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

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14

15 **Abstract**

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

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

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

37 *Conclusions and recommendations* We demonstrate that understanding interactions
38 between USEtox and its users helps guiding model development and dissemination. USEtox-
39 specific recommendations are to (1) respect the application context for different user types,
40 (2) provide detailed guidance for interpreting model and factors, (3) facilitate consistent

41 integration into LCA software and methods, (4) improve update/testing procedures, (5)
42 strengthen communication between developers and users, and (6) extend model scope. By
43 generalizing our recommendations to guide scientific model development in a broader
44 context, we emphasize to acknowledge different levels of user expertise, to integrate sound
45 revision and update procedures, and to facilitate modularity, data import/export and
46 incorporation into relevant software and databases during model design and development. Our
47 fully documented approach can inspire performing similar surveys on other LCA-related tools
48 to consistently analyze user requirements and provide improvement recommendations based
49 on scientific user analysis methods.

50

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

53 **1 Introduction**

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

72

73 1.1 The story of USEtox

74 Between 1993 and 1999, several consensus building activities were conducted by the
75 SETAC¹ Impact Assessment working groups leading to the definition of a framework for
76 assessing fate, exposure and effects of life cycle emissions of toxic chemicals (Udo de Haes,
77 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>)

78 previous and parallel consensus building activities (e.g. Cowan et al., 1995; Fenner et al.,
79 2005), the OMNIITOX project was initiated (Carlson et al., 2004; Guinée et al., 2004;
80 Molander et al., 2004) to develop methods for assessing risks and impacts associated with
81 chemical emissions from product life cycles. The project served to develop a common
82 perception of the field of toxicity characterization modeling and to build the necessary trust in
83 working together in an efficient way towards harmonizing existing toxicity characterization
84 models. In 2003, the UNEP²/SETAC Life Cycle Initiative (LCI) therefore established a Task
85 Force on Toxic Impacts officially launched in Prague on 22-April-2004 to provide clear
86 guidance for assessing human toxicity, ecosystem toxicity, and related categories with direct
87 effects on human and ecosystem health. This task force was largely based on joined forces
88 between members of the previous efforts and identified that existing toxicity assessment
89 models only covered a limited number of substances and that scope, principles and
90 characterization results varied substantially (Dreyer et al., 2003; Pant et al., 2004), entailing
91 that many LCA practitioners ignored toxicity-related impacts in their life cycle impact
92 assessment (LCIA) step (Hauschild, 2005). This led to a process towards developing a
93 scientific consensus model for the characterization of human toxicological and
94 ecotoxicological impacts of chemical emissions (Figure 1), starting from four expert review
95 and framing workshops held between 2003 and 2010 (Aboussouan et al., 2004; Jolliet et al.,
96 2006; McKone et al., 2006; Diamond et al., 2010) and three model comparison workshops
97 organized in 2006 (Hauschild, 2006b, a; Hauschild et al., 2006). In these workshops, models
98 were compared based on investigating a test set of chemicals representing a specific
99 combination of substance properties and identifying those processes and factors influencing at
100 least some chemical groups. This process was oriented in and operated from the state-of-the-
101 art in various fate, exposure and effect modelling communities, the input of which was
102 gathered through the expert workshops. Result was the development and implementation of

² United Nations Environment Programme (<http://unep.org>)

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

116

117 <Figure 1>

118

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

128 provides the scope of this study, while further improvement and dissemination activities are
129 summarized in Figure 1.

130

131 1.2 Assessing user requirements to facilitate further improvements

132 To assess USEtox user perspectives and requirements and to identify different user
133 expectations, we employ state-of-the-art methods from the field of Science and Technology
134 Studies including Actor Network Theory and Requirement Engineering that focus on users'
135 interactions with science and technology (Sismondo, 2010). Thereby, a technological element
136 (here: USEtox) and human actors (here: users) are analyzed as mutually constituted in a
137 socio-technological network where they influence each other (Harty, 2010). Since humans
138 perceive technology differently and apply it in diverse, changing contexts, technology
139 developers can never fully anticipate the ideal product for all users during the development
140 process (Rohracher, 2003). However, assessing user perceptions and practices can help
141 generating priorities for technology development. Rohracher (2003) recommends managing
142 technology development as continuous interaction between developers and users. Actor
143 Network Theory and Requirement Engineering are further detailed elsewhere (Latour, 2007;
144 Nuseibeh and Easterbrook, 2007; Sismondo, 2010). These methods have already been applied
145 to assess socio-technological interactions of different software tools (Harvey, 2001;
146 Takhteyev, 2009; Harty, 2010) and are suited to focus on the many relationships between a
147 restricted set of technology users with the actual technology (Harvey, 2001). However, to our
148 knowledge, such methods have not been applied to develop recommendations for
149 strengthening and improving the application of environmental assessment models, such as
150 USEtox. Aiming at analyzing and harmonizing USEtox user practice and requirements with
151 developer visions in accordance with state-of-the-art methods from stakeholder analysis and

