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The USEtox story: A survey of model developer visions and user requirements

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Abstract

Purpose USEtox is a scientific consensus model for assessing human toxicological and ecotoxicological impacts that is widely used in life cycle assessment (LCA) and other comparative assessments. However, how user requirements are met has never been investigated. To guide future model developments, we analyzed user expectations and experiences and compared them with the developers' visions.

Methods We applied qualitative and quantitative data collection methods including an online questionnaire, semi-structured user and developer interviews, and review of scientific literature. Questionnaire and interview results were analyzed in an actor-network perspective in order to understand user needs and to compare these with the developers' visions. Requirement engineering methods, more specifically function tree, system context, and activity diagrams were iteratively applied and structured to develop specific user requirements-driven recommendations for setting priorities in future USEtox development and for discussing general implications for scientific tool development.

Results and discussion The vision behind USEtox was to harmonize available data and models for assessing toxicological impacts in life cycle assessment and to provide global guidance for practitioners. Model developers show different perceptions of some underlying aspects including model transparency and expected user expertise. Users from various sectors and geographic regions apply USEtox mostly in research and for consulting. Questionnaire and interview results uncover various user requests regarding USEtox usability. Results were systematically analyzed to translate user requests into recommendations to improve USEtox from a user perspective and were afterwards applied in the further USEtox development.

Conclusions and recommendations We demonstrate that understanding interactions between USEtox and its users helps guiding model development and dissemination. USEtox-specific recommendations are to (1) respect the application context for different user types, (2) provide detailed guidance for interpreting model and factors, (3) facilitate consistent integration into LCA software and methods, (4) improve update/testing procedures, (5) strengthen communication between developers and users, and (6) extend model scope. By generalizing our recommendations to guide scientific model development in a broader context, we emphasize to acknowledge different levels of user expertise, to integrate sound revision and update procedures, and to facilitate modularity, data import/export and incorporation into relevant software and databases during model design and development. Our fully documented approach can inspire performing similar surveys on other LCA-related tools to consistently analyze user requirements and provide improvement recommendations based on scientific user analysis methods.

Keywords: user survey; USEtox; toxicity assessment; actor-network perspective; requirement engineering methods

1 Introduction

In life cycle assessment (LCA), several methods, assessment and modeling tools address the characterization of human toxicological and ecotoxicological impacts of chemical emissions (European Commission, 2010; Hauschild et al., 2011). However, toxic chemical emissions are still often not or insufficiently characterized in LCA studies. Perceived or actual differences regarding method or model applicability between developers and users (including LCA practitioners and decision makers) might contribute to the lack of addressing toxicity impacts in LCA practice. This is partly because it is considered fundamentally important that the scientific quality of models is meeting contemporary standard and represents state-of-the-art, while less effort is usually put into qualitative model attributes like usability, maintainability and interoperability, and to meet the requirements of the model users (Nuseibeh and Easterbrook, 2007). To address this gap, we focus in this study on investigating the visions behind developing a scientific consensus model for the characterization of potentially toxic chemical emissions along with investigating how and why users apply this consensus model in practice. By comparing the developers' visions with the users' application practices we develop recommendations helping to further align the process of translating model development and improvement with user practice. This focus aims at ultimately supporting an improved and extended application of the toxicity characterization of chemical emissions in LCA practice.

1.1 The story of USEtox

Between 1993 and 1999, several consensus building activities were conducted by the SETAC[1] Impact Assessment working groups leading to the definition of a framework for assessing fate, exposure and effects of life cycle emissions of toxic chemicals (Udo de Haes, 1996; Udo de Haes et al., 1999b, a; Udo de Haes et al., 2002). Inspired by this and by

[1] Society of Environmental Toxicology and Chemistry (http://setac.org)

previous and parallel consensus building activities (e.g. Cowan et al., 1995; Fenner et al., 2005), the OMNIITOX project was initiated (Carlson et al., 2004; Guinée et al., 2004; Molander et al., 2004) to develop methods for assessing risks and impacts associated with chemical emissions from product life cycles. The project served to develop a common perception of the field of toxicity characterization modeling and to build the necessary trust in working together in an efficient way towards harmonizing existing toxicity characterization models. In 2003, the UNEP[2]/SETAC Life Cycle Initiative (LCI) therefore established a Task Force on Toxic Impacts officially launched in Prague on 22-April-2004 to provide clear guidance for assessing human toxicity, ecosystem toxicity, and related categories with direct effects on human and ecosystem health. This task force was largely based on joined forces between members of the previous efforts and identified that existing toxicity assessment models only covered a limited number of substances and that scope, principles and characterization results varied substantially (Dreyer et al., 2003; Pant et al., 2004), entailing that many LCA practitioners ignored toxicity-related impacts in their life cycle impact assessment (LCIA) step (Hauschild, 2005). This led to a process towards developing a scientific consensus model for the characterization of human toxicological and ecotoxicological impacts of chemical emissions (Figure 1), starting from four expert review and framing workshops held between 2003 and 2010 (Aboussouan et al., 2004; Jolliet et al., 2006; McKone et al., 2006; Diamond et al., 2010) and three model comparison workshops organized in 2006 (Hauschild, 2006b, a; Hauschild et al., 2006). In these workshops, models were compared based on investigating a test set of chemicals representing a specific combination of substance properties and identifying those processes and factors influencing at least some chemical groups. This process was oriented in and operated from the state-of-the-art in various fate, exposure and effect modelling communities, the input of which was gathered through the expert workshops. Result was the development and implementation of

