SETAC-Europe LCA Working Group 'Data Availability and Data Quality'

Guidelines for Consistent Reporting of Exchanges from/to Nature within Life Cycle Inventories (LCI)

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Abstract. Data availability and data quality are still critical factors for successful LCA work. The SETAC-Europe LCA Working Group 'Data Availability and Data Quality' has therefore focused on ongoing developments toward a common data exchange format, public databases and accepted quality measures to find science-based solutions than can be widely accepted. A necessary prerequisite for the free flow and exchange of life cycle inventory (LCI) data and the comparability of LCIs is the consistent definition, nomenclature, and use of inventory parameters. This is the main subject of the subgroup 'Recommended List of Exchanges' that presents its results and findings here:

- Rigid parameter lists for LCIs are not practical; especially, compulsory lists of measurements for all inventories are counterproductive. Instead, practitioners should be obliged to give the rationale for their scientific choice of selected and omitted parameters. The standardized (not: mandatory!) parameter list established by the subgroup can help to facilitate this.
- The standardized nomenclature of LCI parameters and the standardized list of measurement bases (units) for these parameters need not be applied *internally* (e.g. in LCA software), but should be adhered to in *external* communications (data for publication and exchange). Deviations need to be clearly stated.
- Sum parameters may or may not overlap – misinterpretations in either direction introduce a bias of unknown significance in the subsequent life cycle impact assessments (LCIA). The only person who can discriminate unambiguously is the practitioner who measures or calculates such values. Therefore, a clear statement of independence or overlap is necessary for every sum parameter reported.
- Sum parameters should be only used when the group of emissions as such is measured. Individually measured emission parameters should not be hidden in group or sum parameters.
- Problematic substances (such as carcinogens, ozone depleting agents and the like) may *never* be obscured in group emissions (together with less harmful substances or with substances of different environmental impact), but *must* be determined and reported individually, as mentioned in paragraph 3.3 of this article.
- Mass and energy balances should be carried out on a unit process level. Mass balances should be done on the level of the entire mass flow in a process as well as on the level of individual chemical elements.
- Whenever possible, practitioners should try to fill data gaps with their knowledge of analogous processes, environmental expert judgements, mass balance calculations, worst case assumptions or similar estimation procedures.

Keywords: Data availability; Data quality; Exchanges; Guidelines; LCI data; Life Cycle Inventory (LCI) data; Nomenclature; SETAC LCA-WG, Data Availability and Data Quality; SETAC LCA-WG, Subgroup Recommended List of Exchanges

1 Foreword

Data availability and data quality are still critical factors for successful LCA work. The founding members of the SETAC-Europe LCA Working Group 'Data Availability and Data Quality' took up the spirit towards a standardization and a free data flow, originated by e.g. the SPOLD data exchange format (SPOLD 1997). The goal of the workgroup is therefore to focus ongoing developments towards a common data exchange format, public database and accepted quality measures and to find scientifically sound, multidisciplinary, creative solutions than can be widely accepted. To this end, the workgroup prepares a guidance document (De Beaufort &

Bretz 2001) which will help practitioners and will increase the usefulness and credibility of LCA.

From a long list of pertinent questions, the points of major interest were chosen as topics for the five subgroups formed within the workgroup, among those the subgroup 'Recommended List of Exchanges'. The parameters discussed in this subgroup were restricted to interactions with the natural environment and did not cover flows to and from other technical systems. They comprise therefore material inputs from nature (resources), material outputs to nature (emissions), non-material outputs (energy/heat, radiation , noise etc.), and other, non-flow-related effects (such as land use). Concerning the denomination of all these parameters, a variety of different terms were discussed and rejected during the last three years. Our goal was to stay consistent both with ISO 14048 (2001) and with the SETAC LCIA working group (Udo de Haes 1999). ISO has choosen the preliminary name 'data categories' which convinced neither of the two subgroups, because of possible confusion with the term 'impact categories'. The LCIA working group retained the old expression 'interventions' and posponed a discussion of this point to the upcoming UNEP-SETAC-Initiative. Therefore, we decided to keep the term '*exchanges*' from the first working draft of ISO 14048 (ISO 1999).