152 technology development, we focus together with two USEtox developers³ on three objectives:
153 (1) To apply selected data collection methods. This helps to understand on the one hand the
154 developers' original vision behind building USEtox. On the other hand, this helps to
155 understand the aims and practical experiences of users applying USEtox model and factors.
156 (2) To categorize and evaluate collected data for identifying and characterizing the general
157 application trends of USEtox. Trends are then compared with the developers' original visions
158 and development perspectives. (3) To use requirements engineering methods for establishing
159 a set of specific recommendations to harmonize USEtox developer aims and user
160 requirements. We then generalize our recommendations in support of an improved
161 consideration of user requirements when developing and disseminating scientific modeling
162 tools more generally. Comparing expectations and experiences of users with developer
163 visions of applying USEtox will help to improve and extend the application of the
164 characterization of toxic impacts induced by chemical emissions in LCA and will further help
165 to guide future model development based on user requirements.

166

167 **2 Methods**

168 To investigate user requirements and the actor network relations around USEtox, we
169 applied a mixed-method design (Frechtling, 2010) including both qualitative and quantitative
170 data collection methods as shown in Figure 2. We combined four different starting points to
171 collect information about user practice and the developers' visions and perspectives of
172 developing USEtox: (1) We analyzed basic statistics over users that have registered at
173 <http://usetox.org> and downloaded the USEtox model and databases. (2) We developed an
174 online questionnaire, which was disseminated via an LCA forum list and a list of email
175 addresses collected from users downloading USEtox. (3) We prepared a set of additional,
176 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.

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

185

186 <Figure 2>

187

188 2.1 Data inputs and questionnaire for assessing general user practice

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

195 An online questionnaire was designed using the online survey service
196 <http://obsurvey.com>. Combining the list of users of the USEtox website with the list of about
197 2500 individuals⁴ registered at the LCA forum (<http://pre.nl>), an invitation was sent to more
198 than 3000 potential respondents. The survey scheme was made accessible for 24 days in
199 November 2011. During this period, 131 responses were received. The questionnaire was
200 developed to get more detailed and quantitative information regarding the usage of USEtox,
201 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.

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

214 215 2.2 Detailed interviews of users and developers

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

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

237

238 2.3 Assessing developer visions and user requirements

239 Interviews with USEtox developers about the consensus building process and the visions
240 behind developing the model were complemented with the review of scientific publications
241 related to the development of USEtox. Expert review and model comparison workshop
242 reports (Aboussouan et al., 2004; Hauschild, 2006b, a; Hauschild et al., 2006; Jolliet et al.,
243 2006; McKone et al., 2006; Diamond et al., 2010) along with the two framing USEtox peer-
244 reviewed publications (Hauschild et al., 2008; Rosenbaum et al., 2008) were analyzed.

245 To identify requirements of USEtox users, we iteratively applied and combined different
246 Requirement Engineering methods. Questionnaire and interview results were analyzed and
247 structured into user requests about missing features regarding model structure and functions,
248 and qualitative attributes regarding user requests about model usability, maintainability and
249 interoperability (Sommerville, 2011). Function tree diagrams were applied as a structural way
250 to identify recommendations based on the requested features and quality attributes (Cross,
251 2008). System context diagrams were applied to get an overview of present contexts in which
252 USEtox is applied in order to help identifying potential user interaction improvements

