Development of an LCA tool for the evaluation of environmental performances and eco-design of drinking water treatment plants

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Abstract The variability of water resources requires the development of specific technological solutions, hence the difficulty in getting a generic LCI of water treatment. An LCA tool is currently being developed, aiming to accurately assess the environmental and sanitary performances of drinking water treatment plants. The tool is based on an integrated technological-LCA modelling implemented in Umberto®. Detailed unit process modelling, using high parameterization, enables one to obtain a more specific, realistic and predictive LCI. Beyond performing a proper LCA, this tool will support process eco-design. Programmed in Python™, it is linked with external specialised software tools for specific calculations. A script for sensitivity analysis of the design parameters has been coded following the Morris method. Key parameters for environmental impacts can then be detected and tagged as priority action levers for the project under consideration.

1 Introduction

The water industry is more and more facing emerging problems (e.g. regional water scarcity or water quality deterioration). At the same time, increasing social awareness of environmental problems is expecting water industry to take into consideration environmental constraints and sustainability policies [1-3]. A big challenge is to bring the political class, the water industry managers and the scientific community together to discuss these problems. Another challenge is to develop technical tools and practical methodologies to provide decision-makers with clear information to support decision making processes. There is clearly a need to fill the gap between affirmed intentions and the means to apply them [4]. Except for a few recent examples [5-10], there is a lack of tools for assessing the environmental performances of industrial projects involving process engineering. The EVALEAU research project addresses these challenges, aiming at developing an assessment tool for both environmental and sanitary performances of drinking water treatment plants. The high process variability involved in water treatment is a major difficulty in establishing a generic Life Cycle Inventory (LCI), this is the rationale to develop a flexible modelling tool for LCI calculations of drinking water production.

The overall objective is to develop a tool able to consider any local situations, technical constraints and water sources. The flexibility of the tool is a key feature to come up against the context and the project's characteristics. Two approaches may be available within the tool. The first one is the calculation with real inventory data from an existing plant, as currently done by the existing LCA software tools. Specific technical improvements could then be studied. The second approach consists in the modelling of LCI for a future plant currently at the design stage or when studying different technological solutions. Model accuracy and strong reliability in the LCI modelling are crucial to convince decision-makers about the project's feasibility and the modelling realism. This is definitely a condition to perform eco-design at an industrial scale.

2 Means and methods

The working environment is based on the Umberto® software. Unit processes are modelled as input-output models and coded into Python™ scripts [11]. These scripts run the corresponding calculations and are located into the Umberto® module specifications. The modelling work was based on a bibliographic survey, scientific and industrial expertise. A module script contains a brief description of the unit process model and its parameters, bibliographical sources, comments about the modelling principles, assumptions and warnings. These models are stored into a module library which constitutes the bedrock of the tool. In order to carry out an LCA, background processes and Life Cycle Impact Assessment (LCIA) evaluation methods are imported from the Ecoinvent database. Umberto® has been selected for its ability to model complex industrial systems and for the possibility to do integrated scripting and numerical calculations.