2 Introduction

The choice of reported *exchanges* and their nomenclature may cause a severe problem in the comparability of LCI results: Older studies used to report only relatively few key emissions and coarse measures of raw material consumption (e.g. primary energy), whereas recent LCIs (especially those for energy systems) provide detailed lists of parameters (emissions and extractions, sometimes broken down to single molecule species, elements or isotopes). The number of parameters first saw some 'inflation', then a reduction due to practical considerations, as it can be seen in Table 1.

A parallel development occurred in the parameter requirements of contemporary impact assessment (LCIA) methods, as shown in Table 2.

Obviously, it makes no sense neither to collect as many different *exchanges* as possible, nor to assess old inventories with modern, comprehensive LCIA methods. Besides, the use of synonyms or related, overlapping terms makes it tedious or even impossible to compile a meaningful inventory for a complex process chain from unit processes originating from various sources using different nomenclatures. The consistent connection of *exchanges* with their appropriate weighting factors for impact assessment (as in Foerster 1998) is hardly feasible, if the nomenclature of *exchanges* is ambiguous.

First, the subgroup studied the possibility of compiling a compulsory standardized list of *exchanges*. The idea was to choose and clearly define the optimal one among synonymous, similar or related parameters, and put all others on a 'discouraged' list. The valid parameters were then to be prioritized to obtain a minimal as well as a recommended list. However, strong objections were raised against such a prescriptive approach. Standardized parameter lists could unduly interfere with the freedom to set the goal and scope of an LCA study, and/or pose insurmountable problems in data acquisition. Furthermore, a 'minimum' list could be mistaken as an excuse to omit parameters potentially important for a given study. Both potential effects of a predefined parameter list would violate the ISO standards 14040 (1997) and 14041 (1998). Therefore, the project of a mandatory minimum parameter list of *exchanges* to be used in every LCA was abandoned.

Rather, a list of parameters with their preferred nomenclature is proposed (together with rules for the naming of new, additional parameters). This list shall help the practitioner to make a reasonable choice of *exchanges* that the process owners or participating companies may be willing to provide (under the time and money constraints of practical LCA work). The selection shall contain sufficient *exchanges* to calculate the main classes of impact categories; nevertheless, the final responsibility lies with the practitioner. The following guidelines and rules have been developed to promote the exchangeability of LCI data:

- nomenclature rules for parameters and the avoidance of synonyms: see paragraph 3.1
- appropriate measurement units (example: nitrate as such vs. nitrate as N): see paragraph 3.2
- rules for the treatment of sum parameters (parameter hierarchies, individual to sum): see paragraph 3.3
- guidelines dealing with missing or incomplete information: see paragraph 3.4

Table 1: Parameters reported in LCA studies of the last decade

LCIA Method (Year)	Parameters used	Example Process	Source
BUWAL No. 132 (1991)	24	Electricity	BUWAL 1991
APME Vol. 2 (1993)	42	Ethylene	APME 1993
ETH-ESU 1st Ed. (1994)	~240	Electricity	ETH 1994
BUWAL No. 250 (1996)	67	Electricity	BUWAL 1998

Table 2: Parameters used in LCIA methods published within the last decade

LCIA Method (Year)	Parameters used	Remark	Source
BUWAL No. 133 (1990)	16	No classification	BUWAL 1990
CML (1992)	~450	+320 for pesticides	CML 1992a & b
Eco-indicator 95 (1995)	154	Full classification	PRé 1995
BUWAL 297 (1997)	94	Some classification	BUWAL 1997
Eco-indicator 99 (1999)	~200	Full classification	PRé 1999

The future success of LCI exchangeability relies upon a 'self-commitment' by the author(s) of LCA studies about the choice of parameters and the completeness of the inventory as well as recommendations for 'good practice', described in paragraph 4. The use of deviant synonyms or units may be appropriate for *internal* purposes (reflecting legal requirements or traditions of any particular site or country), but should be strictly avoided in data sets prepared for publication or (electronic) data exchange. Their conversion is in most cases very easy. The necessary translations can be achieved either manually, with standard (spreadsheet) software, or – preferentially – with a reporting feature of commercial LCA tools.

