Simplifying an application for LCIA by conducting a usability study

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Abstract— This paper describes the methodological background which enables calculation of environmental impact indicators for chemicals without knowledge on their production processes. Subsequently, it is described how these can be calculated in batch mode in order to set up a database containing a large number of chemicals. The project included a usability study. The approach of this study and how it enhanced the overall project outcome is presented.

Keywords— LCA; data gaps; chemicals; usability

I. INTRODUCTION

Data gaps are unavoidable when a complex Life Cycle Assessment (LCA) is conducted. Within the project 'StUChem', a web based database was developed to provide calculated Life Cycle Inventory (LCI) and Life Cycle Impact Assessment (LCIA) indicators for large numbers of chemicals.

The aim of the project was to enable a broad target group to use the results which were achieved when the so-called FineChem-Tool [1] was developed for environmental impact assessment of chemicals based on their molecular structure. Consequently the project was set up including a usability study to ensure user-friendliness of the developed website.

II. METHODS

A. *Approaches to meet data gaps in LCAs*

Life Cycle Inventory (LCI) databases (as for example [2]) are commonly used in LCAs to identify the background and thus to set the system boundaries. Though, depending on the subject studied, the availability of data is not always sufficient and especially scarce for chemicals.

While several approaches have been developed to meet data gaps these are mostly connected to high uncertainty while still demanding considerable effort.

Wernet et al. [3] showed that Life Cycle Impact Assessment (LCIA) indicators for chemical compounds, which normally are calculated from a complex material flow network model, can be estimated using Artificial Neural Networks. The Neural Networks were trained to calculate Global Warming Potential (GWP), Cumulated Energy Demand (CED) and Ecoindicator 99 from a set of molecular descriptors without requiring knowledge about the production process. The results were made freely available as 'FineChem Tool' [1]

B. *Use of the FineChem Method*

Despite the possibilities to close data gaps by the FineChem method, it did not achieve wide distribution. We assume that this is partly due to the fact that the method asks for molecular descriptors requiring users to have training in chemistry. To our knowledge, work about the FineChem Tool was presented at LCA XIV [4]. Wernet et al. [5] presented an approach to use calculated values for priority-setting. Throughout the course of the project, some interested parties were supplied with calculated LCI(A) values. To our knowledge, no further LCAs using calculated LCIA values of chemicals have been published.

The FineChem approach provides a powerful tool to close data gaps. LCIA data can be estimated quickly and without knowledge on the production process. By automated evaluation of molecular descriptors and thus enabling bulk handling of molecules, this approach was made available for a considerably broader target group. Non-experts on the chemical field are now able to use this approach.

C. *Developing the database EstiMol*

As the project aimed at enhancing the accessibility of the FineChem approach, the evaluation of the required molecular descriptors was automated. SMiles ARbitrary Target Specification (SMARTS) was identified as a suitable language to count the different functional groups. A Python Script was used in order to enable bulk evaluation. In order to provide a large number of chemicals, [6] was chosen to provide the molecular structures that were used to set up a database for the project. Subsequently, the implemented methods were run on 40,000 molecules for which the indicator values were afterwards calculated using the FineChem-Tool.

For the user interface, the web tool EstiMol was developed. EstiMol features cradle-to-gate GWP, CED and EcoIndicator 99 for roughly 14.000 substances. The workflow starts with an introduction to the methodology of the FineChem-Tool. Users can search the database for chemicals

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by either name, trivial name, CAS (Chemical Abstracts Service) Number using a full text search. Furthermore molecular structures can be searched using the chemical editor Marvin [7]. It is integrated in the search page to enable the users to draw molecules. Search results are presented on the following page. For each chemical, the reason why it was found is indicated. By clicking on a substance, the result page is opened. Here, the calculated values, as well as name, CAS numbers and the molecular structure are shown. In the case of molecules not being valid for the FineChem methodology, this information is displayed and the reason is given. The website can be accessed via http://www.umberto.de/en/estimol/estimol-data/.