[2] United Nations Environment Programme (http://unep.org)

USEtox, a combination of a characterization factors (CF) database and a model to characterize human toxicity and ecotoxicity of chemical emissions (Hauschild et al., 2008; Rosenbaum et al., 2008). More details of the full consensus building process including previous and parallel consensus activities are given in Hauschild et al. (2008), while a full description of considered factors significantly influencing characterization modeling for different chemical classes is provided in Rosenbaum et al. (2008). USEtox was officially announced on 25-May-2010, but version 1.0 was already made freely available via http://usetox.org on 18-Nov-2009. Model and factors have since been applied in multiple comparative impact assessments as further discussed in a special issue of The International Journal of Life Cycle Assessment dedicated to USEtox (Hauschild et al., 2011), USEtox characterization factors have been implemented in LCA software (e.g. GaBi, SimaPro, OpenLCA, Quantis Suite) and some LCIA methods (e.g. ILCD LCIA, Impact World+, TRACI 2).

<Figure 1>

USEtox is continuously being improved and further developed in international efforts with the aim at meeting current and future user needs and expectations, facing market developments and addressing unresolved scientific challenges. Tox-Train (http://toxtrain.eu), a four-year EU project (November 2011 to October 2015), is designed (a) to assess and develop state-of-the-art tools and data for use in comparative toxicity assessment that will be proposed to be integrated in USEtox and (b) to further disseminate USEtox via training and outreach, via re-designing the official website including the introduction of a user forum and developing a transparent update proposal procedure including peer-review, and via investigating user requirements and improving the usability of USEtox in practice. The latter provides the scope of this study, while further improvement and dissemination activities are summarized in Figure 1.

1.2 Assessing user requirements to facilitate further improvements

To assess USEtox user perspectives and requirements and to identify different user expectations, we employ state-of-the-art methods from the field of Science and Technology Studies including Actor Network Theory and Requirement Engineering that focus on users' interactions with science and technology (Sismondo, 2010). Thereby, a technological element (here: USEtox) and human actors (here: users) are analyzed as mutually constituted in a socio-technological network where they influence each other (Harty, 2010). Since humans perceive technology differently and apply it in diverse, changing contexts, technology developers can never fully anticipate the ideal product for all users during the development process (Rohracher, 2003). However, assessing user perceptions and practices can help generating priorities for technology development. Rohracher (2003) recommends managing technology development as continuous interaction between developers and users. Actor Network Theory and Requirement Engineering are further detailed elsewhere (Latour, 2007; Nuseibeh and Easterbrook, 2007; Sismondo, 2010). These methods have already been applied to assess socio-technological interactions of different software tools (Harvey, 2001; Takhteyev, 2009; Harty, 2010) and are suited to focus on the many relationships between a restricted set of technology users with the actual technology (Harvey, 2001). However, to our knowledge, such methods have not been applied to develop recommendations for strengthening and improving the application of environmental assessment models, such as USEtox. Aiming at analyzing and harmonizing USEtox user practice and requirements with developer visions in accordance with state-of-the-art methods from stakeholder analysis and technology development, we focus together with two USEtox developers[3] on three objectives: (1) To apply selected data collection methods. This helps to understand on the one hand the developers' original vision behind building USEtox. On the other hand, this helps to understand the aims and practical experiences of users applying USEtox model and factors. (2) To categorize and evaluate collected data for identifying and characterizing the general application trends of USEtox. Trends are then compared with the developers' original visions and development perspectives. (3) To use requirements engineering methods for establishing a set of specific recommendations to harmonize USEtox developer aims and user requirements. We then generalize our recommendations in support of an improved consideration of user requirements when developing and disseminating scientific modeling tools more generally. Comparing expectations and experiences of users with developer visions of applying USEtox will help to improve and extend the application of the characterization of toxic impacts induced by chemical emissions in LCA and will further help to guide future model development based on user requirements.

2 Methods

To investigate user requirements and the actor network relations around USEtox, we applied a mixed-method design (Frechtling, 2010) including both qualitative and quantitative data collection methods as shown in Figure 2. We combined four different starting points to collect information about user practice and the developers' visions and perspectives of developing USEtox: (1) We analyzed basic statistics over users that have registered at http://usetox.org and downloaded the USEtox model and databases. (2) We developed an online questionnaire, which was disseminated via an LCA forum list and a list of email addresses collected from users downloading USEtox. (3) We prepared a set of additional, more detailed questions and interviewed selected USEtox users and developers. (4) We

[3] USEtox developers helped to develop the user questionnaire, gave access to the usetox.org statistics, and provided details on the consensus building process of USEtox.

extracted additional information about the developers' visions from relevant peer-reviewed literature. Results from all four approaches were categorized and evaluated in an actor-network perspective to identify different user types. Actual practices of the users were then compared with the developers' original visions about USEtox users. The outcome of the evaluation is used to develop and focus specific recommendations to aid setting priorities in the continuous USEtox development and improvement process and also discuss general implications for scientific tool development. The applied methods are detailed in the following.

<Figure 2>

2.1 Data inputs and questionnaire for assessing general user practice

With permission from the USEtox development team and strictly respecting the confidentiality of the data ensured by inviting two USEtox developers as co-authors, we accessed the user statistics of their official website containing name, affiliation, and country per user. We applied basic statistics to identify the geographical and sectorial distribution of USEtox users. On 1-Nov-2011, i.e. within the first 24 months after model and factors became available online, we counted 551 distinct users registered at http://usetox.org.