3 Recommended Guidelines for the Inventory of Exchanges

3.1 Nomenclature for parameter list

In order to create a recommended list of parameters, over 20 parameter lists were obtained from LCA practitioners and software suppliers in the whole workgroup. Many of the parameter lists were originally based on the ETH-ESU energy database (ETH 1994) with about 300 *exchanges*, incl. 60 radioactive substances and land use, and the BUWAL 250 packaging study (BUWAL 1998) with 140 *exchanges*, partly summarized from ETH. These two lists seem to present a 'state of the art' compilation of the commonly used parameters in LCA. A further 150 other parameters were used by various practitioners. In the SPOLD data exchange software (SPOLD 1997 and 1999), a name list is given that contains more than 150 inputs and almost 300 emission parameters, many – not all – corresponding to the two mentioned parameter lists.

For the list of *exchanges*, a set of simple rules for the naming and identification of substances was developed (see Box 1), based on the original SPOLD naming conventions, which were adapted to ensure the necessary precision. For chemicals, SPOLD uses CAS numbers and CAS INDEX names (STN 2000) for identification. A closer inspection of the CAS REGISTRY system reveals, however, that for many CAS numbers, several CAS INDEX names are given in apparently random order. For the original SPOLD list, the shortest notation was chosen. But under this rule, closely related chemicals were named inconsistently. Our subgroup therefore re-examined the original SPOLD list; synonymous entries were deleted and the nomenclature standardised according to the developed rules. Secondly, the list was matched to the mentioned parameter lists and missing parameters were added, following again the standardised nomenclature. Consequent use of the CAS numbers as primary identifiers ensures that synonymous entries were avoided. The resulting recommended list of parameters will be part of the working group report (De Beaufort and Bretz 2001).

Obviously, such a list cannot be comprehensive (in spite of the broad information base processed), but must be amended, when new parameters will gain attention, as environmental science progresses. But new parameters should be added with great care only, and named according to the Nomenclature rules in Box 1. In any case of doubt, it is advisable to search the list for analogous compounds, and name new substances accordingly.

3.2 Appropriate measurement units

The occurrence of non-SI units is not the subject of this paragraph (see introduction to paragraph 2). But even when SI units are employed, many parameters used in LCI can still be expressed in ambiguous ways (e.g. nitrate may be reported as 'kg nitrate as N' or as 'kg nitrate as such', which differ by a factor of 4.4). Insecurity about the underlying measurement base impedes the exchange of LCI data between practitioners, and can introduce serious errors in the compilation of inventories, if the base units are accidentally confused.

Box 1: Nomenclature rules

Principle:

The parameter **name that gives rise to the least possible misunderstandings** is chosen. The name must indicate what is actually measured (especially in sum parameters and indicators).

All parameters are therefore first sought in the CAS REGISTRY system. If ever possible, one of the index names registered in CAS has to be used. This needs not be the shortest CAS name; the choice is made according to the following rules:

1. Inorganic anions reported as such (not as salts) carry their trivial names, which also indicate the oxidation level of the central element.
2. Ores (mineral resources) are normally expressed as the element that is extracted from them. However, ores of different composition or 'richness' as well as mixed ores that yield more than one element or other minerals obtain their mineralogic name.
3. In the cases of (a) very common trivial names and (b) pesticide names that are much shorter or simpler than the systematic names, these trivial names may be used.
4. Chlorofluorocarbons (CFCs and HCFCs) and halons must be identified by their CFC/ halon name, in addition to their chemical name.
5. Qualifying information follows the parameter name, separated by commas. Depending on the substance – the following possibilites occur:
   - Organics: 'parent hydrid' (principle chain, ring) comes first, the substituents follow. One characteristic group or functional class name can follow immediately (without blank) behind the principal chain or ring, before other substituents.
   - Salts of O-containing acids: Acid appears first, followed by the cation – if necessary including its oxidation level or a counting prefix
   - Esters of organic acids: Acid appears first, followed by the alkyl group, possibly with a counting prefix.
   - Isotopes: Name of parent element, followed by a dash and the mass number
   - Metals: First comes always the parent metal, then a specification such as (i) 'ion' plus oxidation level for ions, (ii) roman numerals for oxidation levels of the metal, (iii) name of the counter-anion for metal oxides and salts or (iv) 'in ground' for metal resources. Ions are only reported as separate parameters if they need to be distinguished from the parent metal, e.g. for toxicological reasons.
   - Hydrogen compounds: Simple hydrogen compounds follow the same rule as the analogous metal compounds (see above).
6. Chemical formulae should be given whenever possible, but in a separate field and not in the name field. For complicated chemicals, sum formulae can be used. The sequence of elements in such sum formulae must be adhered to: C, H, N, O, P, Br, Cl, F, I, to make them searchable.
7. Salt formulae are written conventionally with the cation first. Formulae of ions indicate the charge as +, ++, 3+, -, --, 3-. To avoid confusion, a blank is left before the charge in complex anions.