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

260

261 **3 Results and Discussion**

262 3.1 Developer visions and perspectives

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

278 From interviews with four of the USEtox developers, we derived more individual
279 developer perspectives on the original vision. The interviews revealed that not all developers
280 have the same perception of the overall vision in its details. Different ideas were expressed of
281 what is supposed to make the model transparent for the user. For some developers
282 transparency is clearly related to usability and that users with different levels of expertise and
283 experience are able to apply model and factors. In contrast to that, for one developer
284 transparency is related to visibility of numbers and equations in the model to allow users to
285 understand the modeling principles. This originates in different opinions about the level of
286 user expertise. While one developer expressed that he was satisfied with the complexity of
287 USEtox and that he would not encourage users without profound knowledge in environmental
288 chemistry to apply the model, other developers want the model to be as widely applicable to
289 users with different levels of expertise as possible. This would include users that only want to
290 use the model results without fully understanding the model in its complexity. However, all
291 developers agreed that there is a limit to how easy it can be made to calculate characterization
292 results, for which at least a basic understanding of chemicals and toxicity is required.
293 According to one developer, guidance should ideally be available via an interface that helps
294 identifying required data input and guides through the essential calculation steps. However,
295 such interface had not been developed, since having an intuitive user interface was not the
296 first priority upon implementing USEtox. The developer interviews also revealed that despite
297 the intent to simplify the inclusion of toxicity-related impacts into LCA, it was unforeseen
298 that USEtox became as widely spread geographically and among different users across
299 various sectors as we can see it today with about 200 and 325 citations of the USEtox
300 development publications at <http://scopus.com> and <http://scholar.google.com>, respectively
301 (the latter representing also non-peer reviewed literature including books, reports and
302 presentations), as of June 2014. It was further mentioned that USEtox becomes increasingly
303 applied and recognized also at the regulatory level, e.g. in France, where USEtox is

304 considered the model of choice for ecotoxicity product labelling for the “Grenelle” legislation
305 (Van Hoof et al., 2011), or in the United States, where USEtox is evaluated by the U.S.
306 Environmental Protection Agency for exposure-based chemical prioritization (Wambaugh et
307 al., 2013). The developers’ reflections about the use of USEtox must be seen in the context
308 that originally, the USEtox model was foreseen to be primarily applied by the developers
309 themselves and to provide only a list of pre-calculated characterization factors to the user
310 community. However, in the end of the initial USEtox development process it was perceived
311 more appropriate to also allow users to calculate their own factors e.g. for chemicals that are
312 currently not covered in USEtox, thereby also providing the full model.

313

314 3.2 User application practice and perspective

315 Among the 551 users registered at the USEtox website, a wide range of sectors was
316 covered including academia (49%) and non-academic research institutes (6.5%), consultancy
317 (18%), enterprises (12%), regulatory bodies (9%), associations (2.4%), private persons
318 (1.5%), and non-governmental organizations (NGO). The remaining 1.6% of users did not
319 state their sector affiliation. Geographically, users were from Europe (57%, where France and
320 Denmark alone account for almost half of all European users), North America (33%, mainly
321 USA), Asia (5%), South and Central America (2.4% each), and finally Australia (1.3%) and
322 Africa (0.7%). The 131 users responding to the online questionnaire were found to cover all
323 listed sectors (see

324

325

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

329

330

331 Figure 3.

332

333 <Figure 3>

334

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

338

339

340 Figure 3A). This is in line with

341

342

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

352

353

354 Figure 3C). In interviews, it was also stated that its status in the French regulation gave
355 inspiration for using USEtox. Most users learned to use model and factors via the user manual
356 (Huijbregts et al., 2010) and the instructions directly provided in the model file (
357
358
359 Figure 3B). However, several users asked for a more intuitive user interface, supported by
360 some interviews detailing that the manual is difficult to understand and to apply as guide
361 through the modeling steps. This is consistent with the fact that almost 50% of users do not
362 particularly agree that “USEtox is easy to use” (
363
364
365 Figure 3E) and some users even used the interviews as opportunity to ask questions around
366 how to apply the model. However, the majority of users found that “USEtox is useful” (
367
368
369 Figure 3E) and explained in interviews that particularly the scientific foundation was
370 appreciated. Almost 50% of users reported to only apply USEtox characterization factors and
371 17% to access chemical data (
372
373
374 Figure 3F), for which the substance data and results databases are sufficient. About 14% of
375 users indicated not to directly use either model or results, but e.g. included USEtox as
376 reference or list of available toxicity models or in their teaching. Other users access USEtox
377 characterization factors via LCA software, which is especially preferred by unexperienced
378 users as stated in interviews, but also by more experienced users, due to the direct use in LCA
379 studies. However, various users directly apply USEtox for either calculating interim factors

380 for fate, exposure and/or effects (14%) or for calculating characterization factors (20%) for
381 new chemicals not yet covered in USEtox (
382
383
384 Figure 3F). These users need to understand and apply the model itself. Interviews uncovered
385 that some users experienced problems because USEtox results are not integrated in all LCIA
386 methods. This has implications in the form of inconsistent substance coverage in the case of
387 LCAs including chemicals found in other models than USEtox. Along with that, it was stated
388 to be problematic especially for non-experts how to correlate or compare USEtox results with
389 results from other LCIA models for toxicological impacts that were e.g. used before USEtox
390 was available. Finally, some users indicated via their interviews that they had problems with
391 implementing USEtox results into LCA software, thereby missing a way to automatically
392 update the software whenever they calculated new characterization factors.