An online questionnaire was designed using the online survey service http://obsurvey.com. Combining the list of users of the USEtox website with the list of about 2500 individuals[4] registered at the LCA forum (http://pre.nl), an invitation was sent to more than 3000 potential respondents. The survey scheme was made accessible for 24 days in November 2011. During this period, 131 responses were received. The questionnaire was developed to get more detailed and quantitative information regarding the usage of USEtox, including specific usage patterns and user perspectives and requirements when applying the

[4] Most potential USEtox users were invited via usetox.org. The few potential users that accessed USEtox not directly via usetox.org, but e.g. via a colleague's download copy were invited via the LCA forum.

USEtox model and/or factors. All questions are assigned specific answering options. Detailed questions focus on user affiliation, how users got aware of USEtox and how they learned to apply model and factors, users' purpose or field of application for using USEtox, and finally what parts or aspects users effectively use from the USEtox package (only applying characterization factors, getting access to substance data, calculating factors for new substances, etc.). Two specific questions address the user perspective of applying USEtox and focus on the degree of agreement regarding the perceived usefulness and applicability (ease to use) of model and factors. Whenever appropriate, an open text field was available for additional or more detailed user feedback. We also used the questionnaire to identify 32 users that were interested in further discussing their perspectives. For conducting detailed follow-up user interviews, ten were selected with the aim to cover different sectors and geographical regions as broadly as possible.

2.2 Detailed interviews of users and developers

Aiming at supporting the questionnaire's outcome and deepening our understanding of both USEtox developer visions and user perspectives, we prepared a set of detailed questions used for interviewing four developers as well as ten users from different stakeholder sectors and regions. All interviewed users had previously completed the questionnaire. The interviews were semi-structured, allowing an open, but focused, conversational process (Rabionet, 2011). Furthermore, this method enabled us to ask in-depth questions whenever interesting and relevant viewpoints and comments emerged during the conversations. Main focus points of the interviews were the users' acquisition, application practice and perspectives regarding strengths and weaknesses of the USEtox model and results with respect to its practicability. Eleven persons were interviewed via internet phone calls, while three persons were interviewed face-to-face.

All interviews were recorded and subsequently transcribed. To link and categorize transcription fragments with certain topics, viewpoints or other elements in common, all transcriptions were divided into segments, which were then coded, i.e. descriptive headers or keywords were added to linked segments (Coffey and Atkinson, 1996). This procedure gave an overview of the comments given on different topics. To aggregate the information of different segments per category, segments were “condensed” (Kvale, 1996) until all information could be allocated to three main categories, namely one category containing user background, one containing users perspectives structured against different topics and finally one containing the developers perspectives structured against topics. This procedure provided an appropriate overview of user and developer perspectives of USEtox.

2.3 Assessing developer visions and user requirements

Interviews with USEtox developers about the consensus building process and the visions behind developing the model were complemented with the review of scientific publications related to the development of USEtox. Expert review and model comparison workshop reports (Aboussouan et al., 2004; Hauschild, 2006b, a; Hauschild et al., 2006; Jolliet et al., 2006; McKone et al., 2006; Diamond et al., 2010) along with the two framing USEtox peer-reviewed publications (Hauschild et al., 2008; Rosenbaum et al., 2008) were analyzed.

To identify requirements of USEtox users, we iteratively applied and combined different Requirement Engineering methods. Questionnaire and interview results were analyzed and structured into user requests about missing features regarding model structure and functions, and qualitative attributes regarding user requests about model usability, maintainability and interoperability (Sommerville, 2011). Function tree diagrams were applied as a structural way to identify recommendations based on the requested features and quality attributes (Cross, 2008). System context diagrams were applied to get an overview of present contexts in which USEtox is applied in order to help identifying potential user interaction improvements

(Sommerville, 2011). Activity diagrams were additionally applied to visualize imagined and actual steps in the user-technology interaction (Bhattacharjee and Shyamasundar, 2009). All diagrams were iteratively applied and adjusted to the results from the questionnaire and interviews. Results of all user requirement methods were combined to systematically compare USEtox developer visions with user perspectives and requirements, finally yielding a set of recommendations to harmonize developer visions and user practice in the further development of USEtox.

3 Results and Discussion

3.1 Developer visions and perspectives

From development-related publications, we compiled the original vision to develop and implement USEtox. The overall vision behind developing the scientific consensus model USEtox was that the data, methods and factors of characterizing human toxicological and ecotoxicological impacts are harmonized and are made globally available and applicable for LCA practitioners for a large number of chemicals. To implement this vision, the developers aimed at establishing a universally acceptable modeling practice and developing a consensus-based model as joint effort of all participating parties. This model was foreseen to (a) provide characterization factors as strongly correlated to the factors provided by other models as their characterization factors are to each other, (b) produce output that falls within the output range of the existing characterization models, (c) be parsimonious in the sense that it contains only those elements that the comparison of the existing characterization models identified as the most influential, (d) provide a repository of knowledge through evaluation against a broad set of existing models, and (e) be endorsed by all contributors. Finally, model and resulting factors should be more transparent and better documented than existing tools to increase practicability and usability.