Box 2: Rules for choice of appropriate measurement base

1. Wherever possible, the measurement base should be identical to the name of the parameter: Salts and other compounds (e.g. halogenated hydrocarbons) are reported 'as such', not as the underlying element.
2. As an exception to rule 1, results 'as xxx' may be reported, when various molecular species are in chemical equilibrium and cannot easily be quantified as individual molecules. Examples: nitrogen oxides as NO_2, sulfur oxides as SO_2. Such cases should be restricted to the necessary minimum, and great care has to be taken (i.e. the expression CO_x as CO_2 is chemically meaningless).
3. Sum parameters sometimes need to be expressed as an underlying element (TOC, DOC, N organic bound, N total, AOX), since this is the only parameter actually measured, whereas the individual species cannot be quantified.
4. Extraction of ores (having a highly variable composition) should be given as mass of the extracted element, to facilitate comparability. Exception: If a rich ore (high concentration) and a light ore (low concentration) form two clearly distinct resources, which cannot easily be substituted for each other, they should be reported as such.
5. Emission classes that have a distinct environmental effect independent from their mass may be quantified (and aggregated) on the basis of this quality (polychlorinated dibenzo-p-dioxins as 2,3,7,8-TCDD – tox equivalents).
6. Natural isotopes that reach the biosphere due to anthropogenic interventions should be accounted for in kBq. However, radioactive substances should not be aggregated as kBq, because the number of decays per second does not correlate with the different health effects caused by the individual isotopes (Frischknecht 2000).
7. As long as the strategies to report and classify solid wastes are not better defined, wastes should be reported both as volume and as mass, if ever possible. This conversion can only be performed at the level of each individual waste, since the respective densities must be known. Clearly, the two parameters 'waste as volume' and 'waste as mass' are not additive.

Therefore, general rules for the choice of the underlying units are presented below. The objective is to choose the most intuitive and least error-prone unit for each parameter. In case of parameters that are not exactly synonyms, but mean the same thing (such as 'nitrate' and 'nitrate-N'), the parameter name that gives rise to the least possible misunderstandings is recommended. The set of rules in **Box 2** describes the principles for the choice of the appropriate measurement base.

3.3 Treatment of sum parameters

Sum parameters are frequently found in LCI and considered useful both by practitioners and authorities due to the fact that in most studies, individual substance measurements are not necessary or not even feasible. Nevertheless, they can create serious problems in LCA work:

- Overlap with concurrent determinations of individual molecules
- Partial overlap with other, similar sum parameters
- Difficulties to attribute one appropriate damage factor in LCIA to a mixture of compounds with different chemical, toxicological, and fate properties

Frequently occurring sum parameters were investigated individually and are described in detail in the working group report (De Beaufort and Bretz 2001). The main points are summarised in **Box 3**. As a general rule, sum parameters should only be used when the group as such is measured. Individually measured emission parameters should not be hidden in group or sum parameters such as NMVOC or VOC. In the case of really problematic substances (carcinogens, ozone depleting agents, etc.), they may never be obscured in group emissions, but must be determined and reported individually.

When individual molecules and sum parameters are determined in the same sample, overlap occurs inevitably. This overlap can only be overcome, when corrected sum parameter are reported. Such a correction of sum parameters is the only consistent way to make them additive. Obviously, the practitioner who analyses a certain process and prepares its inventory is the only one who can resolve overlaps. If the process data are later used by others, sum parameters reported as such can no longer be corrected and become meaningless, even though they may be marked that they are not corrected for individually reported species.