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

396

397 <Table 1>

398

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

406

407 3.3 Comparison of developer visions with user requirements

408 The overall vision that methods and factors to characterize human toxicological and
409 ecotoxicological impacts in LCIA should become globally available has been achieved within
410 the first years after publishing USEtox. Users apply model and factors in several contexts,
411 sectors and regions, partly because of its consensus status (see also

412

413

414 Figure 3). However, the vision to be more transparent and better documented than existing
415 tools to increase practicability and usability has only partly been achieved as shown from user
416 experiences and expectations in the previous section. As an input for potentially improving
417 the usability of USEtox, we therefore conducted a more detailed analysis of user
418 requirements. Figure 4 illustrates how function tree diagrams, system context diagrams and
419 activity diagrams were iteratively applied to structure usability-related user requirements
420 based on the data from the questionnaire and interviews with users.

421

422 <Figure 4>

423

424 In a function tree diagram (Figure 4A) we propose possibilities to improve the graphical
425 user interface (GUI) of USEtox towards a more intuitive and transparent application and give
426 examples of the level of increasing applicability, such as to adapt the GUI until a specific user
427 has gained a certain level of expertise to apply model and factors without any manual. This
428 can be achieved via a step-wise GUI guidance system that is accompanied with hints of where
429 to e.g. find and insert relevant input data. Combining requirements of different user types
430 (Table 1) with the contexts in which users apply USEtox yields a specific set of
431 interconnected sub-systems illustrated in the system context diagram (Figure 4B). Users

432 typically interact manually (denoted “M”) with the front end sub-system for inserting user
433 input and reading model output, whereas other sub-systems like model equations describing
434 specific fate processes are usually of less importance for direct user access. A detailed
435 proposal of an improved procedure of users interacting with different USEtox sub-systems is
436 presented in the activity diagram (Figure 4C). Starting with searching for a specific chemical
437 of interest, this diagram guides the user through the different steps until the desired result (e.g.
438 a set of characterization factors, CFs) is reached, thereby passing various sub-systems.
439 Missing data and extrapolations between data are also included as requiring further guidance.

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

443

444 **4 Recommendations**

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

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

- 457 2) More specifically for basic users (see Table 1) a model user interface should be provided
458 as detailed guidance system allowing to follow different calculation steps and other
459 actions step-by-step including interpretation of intermediate and final results,
460 implementation of new substances, customization of implemented substances and
461 landscape data (see Figure 4C). This would help to improve the acceptability of toxicity
462 assessment with USEtox among affected users. Furthermore, USEtox results should be
463 consistently incorporated in all relevant LCA software systems.
- 464 3) More specifically for LCA software developers and instructors (see Table 1) additional
465 guidance and communication options should be provided by the USEtox developers to
466 simplify the interpretation and manual or automatized implementation of final results (i.e.
467 characterization factors) into LCA software tools and LCIA methods.
- 468 4) It should be clear and transparent how users can contribute to improving (updating
469 implemented data upon the availability of e.g. improved substance data), correcting
470 (finding bugs in the technical functionality, errors in data and/or equations), and further
471 developing USEtox by for example extending substance coverage and/or model scope.
472 Any update, however, should be in line with the consensus status of model and factors.
- 473 5) In support of further improving and further developing USEtox, a clear user
474 communication and information strategy needs to be established by the USEtox
475 developers. More specifically, dedicated user meetings and forums allowing for direct
476 contact between users and developers should be established to improve user feedback
477 possibilities that can be considered in future development steps.
- 478 6) The scope of USEtox in terms of substance, compartment, exposure pathway and effect
479 coverage and disaggregation should be increased to facilitate an extended application of
480 model and factors in LCA studies. However, all additional aspects should be
481 implemented in accordance with the consensus building quality criteria detailed in
482 (Hauschild et al., 2008; Rosenbaum et al., 2008).