From interviews with four of the USEtox developers, we derived more individual developer perspectives on the original vision. The interviews revealed that not all developers have the same perception of the overall vision in its details. Different ideas were expressed of what is supposed to make the model transparent for the user. For some developers transparency is clearly related to usability and that users with different levels of expertise and experience are able to apply model and factors. In contrast to that, for one developer transparency is related to visibility of numbers and equations in the model to allow users to understand the modeling principles. This originates in different opinions about the level of user expertise. While one developer expressed that he was satisfied with the complexity of USEtox and that he would not encourage users without profound knowledge in environmental chemistry to apply the model, other developers want the model to be as widely applicable to users with different levels of expertise as possible. This would include users that only want to use the model results without fully understanding the model in its complexity. However, all developers agreed that there is a limit to how easy it can be made to calculate characterization results, for which at least a basic understanding of chemicals and toxicity is required. According to one developer, guidance should ideally be available via an interface that helps identifying required data input and guides through the essential calculation steps. However, such interface had not been developed, since having an intuitive user interface was not the first priority upon implementing USEtox. The developer interviews also revealed that despite the intent to simplify the inclusion of toxicity-related impacts into LCA, it was unforeseen that USEtox became as widely spread geographically and among different users across various sectors as we can see it today with about 200 and 325 citations of the USEtox development publications at http://scopus.com and http://scholar.google.com, respectively (the latter representing also non-peer reviewed literature including books, reports and presentations), as of June 2014. It was further mentioned that USEtox becomes increasingly applied and recognized also at the regulatory level, e.g. in France, where USEtox is considered the model of choice for ecotoxicity product labelling for the “Grenelle” legislation (Van Hoof et al., 2011), or in the United States, where USEtox is evaluated by the U.S. Environmental Protection Agency for exposure-based chemical prioritization (Wambaugh et al., 2013). The developers’ reflections about the use of USEtox must be seen in the context that originally, the USEtox model was foreseen to be primarily applied by the developers themselves and to provide only a list of pre-calculated characterization factors to the user community. However, in the end of the initial USEtox development process it was perceived more appropriate to also allow users to calculate their own factors e.g. for chemicals that are currently not covered in USEtox, thereby also providing the full model.

3.2 User application practice and perspective

Among the 551 users registered at the USEtox website, a wide range of sectors was covered including academia (49%) and non-academic research institutes (6.5%), consultancy (18%), enterprises (12%), regulatory bodies (9%), associations (2.4%), private persons (1.5%), and non-governmental organizations (NGO). The remaining 1.6% of users did not state their sector affiliation. Geographically, users were from Europe (57%, where France and Denmark alone account for almost half of all European users), North America (33%, mainly USA), Asia (5%), South and Central America (2.4% each), and finally Australia (1.3%) and Africa (0.7%). The 131 users responding to the online questionnaire were found to cover all listed sectors (see

Figure 3A) and all geographical regions except Africa (Europe: 67%, North America: 27%, Asia: 4%, Australia and South and Central America: 1% each). All questionnaire results are summarized in

Figure 3.

<Figure 3>

Respondents applying USEtox were predominantly consultants or academic researchers, whereas the model is used to a much lesser extent in the public sector including government agencies, NGOs, or non-university research dominating the “other” category (

Figure 3A). This is in line with

Figure 3D showing that USEtox is mainly used in research including teaching (44%) and in management applications including life cycle and supply chain management and corporate social responsibility. Only few users apply USEtox in the context of marketing including public relations or regulation. The ten detailed user interviews revealed that users across sectors appreciate the status of USEtox as a scientific consensus model covering a large number of chemicals and that some researchers use the model structure as inspiration to develop their own models. USEtox was mainly known via colleagues or from scientific publications, and only for less than 5% of users via the official website, or “other” sources including professional network, LCA discussion forums or conferences (

Figure 3C). In interviews, it was also stated that its status in the French regulation gave inspiration for using USEtox. Most users learned to use model and factors via the user manual (Huijbregts et al., 2010) and the instructions directly provided in the model file (

Figure 3B). However, several users asked for a more intuitive user interface, supported by some interviews detailing that the manual is difficult to understand and to apply as guide through the modeling steps. This is consistent with the fact that almost 50% of users do not particularly agree that "USEtox is easy to use" (

Figure 3E) and some users even used the interviews as opportunity to ask questions around how to apply the model. However, the majority of users found that "USEtox is useful" (

Figure 3E) and explained in interviews that particularly the scientific foundation was appreciated. Almost 50% of users reported to only apply USEtox characterization factors and 17% to access chemical data (

Figure 3F), for which the substance data and results databases are sufficient. About 14% of users indicated not to directly use either model or results, but e.g. included USEtox as reference or list of available toxicity models or in their teaching. Other users access USEtox characterization factors via LCA software, which is especially preferred by unexperienced users as stated in interviews, but also by more experienced users, due to the direct use in LCA studies. However, various users directly apply USEtox for either calculating interim factors for fate, exposure and/or effects (14%) or for calculating characterization factors (20%) for new chemicals not yet covered in USEtox (Figure 3F). These users need to understand and apply the model itself. Interviews uncovered that some users experienced problems because USEtox results are not integrated in all LCIA methods. This has implications in the form of inconsistent substance coverage in the case of LCAs including chemicals found in other models than USEtox. Along with that, it was stated to be problematic especially for non-experts how to correlate or compare USEtox results with results from other LCIA models for toxicological impacts that were e.g. used before USEtox was available. Finally, some users indicated via their interviews that they had problems with implementing USEtox results into LCA software, thereby missing a way to automatically update the software whenever they calculated new characterization factors.