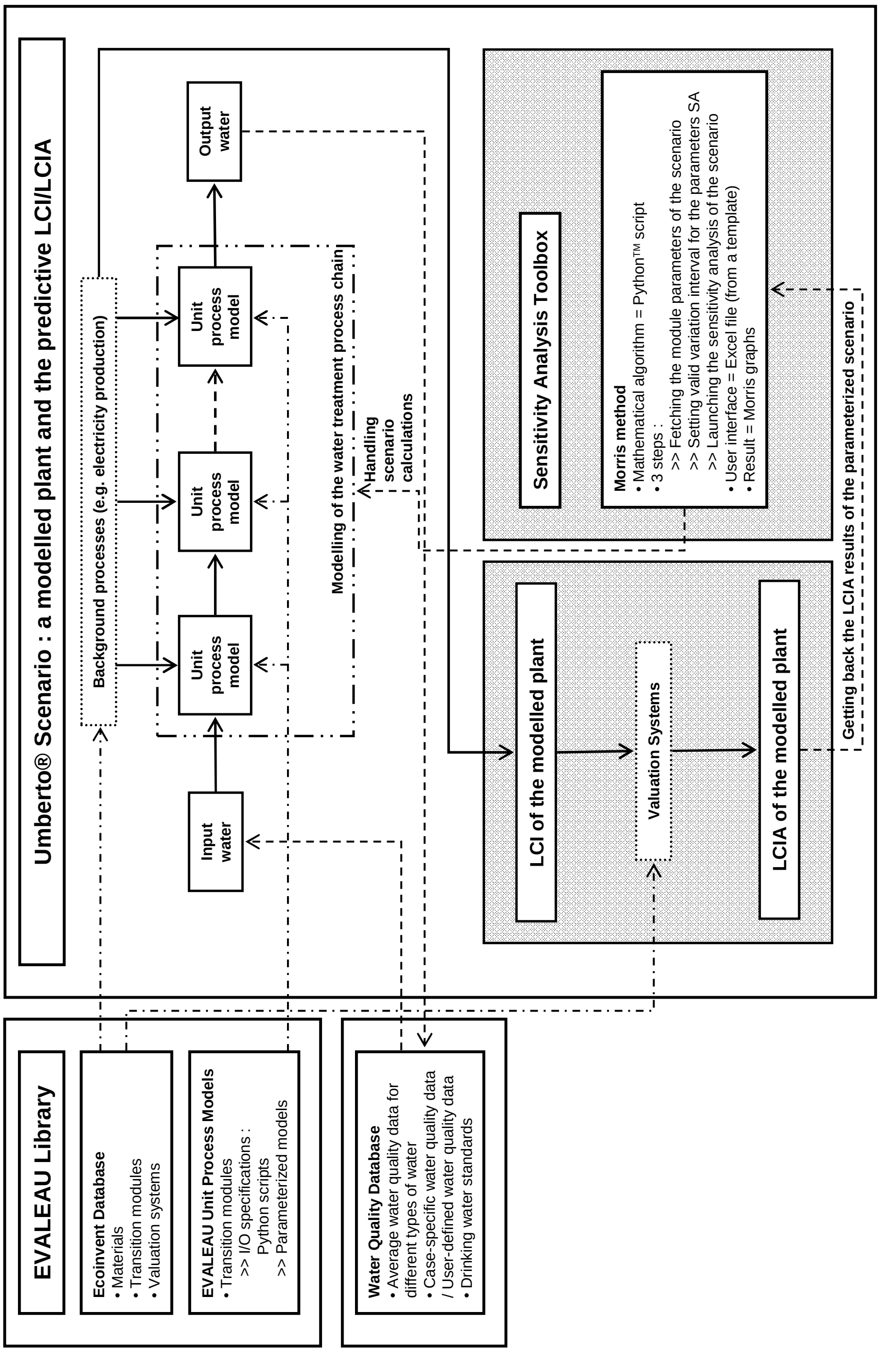

Fig.1: **Framework of the EVALEAU tool**

Python™ scripting provides the ideal framework for further developments of the tool. For instance, mathematical algorithms for parameter sensitivity analysis have been implemented. Object-oriented programming significantly enhances the current version of Umberto®. The framework of the tool is represented on Figure 1. Besides, depending on LCA expert's recommendations, the tool must be able to evolve. So, the computer framework is organized in a far-sighted way and special attention has been dedicated to writing good quality codes. It ensures that further developments of the tool (e.g. to include technological advances and complementary software features) could be achieved without excessive efforts.

3 Mathematical modelling of water treatment plants

3.1 System boundaries and functional unit

For all unit processes, it is assumed that the construction and the decommissioning phases are negligible. Only the operation phase is taken into account and modelled. Friedrich [12] and Raluy et al. [13] evaluated the environmental impact contribution of these phases. Both found that the decommissioning phase is negligible in comparison with the operation one (<1%). The construction phase shows a higher environmental impact, 15% in the first paper and about 5% in the latter. The result of Raluy et al. [13] is lower probably because only desalination technologies were studied. As a matter of fact these processes are much more energy-consuming than conventional treatments, i.e. they generate higher environmental impacts. However in order to test the assumption, the LCA of two drinking water treatment plants currently performed within the EVALEAU project includes the construction and the operation phases. Preliminary results showed that the environmental impacts of the construction phase represent about 10% of the total environmental impacts. As a result the modelling of the construction phase for predictive LCI is not a priority task by now and will be neglected.

The study has therefore focused on the drinking water treatment plant including only the operation phase. The functional unit is 1 m3 of potable water exiting the plant. Potable water distribution is not considered.