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

488 1) As part of developing scope and context of a model, developers should familiarize
489 themselves through different types of dialogues with the backgrounds, levels of detail
490 regarding scientific knowledge and technical know-how, and application fields of all
491 actors they imagine as potential users. This can be facilitated by applying Actor Network
492 Theory methods. Requirement Engineering methods can then be used to define
493 appropriate user interfaces along with required guidance and documentation material (see
494 (Figure 4), thereby improving interpretability and applicability aspects and model
495 integrity and reliability from the user perspective. This is relevant for all types of model
496 development, including the development of software-based models as defined by van
497 Vliet (2008).

498 2) Depending on the desired accessibility, dissemination and application context of a
499 scientific model, a clear, transparent, and logical revision and update procedure should be
500 an inherent part of the model design. Users as well as developers will benefit from this
501 strategy as on the one hand maintainability and testability will be increased, while on the
502 other hand strengthening the flexibility regarding different user types and application
503 scopes. This is mainly related to revision of software-based models (van Vliet, 2008).

504 3) Along with underlying scientific robustness and correctness, it is recommended to
505 integrate the technological context of a scientific model into the design and development
506 phases. Aspects of re-usability based on a modular model structure, interoperability and
507 portability between different software and operating systems, and finally technological
508 interface design for incorporating parts of a model or its results into relevant software or

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

511

512 **5 Conclusions and Outlook**

513 Our experiences from the detailed and complex analyses of user expectations and
514 experiences with USEtox and the further development of USEtox based on these analyses
515 show that understanding the interactions of users with and requirements on a scientific model
516 and the comparison with the developers' visions about users and model application can guide
517 the further development process. The variety of user types with their differences in specific
518 expertise and application contexts plays a significant role in designing model guidance
519 material. While some of our recommendations might seem intuitive, we provide a consistent
520 and formal analysis of the relationships between user expectations, developer visions and tool
521 applicability. Thereby, we ensure that no important relationships are ignored even though they
522 are not intuitive. This is in line with the rationale of using LCA as comprehensive scientific
523 method yielding results that might in some cases also be intuitive, while in other cases
524 revealing rather unexpected conclusions (e.g. Quantis, 2011). A limitation of our study is the
525 restricted number of surveyed and interviewed users, where additional users with their
526 specific requirements and practices might provide additional insight into existing applicability
527 and usability issues and constraints, expectations and experiences. On the other hand, the
528 respondents offered a reasonable coverage of the different known user types, sectors and
529 geographical regions. The consensus status of USEtox is generally much appreciated by
530 interviewed users, whereas some of the consensus-building criteria, such as well-documented
531 model and factors, are still not met. We conclude from the results of our analysis of the
532 restricted set of USEtox users that usability aspects are as important as scientific correctness
533 to build trust among users and to facilitate a broad and meaningful application of model and
534 factors. While a more transparent communication strategy with the user community is still

535 desirable including a clear time plan for future updates and releases, current improvement
536 efforts have already lead to features that were requested by surveyed users. These efforts
537 include the implementation of a user forum with regular input by the USEtox team and a
538 frequently asked questions (FAQ) page (part of the re-designed USEtox website), regular
539 USEtox Community of Users meetings at international conferences, and a form and procedure
540 to propose and adopt improvements or updates of model and/or factors (see <http://usetox.org>).
541 The development of a USEtox user interface wizard that will provide guidance regarding
542 model calculation steps and implementation/customization of substances is in progress as this
543 was requested by various users. Furthermore, USEtox-based characterization factors are
544 implemented in several LCIA methods including IMPACT World+ (Bulle et al., 2012),
545 TRACI 2.0 (Bare, 2011), CML-IA (Guinée et al., 2002), and recommended in the ILCD
546 handbook (European Commission, 2011), whereas ReCiPe (Goedkoop et al., 2009), LIME2
547 (Itsubo and Inaba, 2012) and the earlier methods EDIP2003 (Hauschild and Potting, 2005)
548 and CML2002 (Guinée et al., 2002) rely on other models for toxicological impacts (of which
549 CML2002 also proposes USEtox factors as a user choice). Since May 2013, USEtox is
550 officially endorsed by the UNEP/SETAC Life Cycle Initiative (ILCB, 2013). It remains to be
551 seen how the new USEtox features will contribute to further improving the consideration of
552 toxicity-related impacts in LCA. Overall, scientific model design and development processes
553 can greatly benefit from a close and continuous interaction between developers and users. The
554 thorough documentation of the survey and how it was performed in order to document how
555 the results were obtained will possibly inspire readers with aspirations of performing similar
556 surveys on other LCA-related tools.

557

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564 confidentially.