One possibility to make such corrections is the use of a hierarchy of parameters. Such a hierarchy creates an open architecture for new findings and ensures the transparency of the structure of sum parameters; the structure proposed in De Beaufort and Bretz (2001) is shown in **Fig. 1**. This hierarchy has to fulfil the following requirements:

Box 3: Conclusions concerning the treatment of sum parameters (for more details concerning specific factors, see De Beaufort & Bretz 2001)

- In the absence of individually speciated NMVOC emissions, default compositions of VOC-emissions of technologies should be applied, which correspond to the technology at stake.
- In the absence of individually speciated PAH emissions, generic PAH fingerprints of technologies should be applied, which correspond to the technology at stake.
- If PCB emissions cannot be quantified individually, the Beck standard should be used. In this case, the estimanted total amount of PCBs is obtained by multiplying the amount measured with the factor 5 (if not already done in the original data source).
- When individual dioxins and furans cannot be reported, the toxic equivalents (TEQ) may be used, determined on the basis of the toxic equivalency factors (TEF).
- The use of the sum parameter 'monocyclic aromatic hydrocarbons' (MAH) is discouraged.
- The sum parameter adsorbable 'organically bound halogens' (AOX) is hard to interpret. Rather, at least the main individual substances should be reported.
- Individually measured and/or reported ozone depleting substances and partly halogenated hydrocarbons must not be pooled, but individual substances should be quantified.
- Individually measured and/or reported radionuclide emissions must not be pooled, but individual isotopes need to be reported. Similarly, emissions of an isotope to air must not be combined with its emissions to water.