3.2 Adaptability of the modelling tool

A water treatment plant consists of a sequence of unit processes. Each unit process changes the water quality and consumes energy and/or chemicals (Fig.2). The water treatment plant will be a different sequence of unit processes depending on the raw water quality; this is why numerous unit processes are developed by the water treatment industry. The objective of these plants is to work on a raw material (i.e. source water) and to change it into a commercial product (i.e. drinking water).
The EVALEAU tool is based on an exhaustive library of computational models, each of them representing a unit process. By using this library the user can build any process chain (Fig.1) within the constraint of respecting the quality criteria of the final product, i.e. treated water must respect the regulatory standard.
Mueller et al. [5] developed a methodology which consists in generating the LCI from a parameterized LCI model. The approach is slightly different. The parameterized LCI model of the product is obtained using mathematical regression from initial inventory data of several manufacturers' products. Once the LCI model is established, the LCI of a product's manufacturing is proportional to its mass. The EVALEAU modules are deterministic models describing the process, i.e. energy and mass balance equations for design and functioning, using a set of physical and chemical parameters, thus enabling the parameterization of the respective LCI.
Next to the input water quality data, the parameters of the unit process models are the starting point for the calculations (Fig.2). But input water quality is a constraint depending on the context of the project, whereas unit process parameters are technical specifications. They correspond to engineering choices and they can be set to any realistic value that makes it possible to meet the project's requirements. The basic version of a unit process model (as imported from the library) uses default parameter values. Those default values come from literature or expert's recommendations. The parameters can be design parameters (e.g. water filtration speed), technical and legal constraints (e.g. disinfection requirements) or specific choices (e.g. pipe materials). This basic version can be seen as a generic one which corresponds to average working conditions of the unit process.

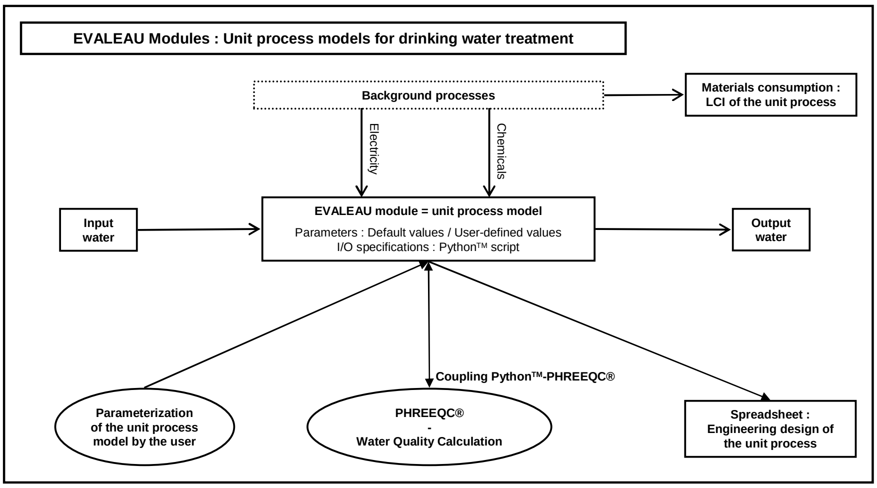

Fig.2: Diagram of the EVALEAU modules

Thanks to the modelling parameterization, the simulated project can stick better to the reality of the industrial project. The user has to make choices about the parameter values like an engineer would have to make technical choices during the plant's design, prior to its construction. Defining the parameter values enables the user to modify the generic version of the model and to get a very specific model, more representative of the case under study. The extensive parameterization of the unit process models leads to stronger capacity to adapt to specific situations, which is a key feature of the tool.

The most important challenge of such eco-design tool is the realism of the modelling results. Modelling flexibility has been boosted in order to fit any engineering design related to project constraints. The tool allows accurate design of the processes from raw water quality and user-defined parameters, thus simulating a process chain within any specific project context. Accurate calculations of matter and energy balances are sought in order to establish a predictive and reliable LCI of drinking water production, thus leading to a more robust eco-design tool.

4 Enhancement of the EVALEAU tool: linking to other software tools

4.1 Saving engineering design data into spreadsheets

Within a unit process model, engineering design data are calculated, such as the size of facilities or machine electrical power. They are not part of the LCI but they are fundamental for the eco-design of a future plant. As they are not useful for LCIA, they are not part of the Umberto® results but they are saved into Microsoft Excel® spreadsheets. One spreadsheet is automatically created for each unit model of the Umberto® scenario, i.e. one for each modelled process (Fig.2). By saving the modelling results for a process at the design stage, these spreadsheets are essential for the eco-design approach.

4.2 Running calculations with other software tools

There are some examples of LCI generated using specialised software which is specific of an industrial application [6-8]. But the generated LCI is often used by an LCA software in a second step requiring user intervention. Python™ scripting enables one to link directly and automatically the EVALEAU tool to other software tools. This feature enables the tool to run a complete LCA in one time, or even multiple LCA calculations (see paragraph 5.1).

The tool uses PHREEQC® [14], geochemical software, developed by the U.S. Geological Survey, widely used for water quality calculation and chemical reaction simulation in aqueous phase. Linking the tool to PHREEQC® has been a major step in its development since water quality can therefore be taken into account. In the context of drinking water production, the quality of the product (including the sanitary criteria) is central. In order to get modelling results good enough to be used in a project proposal, the water quality must be checked and validated as potable.