From evaluating questionnaire and user interview results we are able to categorize users into five actual user types with specific characteristics based on their application field, expertise and USEtox application practice (Table 1).

<Table 1>

LCA software developers and instructors do not necessary apply USEtox as practitioners in LCA case studies or for research, but they constitute important user types, since they help implementing USEtox results into other tools including LCA software (LCA software developers) and/or guide practitioners in applying model and results and might even recommend USEtox to other users (instructors). From their close contact to different user fields, instructors hold valuable knowledge about user requirements, which was also a benefit in our questionnaire and detailed interviews.

3.3 Comparison of developer visions with user requirements

The overall vision that methods and factors to characterize human toxicological and ecotoxicological impacts in LCIA should become globally available has been achieved within the first years after publishing USEtox. Users apply model and factors in several contexts, sectors and regions, partly because of its consensus status (see also Figure 3). However, the vision to be more transparent and better documented than existing tools to increase practicability and usability has only partly been achieved as shown from user experiences and expectations in the previous section. As an input for potentially improving the usability of USEtox, we therefore conducted a more detailed analysis of user requirements. Figure 4 illustrates how function tree diagrams, system context diagrams and activity diagrams were iteratively applied to structure usability-related user requirements based on the data from the questionnaire and interviews with users.

<Figure 4>

In a function tree diagram (Figure 4A) we propose possibilities to improve the graphical user interface (GUI) of USEtox towards a more intuitive and transparent application and give examples of the level of increasing applicability, such as to adapt the GUI until a specific user has gained a certain level of expertise to apply model and factors without any manual. This can be achieved via a step-wise GUI guidance system that is accompanied with hints of where to e.g. find and insert relevant input data. Combining requirements of different user types (Table 1) with the contexts in which users apply USEtox yields a specific set of interconnected sub-systems illustrated in the system context diagram (Figure 4B). Users typically interact manually (denoted “M”) with the front end sub-system for inserting user input and reading model output, whereas other sub-systems like model equations describing specific fate processes are usually of less importance for direct user access. A detailed proposal of an improved procedure of users interacting with different USEtox sub-systems is presented in the activity diagram (Figure 4C). Starting with searching for a specific chemical of interest, this diagram guides the user through the different steps until the desired result (e.g. a set of characterization factors, CFs) is reached, thereby passing various sub-systems. Missing data and extrapolations between data are also included as requiring further guidance.

All diagrams were iteratively adapted until a satisfactory level of detail was reached to transform questionnaire and interview results into recommendations for improving USEtox from the user perspective.

4 Recommendations

Recommendations to guide future development activities of the USEtox consensus model with respect to user applicability and functionality are designed on the one hand to be in line with the developers’ original vision to extend the application of characterizing the toxicity of chemical emissions in LCA. On the other hand, our recommendations are designed to help facilitating the correct use and interpretation of the USEtox model and results in different user application contexts. Six specific recommendations were developed:

1) Generally, the USEtox package should contain features to allow all user types to open model and factors, perform the calculation of intermediate and final results for implemented substances, interpret all results, and – if appropriate – insert new substances and/or customize landscape and substance data. Each user type has a different level of understanding of underlying data and methods (see Table 1) and, hence, requires a user type-specific level of detail in the guidance material (see Figure 4A-B).

2) More specifically for basic users (see Table 1) a model user interface should be provided as detailed guidance system allowing to follow different calculation steps and other actions step-by-step including interpretation of intermediate and final results, implementation of new substances, customization of implemented substances and landscape data (see Figure 4C). This would help to improve the acceptability of toxicity assessment with USEtox among affected users. Furthermore, USEtox results should be consistently incorporated in all relevant LCA software systems.

3) More specifically for LCA software developers and instructors (see Table 1) additional guidance and communication options should be provided by the USEtox developers to simplify the interpretation and manual or automatized implementation of final results (i.e. characterization factors) into LCA software tools and LCIA methods.

4) It should be clear and transparent how users can contribute to improving (updating implemented data upon the availability of e.g. improved substance data), correcting (finding bugs in the technical functionality, errors in data and/or equations), and further developing USEtox by for example extending substance coverage and/or model scope. Any update, however, should be in line with the consensus status of model and factors.

5) In support of further improving and further developing USEtox, a clear user communication and information strategy needs to be established by the USEtox developers. More specifically, dedicated user meetings and forums allowing for direct contact between users and developers should be established to improve user feedback possibilities that can be considered in future development steps.

6) The scope of USEtox in terms of substance, compartment, exposure pathway and effect coverage and disaggregation should be increased to facilitate an extended application of model and factors in LCA studies. However, all additional aspects should be implemented in accordance with the consensus building quality criteria detailed in (Hauschild et al., 2008; Rosenbaum et al., 2008).

These recommendations have already been particularly useful for understanding actual user needs that could partly be considered in current update, improvement, and outreach activities around USEtox. From generalizing USEtox-specific recommendations we derived the following three recommendations from the user questionnaire and interview results, which have implications for the scientific model development process in general:

1) As part of developing scope and context of a model, developers should familiarize themselves through different types of dialogues with the backgrounds, levels of detail regarding scientific knowledge and technical know-how, and application fields of all actors they imagine as potential users. This can be facilitated by applying Actor Network Theory methods. Requirement Engineering methods can then be used to define appropriate user interfaces along with required guidance and documentation material (see (Figure 4), thereby improving interpretability and applicability aspects and model integrity and reliability from the user perspective. This is relevant for all types of model development, including the development of software-based models as defined by van Vliet (2008).
2) Depending on the desired accessibility, dissemination and application context of a scientific model, a clear, transparent, and logical revision and update procedure should be an inherent part of the model design. Users as well as developers will benefit from this strategy as on the one hand maintainability and testability will be increased, while on the other hand strengthening the flexibility regarding different user types and application scopes. This is mainly related to revision of software-based models (van Vliet, 2008).
3) Along with underlying scientific robustness and correctness, it is recommended to integrate the technological context of a scientific model into the design and development phases. Aspects of re-usability based on a modular model structure, interoperability and portability between different software and operating systems, and finally technological interface design for incorporating parts of a model or its results into relevant software or

databases are here equally important. This is mainly related to software transition as defined by van Vliet (2008).