565

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742 **Figures and Tables captions**

743

744 Table 1

745 Identified USEtox user types and their characteristics.

746

747 Figure 1

748 USEtox development timeline including consensus building process between 2003 and 2010
749 and current improvement and dissemination activities after 2010. ^aJolliet et al. (2006);

750 ^bAboussouan et al. (2004); ^cMcKone et al. (2006); ^dGuinée and Hauschild (2005); ^eHauschild
751 et al. (2006); ^fHauschild (2006b); ^gHauschild (2006a); ^hDiamond et al. (2010); ⁱHauschild et
752 al. (2008), Rosenbaum et al. (2008); ^jOscarson and Hauschild (2010); ^kHenderson et al.
753 (2011), Rosenbaum et al. (2011); ^lHauschild et al. (2011); ^mThis study, ⁿILCB (2013);

754 ^oOMNIITOX project (EU FP5 contract: G1RD-CT-2001-00501), Carlson et al. (2004),
755 Molander et al. (2004); ^pUSEtoxPI project (LRI-ACC contract: MTH1001-01), Jolliet and
756 McKone (2012), Mitchell et al. (2013); ^qTOX-TRAIN project (EU FP7 contract: IAPP-GA-
757 2011-285286, Bengoa et al. (2014); ^rExpoDat project initiated by LRI-ACC ExpoDat2012
758 workshop, American Chemical Council (2012); ^sQUAN-TOX project (EU FP7 contract:
759 PCIG14-GA-2013-631910).

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761 Figure 2

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

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768 Figure 3

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

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773 Figure 4

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

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User type	User type characteristics
Basic user	<ul style="list-style-type: none"> - 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	<ul style="list-style-type: none"> - 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	<ul style="list-style-type: none"> - 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	<ul style="list-style-type: none"> - 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	<ul style="list-style-type: none"> - 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