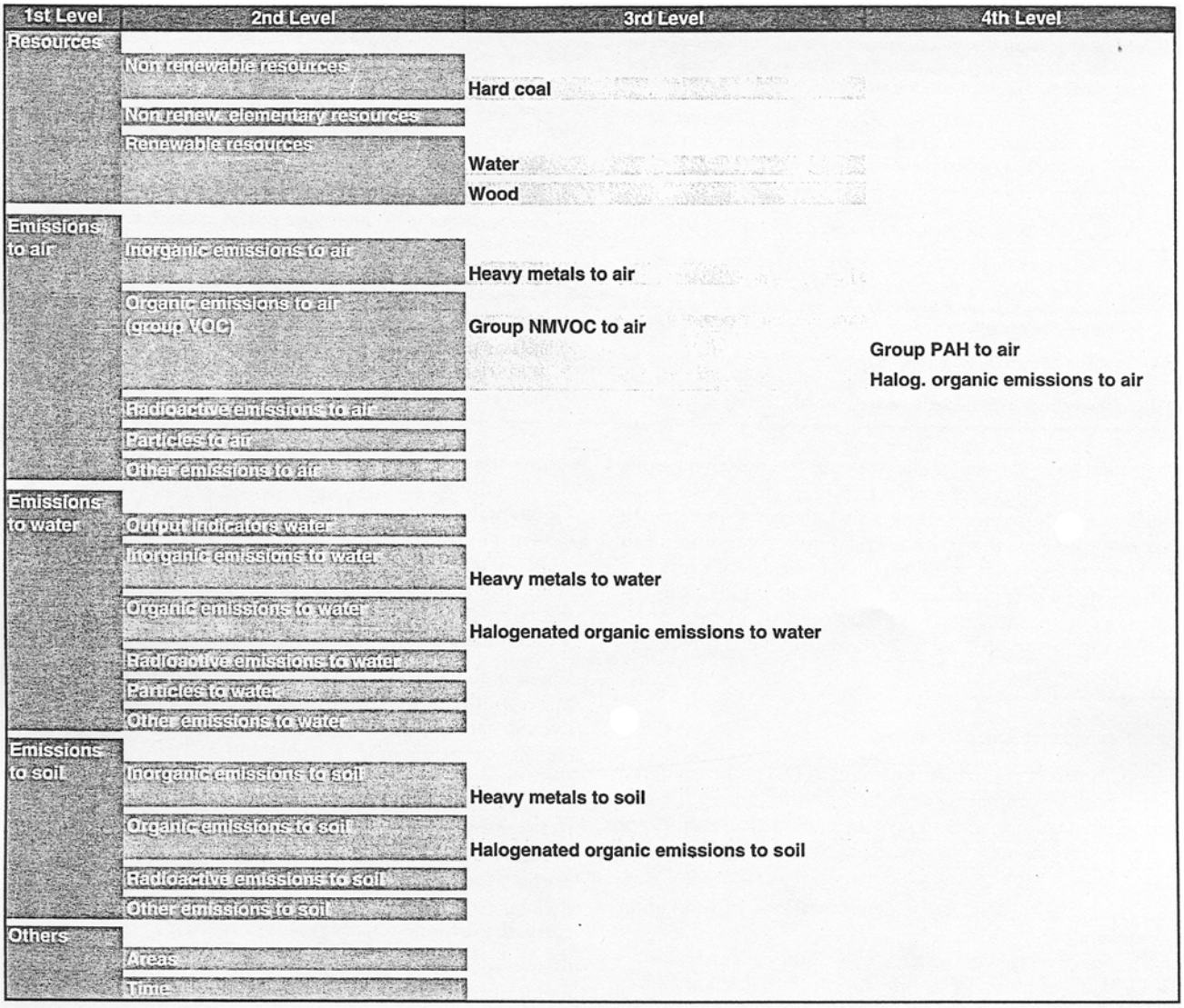

Fig. 1: Overview of the different levels of the hierarchy

- The drive for simplicity should not neglect the complexity which characterises the problem.
- The possibility to analyse a study in detail has to be provided by the structure of the parameter list.
- The standardization list has to consider the needs of a sophisticated description of various industrial sectors.

3.4 Missing/incomplete information and their educated guesses

Two cases of information missing in life cycle inventories may be distinguished: (a) Missing unit processes in LCI process trees and (b) missing *exchanges* (inputs, outputs etc.) in individual unit processes. Generally, case (a) causes more severe errors in the total results, although one can imagine a situation where case (b) may also seriously distort the result of an LCA (e.g. if a very crucial emission is missing).

Generally, missing information in LCI is implicitly set to *zero*, without any assessment of its importance. Errors introduced by such omissions are not stochastic, but cause a distinct bias towards lower values. Ignorance is thereby rewarded. Ways must therefore be investigated to

I) Identify data gaps completely
II) Close such data gaps as far as possible
III) Assess the impact of remaining data gaps on the end result
IV) Counteract the downward bias, e.g. by worst-case assumptions

Ways to deal with the two types of missing information are described in Table 3. Many of the recommendations made there seem very common-place (or ridiculously trivial). However, even in modern LCI publications, such simple measures as mass balances are sometimes not applied to ensure data completeness. In LCI work, almost every reasonable estimate, even a guess, is probably closer to reality than the standard and default 'gap filler' *zero*, since processes with zero emissions are very rare.

Table 3: Ways to deal with missing/incomplete information

	Missing unit processes	**Missing *Exchanges***
I	• All known process steps (incl. steps with unknown individual exchanges) must be considered • Steps with missing data need to be clearly marked, to identify data gaps (→ inventory of missing information) • Gaps should be screened for their importance • Such steps may only be omitted when (i) their mass contribution is below a threshold and (ii) neither extreme materials nor highly critical emissions are expected	• Their identification is generallymore complicated • Adequate book-keeping of raw materials and energy and appropriate analysis of effluents may yield valuable hints, or at least rudimentary information • Comparison of the known inputs and the stochiometry of the process with the resulting goods often reveals gaps in output data
II	• Processes may be described (i) by own process knowledge, (ii) by literature data or (iii) by estimation as discussed in Bretz & Fankhauser (1996) • Processes with lacking information should at least be entered as a 'formal nodes' (only material inputs, but no process energy requirements nor emissions)	• Data gaps can be filled following the law of mass conservation (this probably underestimates the losses and fails to forecast the final fate of wastes or the compartment of emissions, but is clearly superior to a total disregard of the mass balance) • Combustion processes may be characterized by typical VOC fingerprints, described in the literature (e.g. De Beaufort & Bretz 2001)
III	• From the inventory of missing information (see I), the amount of omitted or 'formal node' processes can be quantified • The relation of undefined to well-defined flows is an indication for completeness, data quality and relevance	• Inspection of literature data for similar processes often reveals obvious gaps • Gaps can be filled with data from other sources • Consequences of omission can be estimated with regard to the LCIA method applied