5 Conclusions and Outlook

Our experiences from the detailed and complex analyses of user expectations and experiences with USEtox and the further development of USEtox based on these analyses show that understanding the interactions of users with and requirements on a scientific model and the comparison with the developers' visions about users and model application can guide the further development process. The variety of user types with their differences in specific expertise and application contexts plays a significant role in designing model guidance material. While some of our recommendations might seem intuitive, we provide a consistent and formal analysis of the relationships between user expectations, developer visions and tool applicability. Thereby, we ensure that no important relationships are ignored even though they are not intuitive. This is in line with the rationale of using LCA as comprehensive scientific method yielding results that might in some cases also be intuitive, while in other cases revealing rather unexpected conclusions (e.g. Quantis, 2011). A limitation of our study is the restricted number of surveyed and interviewed users, where additional users with their specific requirements and practices might provide additional insight into existing applicability and usability issues and constraints, expectations and experiences. On the other hand, the respondents offered a reasonable coverage of the different known user types, sectors and geographical regions. The consensus status of USEtox is generally much appreciated by interviewed users, whereas some of the consensus-building criteria, such as well-documented model and factors, are still not met. We conclude from the results of our analysis of the restricted set of USEtox users that usability aspects are as important as scientific correctness to build trust among users and to facilitate a broad and meaningful application of model and factors. While a more transparent communication strategy with the user community is still desirable including a clear time plan for future updates and releases, current improvement efforts have already lead to features that were requested by surveyed users. These efforts include the implementation of a user forum with regular input by the USEtox team and a frequently asked questions (FAQ) page (part of the re-designed USEtox website), regular USEtox Community of Users meetings at international conferences, and a form and procedure to propose and adopt improvements or updates of model and/or factors (see http://usetox.org). The development of a USEtox user interface wizard that will provide guidance regarding model calculation steps and implementation/customization of substances is in progress as this was requested by various users. Furthermore, USEtox-based characterization factors are implemented in several LCIA methods including IMPACT World+ (Bulle et al., 2012), TRACI 2.0 (Bare, 2011), CML-IA (Guinée et al., 2002), and recommended in the ILCD handbook (European Commission, 2011), whereas ReCiPe (Goedkoop et al., 2009), LIME2 (Itsubo and Inaba, 2012) and the earlier methods EDIP2003 (Hauschild and Potting, 2005) and CML2002 (Guinée et al., 2002) rely on other models for toxicological impacts (of which CML2002 also proposes USEtox factors as a user choice). Since May 2013, USEtox is officially endorsed by the UNEP/SETAC Life Cycle Initiative (ILCB, 2013). It remains to be seen how the new USEtox features will contribute to further improving the consideration of toxicity-related impacts in LCA. Overall, scientific model design and development processes can greatly benefit from a close and continuous interaction between developers and users. The thorough documentation of the survey and how it was performed in order to document how the results were obtained will possibly inspire readers with aspirations of performing similar surveys on other LCA-related tools.

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Figures and Tables captions

Table 1

Identified USEtox user types and their characteristics.

Figure 1

USEtox development timeline including consensus building process between 2003 and 2010 and current improvement and dissemination activities after 2010. [a]Jolliet et al. (2006); [b]Aboussouan et al. (2004); [c]McKone et al. (2006); [d]Guinée and Hauschild (2005); [e]Hauschild et al. (2006); [f]Hauschild (2006b); [g]Hauschild (2006a); [h]Diamond et al. (2010); [i]Hauschild et al. (2008), Rosenbaum et al. (2008); [j]Oscarson and Hauschild (2010); [k]Henderson et al. (2011), Rosenbaum et al. (2011); [l]Hauschild et al. (2011); [m]This study, [n]ILCB (2013); [o]OMNIITOX project (EU FP5 contract: G1RD-CT-2001-00501), Carlson et al. (2004), Molander et al. (2004); [p]USEtoxPI project (LRI-ACC contract: MTH1001-01), Jolliet and McKone (2012), Mitchell et al. (2013); [q]TOX-TRAIN project (EU FP7 contract: IAPP-GA-2011-285286, Bengoa et al. (2014); [r]ExpoDat project initiated by LRI-ACC ExpoDat2012 workshop, American Chemical Council (2012); [s]QUAN-TOX project (EU FP7 contract: PCIG14-GA-2013-631910).

Figure 2

Overview of applied data collection and analysis methods to compare USEtox users' practice with developers' visions and develop recommendations for future development of USEtox.

Figure 3

Distribution of answers to the questions posed in the online questionnaire to USEtox users. In questions B, D, and F, multiple choices were allowed. *Responses to all categories but “Other use”. **Additional responses to specify further uses in category “Other use”.