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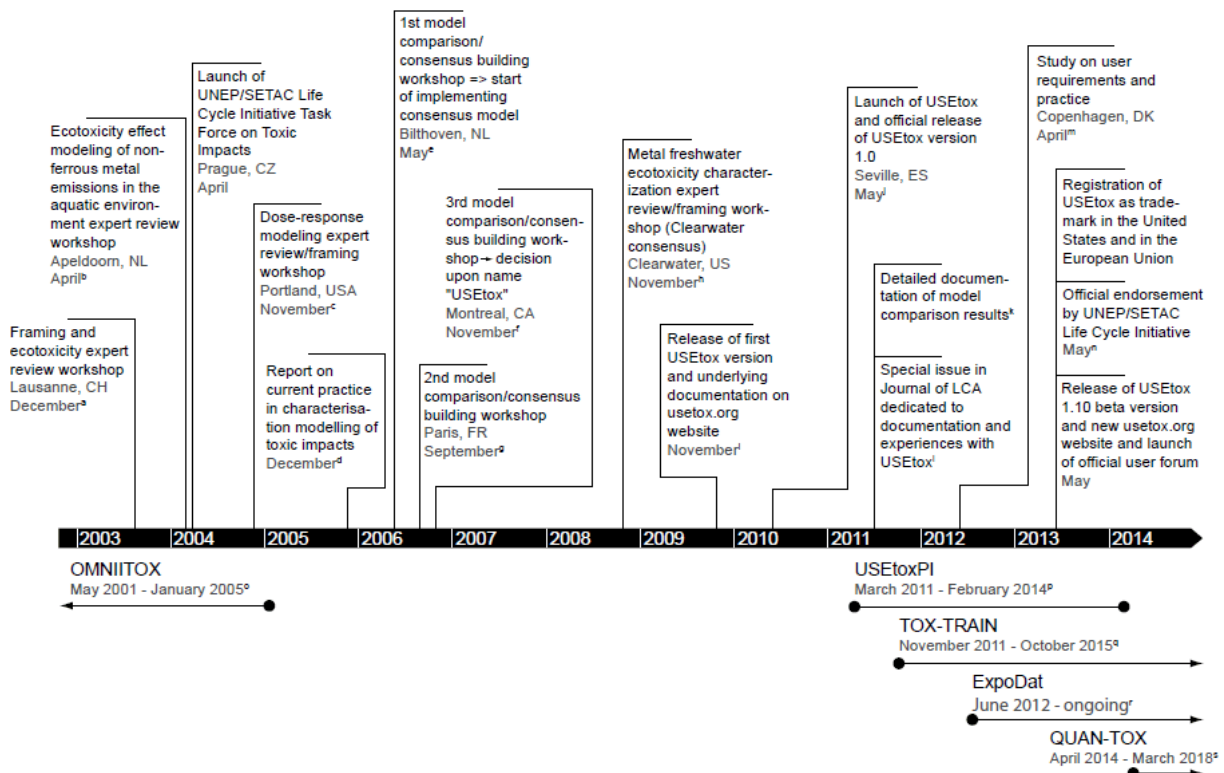
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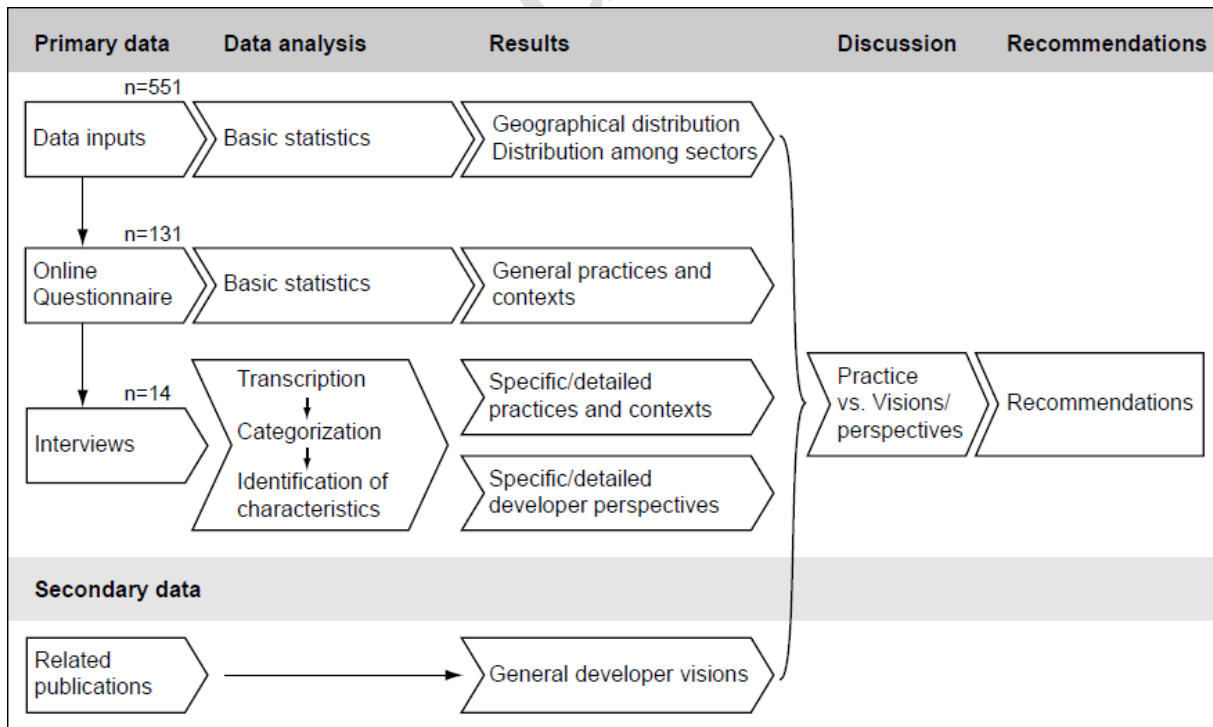
802 Figure 5



