deriving a characterisation factor for use in life cycle impact assessments of toxic releases.

Note that for cases when the OMNIITOX IS can supply existing characterisation factors to a user, but the user nevertheless wants to calculate new characterisation factors for a new data set, the OMNIITOX IS will need to have an updating procedure determining whether the newly calculated characterisation factors are better than the old ones or not, and thus whether the old ones will be updated by the new ones. Expert judgements and expert reviews are indispensable for such a procedure. An outcome of such a judgement and review may of course also be that both sets of characterisation factors (for the same chemical) are included in the OMNIITOX IS, but that they are valid for different geographical areas or environmental circumstances, etc. As



* Possibly the MRLs for the BM and SBM will be differentiated for different chemical groups, e.g. organics, amphiphilics and inorganics.

** While the use of property estimation tools (QSAR) for substance input parameters to the BM is avoided as far as possible, some of the input parameters to the SBM may have to be estimated in order to obtain the desired substance coverage for the SBM.

Fig. 1: Preliminary decision tree for calculating characterisation factors with the OMNIITOX Information System – BM = Base Model; SBM = Simple Base Model; CF = Characteristion Factor; MRL = Minimum Requirement List

it is also important for users that the OMNIITOX characterisation factors are stable from study to study, a solution in the OMNIITOX IS must be found to balance the quest for quality and stability of the characterisation factors.

Basically, it is intended that characterisation factors calculated with the base model and characterisation factors calculated with the simple base model can be used together in one LCA case study. For this mixed use it is important that the uncertainties attached to the characterisation factors of the two different models can be quantified, as the uncertainties of characterisation factors calculated with the SBM are conjectured to be higher than those calculated with the BM.

6 Conclusions and Outlook

The OMNIITOX project is currently developing the base model and the simple base model described above. The base model will include a state-of-the-art multimedia model, whereas the simple base model will be derived from the base model using statistical analyses. The data requirements are likely to significantly differ between these two models, but so do the uncertainties attached to the resulting characterisation factors.

The experience within the OMNIITOX project until today has suggested that data availability is a crucial issue for calculating new characterisation factors. But also data quality is a crucial issue and there is often a trade-off between these two issues. Data availability determines whether calculating characterisation factors is possible at all, whereas data quality determines whether the resulting characterisation factors are reliable. Today, there is not sufficient knowledge and/nor resources to have high data availability as well as high data quality and high model quality at the same time. The OMNIITOX model framework tries to provide a best practice in these respects, proposing a balance between science and practice.

It is foreseen that a first version of the base model will be ready in late Summer of 2004, whereas a first version of the simple base model can be expected a few months later.

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