Figure 4

Function tree diagram (A), system context diagram (B), and activity diagram (C) as applied to user questionnaire and interview results for iteratively analyzing usability aspects of USEtox.

Table 2

User type	User type characteristics
Basic user	– Prefers to access/apply USEtox results via LCA software – Sometimes needs to calculate characterization factors for chemicals not covered in USEtox in LCA studies or as exercise – Has difficulties to correlate/compare USEtox results with results from other LCIA models assessing toxicological impacts – Example users: students, employees of manufacturing companies, early-stage researchers
Experienced user	– Prefers to access/apply USEtox results via LCA software – Sometimes needs to calculate characterization factors for chemicals not covered in USEtox in LCA studies (scientific content is important, but has to be pragmatic) – Time to find characterization factors is often limiting factor in user's work – Example users: experienced consultants, employees of manufacturing companies
Researcher	– Is interested in/needs access to specific features of USEtox model and results – Scientific purposes to apply and/or study USEtox – Reviews and analyzes model and results in detail (scientific content and correctness are very important) – May use USEtox as inspiration to develop new models – Example users: more or less experienced researchers in university, other research institutes, and consultancy companies
LCA software developer	– Is interested in how USEtox is integrated in LCA software and LCIA methods – Has full understanding of LCA software and underlying databases – Uses/needs access to background material (raw data, data documentation) – Example users: developers of LCA software and databases
Instructor	– Assists (LCA) practitioners in applying USEtox model and results – Does not apply USEtox as practitioner, but understands its functionality well from profoundly studying model and results – May recommend practitioners to apply USEtox as function of his (instructor) own credibility in model and results – Has good overview of users and their application fields of USEtox – Example users: employees of governmental agencies