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805 Figure 6

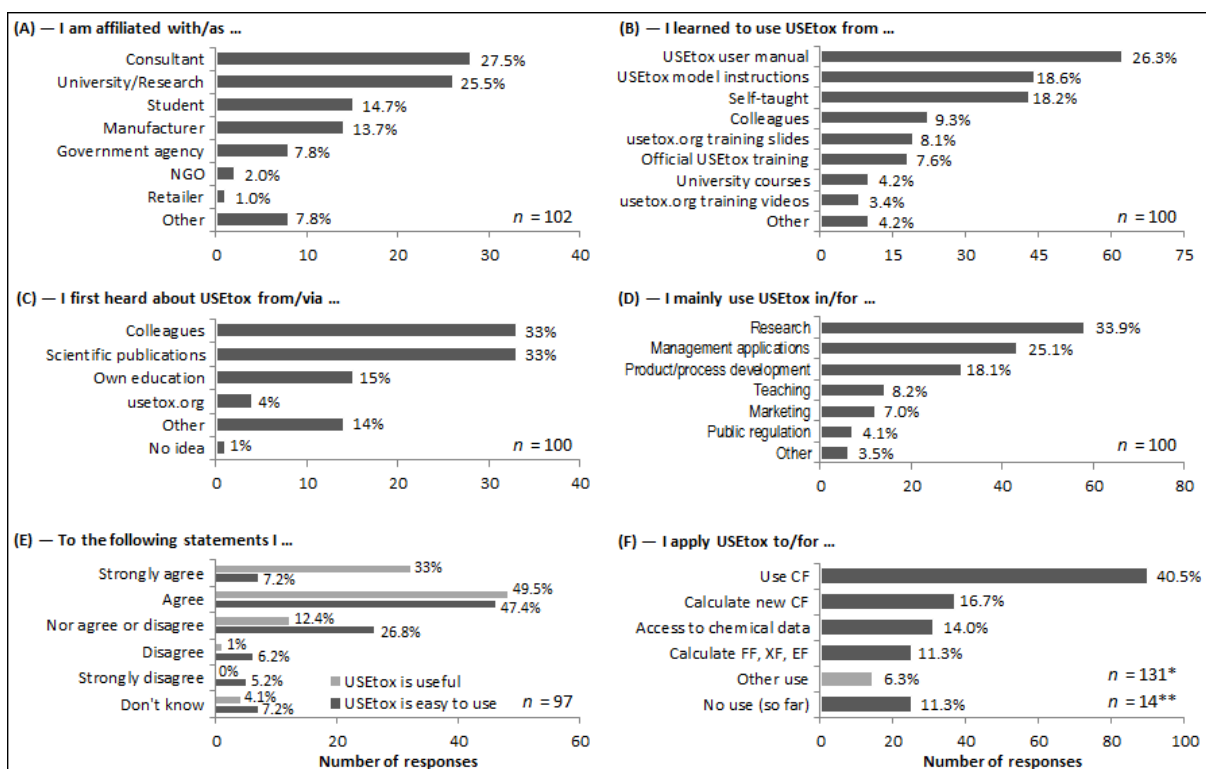


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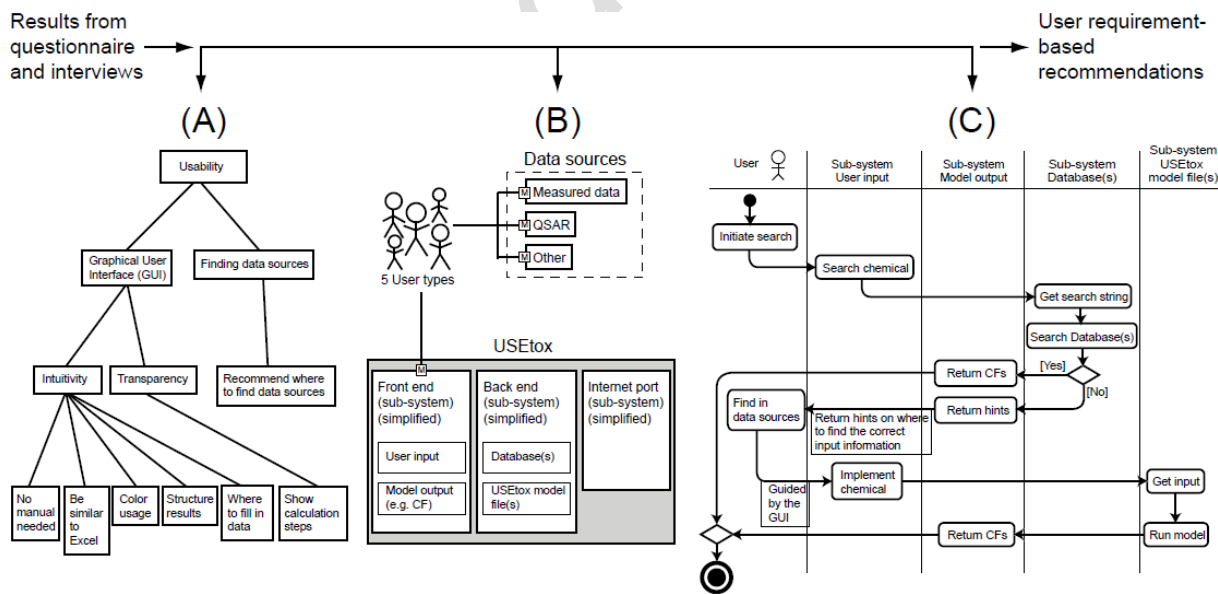
809 Figure 7



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812 Figure 8



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