IV	• When an omitted/poorly documented process is identified as possible problem, then
	  • a worst case guess and a subsequent sensitivity analysis on the overall results should be performed
	  • Further analysis is needed when this sensitivity analysis shows dominant effects on the final result
		• Mass balances (see II) are often blamed as worst case assumptions
		  • Sensitivity analysis can identify cases where mass balance based data cause possible problems
		  • Further analysis is necessary when sensitivity analysis shows dominant effects on the final results

4 Conclusion

The comparability of LCI, the exchange of data between practitioners and the compilation of inventories for complex systems using sub-system data coming from various sources is still severely impeded by inhomogeneous data and inconsistent data acquisition and reporting techniques (see paragraph 3). One conceivable measure to solve that problem and to ensure the free flow of data would be a compulsory list of parameters with a mandatory nomenclature and measurement basis, complemented with strict rules for the use of sum parameters.

However, such a normative approach is not practicable, due to the heterogeneity of goals and scopes in LCA work, the multitude of analytical methods, the variety of legal requirements on reporting parameters and, above all, the flexibility necessary in LCA work. Therefore, in order to achieve as much data compatibility and exchangeability as possible, we propose a **multi-tiered approach based on recommendations that leave room for necessary deviations,** as long as these are **clearly defined and comprehensible** for the recipient of the data. The different steps therefore are:

1. Completeness and scope of the list of Exchanges

In accordance with the goal and scope of their studies, practitioners need the freedom to chose their list of measured and reported *exchanges*, according to their scientific judgement.

2. Nomenclature and synonyms

A standardized nomenclature of *exchanges* has been recommended by the subgroup, based on SPOLD (1997 and 1999). In practical LCI work, the use of deviant nomenclature and local languages cannot be avoided. Furthermore, it is not conceivable that the data existing in individual databases and commercial LCA software can all be converted to the standardized nomenclature. However, the use of the standardized nomenclature should be mandatory in LCI data exchange. Parameters that cannot be mapped to the standardized nomenclature for any reason should therefore be clearly marked.

3. Bases of measurement, units

Together with the standardized nomenclature, a list of measurement bases is proposed. Although practitioners may have good reasons to use different measurement bases or units internally, in data sets prepared for data exchange they should convert the results to the standardized measurement basis. Converted results should be given alongside with the original ones.

4. Sum parameters, overlaps, double-counts or omissions

As stated before, sum parameters should only be used when the group of emissions as such is measured and individually measured emission parameters should not be hidden in group or sum parameters such as NMVOC or VOC. Individual emissions may not be aggregated into sum parameters, if they are known to have a high environmental relevance, different ecological properties (e.g. toxicity), or significantly different weighting factors in any present or foreseeable life cycle impact assessment methods.

Presently, many inventories show partially or fully overlapping individual and/or sum parameters. In individual (unit) processes, the analytical techniques and reporting requirements are normally uniform and overlaps occur only when the analyses are refined to greater detail. In this case, the practitioner should make a clear statement *which param-*

eters are overlapping and may not be added and/or weighted independently by LCIA methods.
In horizontally aggregated (averaged) unit processes and in vertically aggregated process systems, the analytical techniques and reporting requirements are often heterogeneous (site-specific). The only way to cope with this problem is a high degree of transparency, which can be only provided by the author(s) of the study. Once the information is obscured, all attempts to reconstruct it must remain rudimentary.

Especially point 1 must not be mistaken as an invitation to report as few parameters as possible, or even to suppress certain values for which measurements actually exist. Therefore, every report should contain a self-commitment signed by the practitioner(s):

"Included in the inventory were all parameters that can reasonably be expected to occur in the processes under study, and that can have any environmental relevance, especially when judged with present or foreseeable life cycle impact assessment (LCIA) methods."

It should of course be noted that parameters reported in a study *need not* in all cases be measured. Therefore, it is advisable to report the absence of certain critical outputs in a process with a 'zero' entry marked by a quality indicator such as 'calculated from process stoichiometry', 'not present in any process input' or 'not to be expected in this type of process (educated guess)'. This is by far more transparent and scientifically sound than the simple omission from the parameter list.

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