D. Usability Study

At the HTW Berlin, a series of usability studies have already been conducted in the past [8]. In another usability study in April 2014 it was tested if new users can use the frontend of the sustainability search engine for chemicals in an effective, efficient and satisfying way. The case study was performed using the eye tracking method. Particularly the following questions were supposed to be answered:

- Are the users able to find a given substance within 3 minutes?
- How intuitive is the usage of the drawing tool to find a molecule structure?
- How many of the users understand the results page and can name the environmental indicators to a given chemical?

1) Test Settings

To answer these questions, a set of seven tasks was prepared which was conducted by ten test persons. The test persons had basic knowledge of chemistry. The tasks aimed at obtaining different environmental indicators of chemicals by varied ways (full-text search, CAS Number, structure drawing tool).

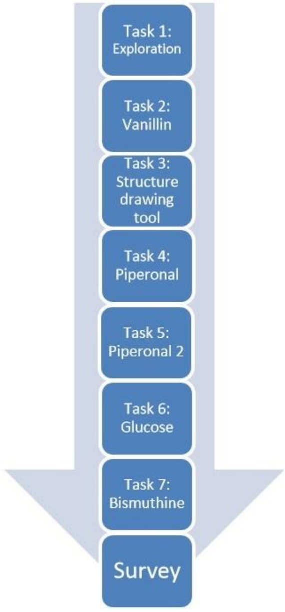

Figure 1: Task sequence of the study

Within these tasks the tool was analyzed according to the three quality attributes defined by [9]. The effectiveness shows the capability of producing a desired result. It is measured by the ratio of how many people completed or failed the tasks. After the task completion the success was evaluated within the categories "with ease", "with complications" and "failed". The target value obviously is that every task is passed with ease.

The efficiency shows how quickly users can work on the tasks. It was measured by the time spend to reach the given task goal. For each task a maximum time limit was specified in which the test person should have passed the task.

The satisfaction illustrates how pleasant it is to use the design of the application. It was covered by two questionnaires by use of the AttrakDiff survey of [10] during the study. It is an instrument to measure the hedonic and pragmatic quality of software in the form of semantic differentials. Besides that, the test persons had been motivated to bring in their thoughts using a think aloud protocol. Furthermore they were asked after the test to say three things which they like most and which they don't like (tops & flops).

III. RESULTS

Even though the tool was relatively small and the number of participants not representative, the usability studies discussed here, led to a series of improvements of the software. A catalog with over 50 items of possible enhancements was the main result of the evaluation. The most important information were gathered by the think aloud protocols and the tops and flops questionnaires. It was shown that the most possible enhancements were evaluated by the users while working on the tasks. Some eye-catching problems were found when analyzing the eye gazes and heat maps of the test persons as well, but generally it was shown that an eye tracking study is not always necessary to find the biggest problems which typical new users have with a software; just showing the tool

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to inexperienced users and asking them what they think helps a lot to see potential problems. Developers and designers of software often do not have the knowledge of the workflow of the users, but make assumptions about it. Also software testers are often not unreserved with a new software version and do not find the same problems that test users in an eye tracking study make obvious.

The whole search engine was overhauled with the findings of the study. Besides that the results of the AttrakDiff surveys were gathered. According to the author's experience, six to ten test persons are generally adequate to show big statistic effects. For statistic effects of small or medium size a larger number of participants would be necessary, but those effects are mostly not the focus of eye tracking studies due to the effort which has to be put into it. In that regard it is obvious that studies made at an early development stage have the benefit of already adding usability practices to the development. The software is still flexible enough to be changed in a short period of time. Therefore it grants the creation of an optimal user-oriented product.

By including a usability study in the project, the user-friendliness of the developed website could be tested and improved within the project. The study enabled the project team to learn about optimization potentials. The involved developers estimated the effort to adapt the website according to the items identified by the study. Afterwards, the items were prioritized in order to use the remaining time as efficiently as possible to improve the usability.

IV. Discussion

Especially for application-oriented projects, including thoughts on usability of the project results already in early phases of the project is a reasonable approach. Usability studies are a rather easy way to find out how to improve the user interface as hurdles are made visible and can be addressed before the release of the software. About 10% of a software project's budget should be spent for usability issues [11]. This increases the learnability, efficiency and the user's satisfaction.

In the end, project results can become more widely spread and used if usability has been taken into account.

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