Figure 5

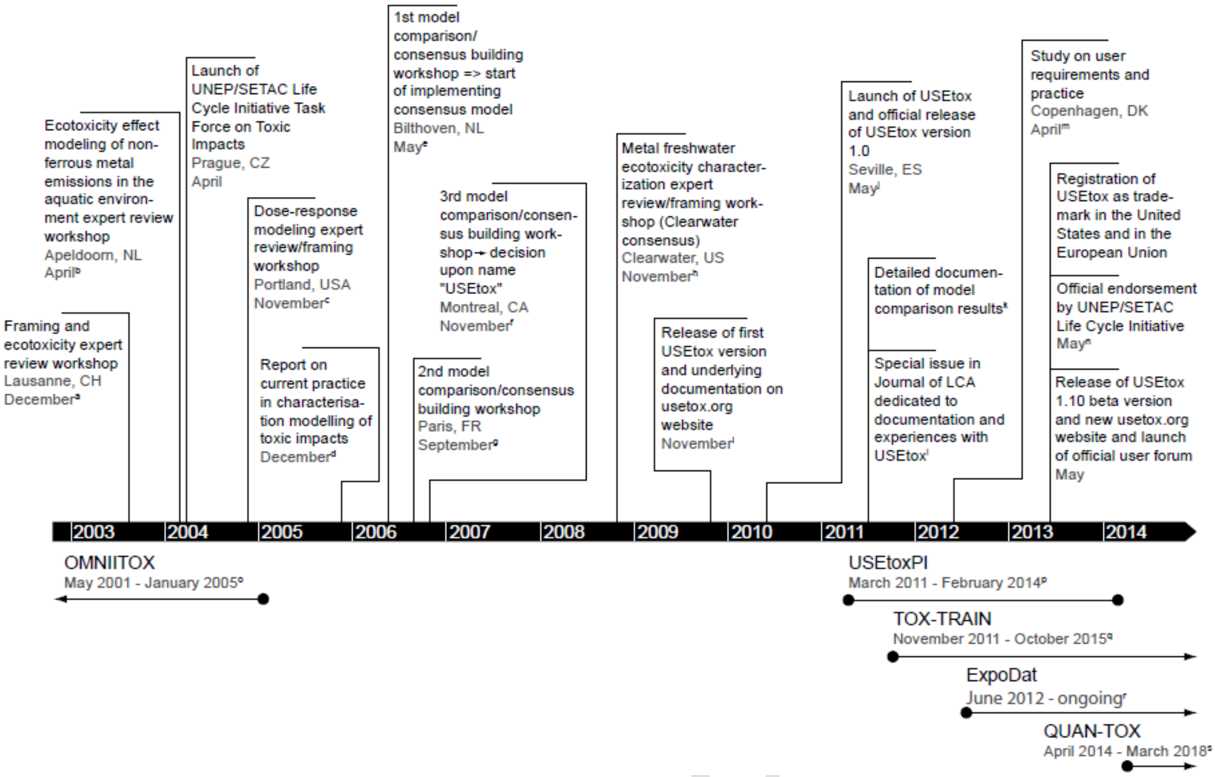

Figure 6

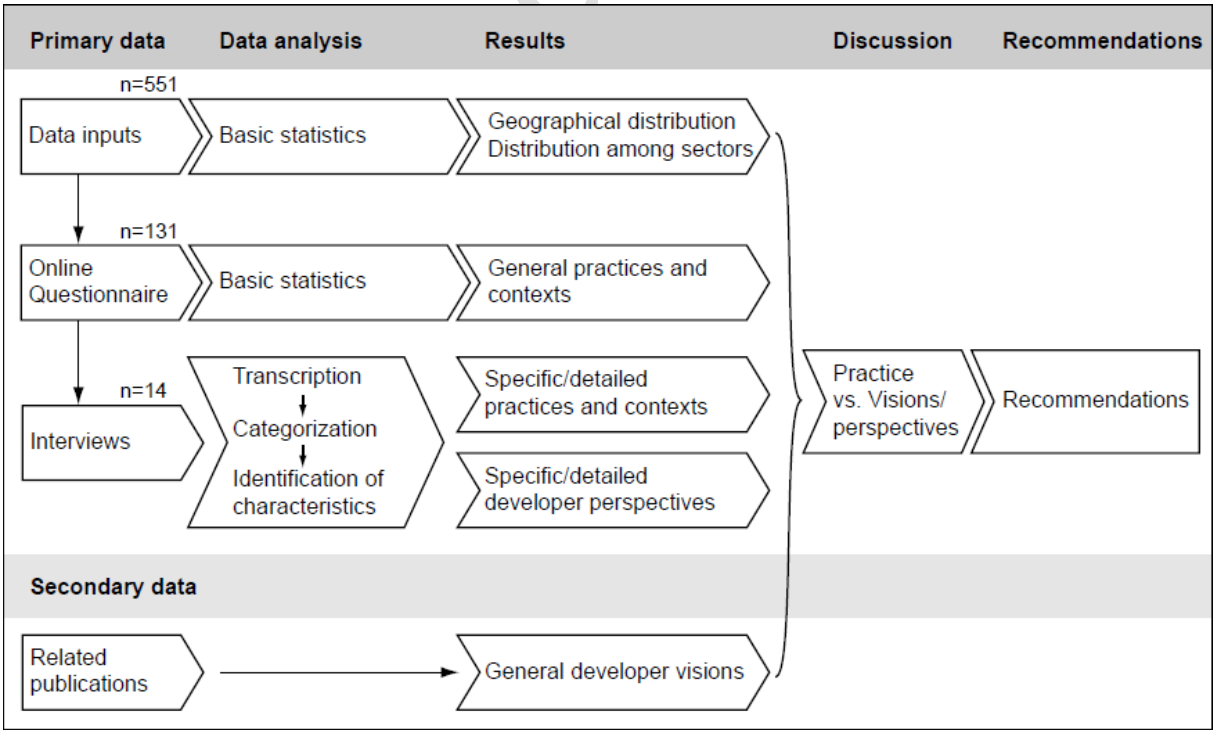

Figure 7

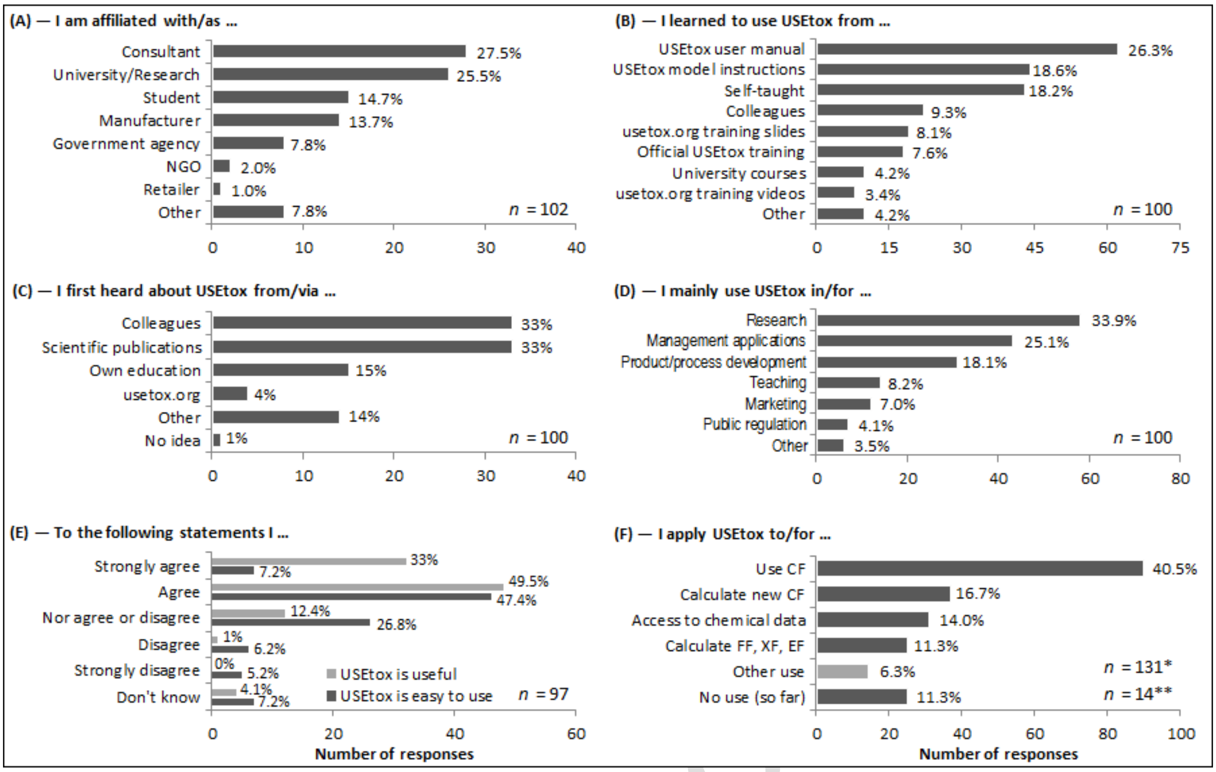

Figure 8