Resource water quality and drinking water quality required by standards are different in each project. The technological solutions necessary to reach project requirements are multiple as well. Then, in every process model, in addition to mass and energy balances, the water's composition change through the process itself is calculated using the software PHREEQC®. The water quality and the chemical consumptions are precisely calculated along the modelled process chain (Fig.2). This way it is possible to detect if the process chain produces a too low or too high water quality. Indeed, too high water quality should be avoided because of useless material consumptions. As it is essential to produce potable water, this feature of the tool is of the highest importance. The accurate determination of the chemical doses makes the resulting predictive LCI more reliable, which is also of the highest importance.

Python™ scripting gives many opportunities to the programmers. As the tool has been linked to the software PHREEQC®, it could be linked to any software dedicated to a particular industrial sector or to a specific application. This will provide the LCA tool with benefits from previous research and modelling efforts, and makes it more reliable.

5 Sensitivity analysis of the model parameters

Sensitivity analysis aims to identify the model parameters which have a significant influence on the results. Different mathematical methods for sensitivity analysis are already applied in the literature. These methods can lead to a better understanding of the industrial reality assuming that the model is realistic enough.

5.1 The Morris method

The principle of the Morris method is to run several model calculations while randomly changing just one parameter value at a time [15]. The objective is to determine qualitatively which parameters have an influence on the model results and the kind of influence (linear or not, interaction with another parameter). Key parameters are then identified.

Foremost, parameter variation intervals must be set in order to avoid incoherent results (e.g. negative energy efficiency). The variations of the modelling results, due to the variation of one parameter at a time, are called "elementary effects" and the sensitivity analysis is based on their calculation. For each parameter, the mean and the variance of its elementary effects are calculated. An influent parameter will have an elementary effect mean that is high. If the variance is high, the signification is that the elementary effects are variable. In this case, the influence of the parameter on the model result is non-linear and/or the parameter has interactions with another one. Finally, the Morris graph sums up all this information: the mean of the elementary effects is represented on the abscissa and the variance on the ordinate. Each parameter of the model is then represented by one point, according to its elementary effects mean and variance. The more a point is on the right of the graph, the more the corresponding parameter has a strong influence on the model. The more a point is up on the graph, the more the influence of the parameter is a non-linear one. The interpretation of the Morris graph is straightforward and that is what makes the method easy to understand.

The Morris method is related to only one result (e.g. a selected environmental impact). But it could be made in parallel for different results in case the LCA model gives many results (e.g. different impact categories). So, for each selected result of the model, a Morris graph will be generated by the tool. Performing a sensitivity analysis on a modelled plant makes it possible to identify the most influencing operation parameters and to prioritize the action levers.

At the current stage of development of the EVALEAU tool, only a Morris method algorithm has been coded. Even if variance-based approaches are more accurate (e.g. E-FAST and Sobol methods), the Morris method offers a good overview of key parameters of a model at a lower computational cost [16-17]. But, if the sensitivity analysis appears to be useful and if the tool needs to use further mathematical methods, the LCA tool could also be linked to SimLab, a free development framework for sensitivity and uncertainty analysis [18]. As for the connection with PHREEQC®, the tool could benefit from previous research and development efforts made by the sensitivity analysis expert community.

5.2 A case study

A sensitivity analysis was carried out on a modelled water treatment plant. The unit processes come in the following order: [coagulation-flocculation] / [sedimentation] / [rapid sand filtration] / [rapid GAC filtration] / [chlorination] / [neutralisation]. This sequence of processes is representative of conventional drinking water treatment. Sludge treatment has not been modelled yet (work is in progress). Water quality data come from the database developed during the project with the industrial partner (i.e. Suez Environnement) and are representative of an average river.

Parameter variation intervals are calculated by applying a +/-25% ratio on the default values and avoiding incoherent boundaries when necessary. 77 parameters are part of the parameter sensitivity analysis, and 6 are excluded because of inconsistencies. For instance, the treated water flow exiting the plant is considered as a project requirement that must be respected when designing the plant. Changing its value to observe its influence on the LCA modelling results does not make sense. So, it has been excluded from the study. The valuation method chosen for this example is "Impact2002+, EndPoint (H,A)". This method gives 4 results (climate change, ecosystem quality, human health and resources) and the Morris method is applied to each. 4 Morris graphs have been generated from the sensitivity analysis, but only the result concerning the impact category "Resources" is presented here. Other model results show similar graph aspect.

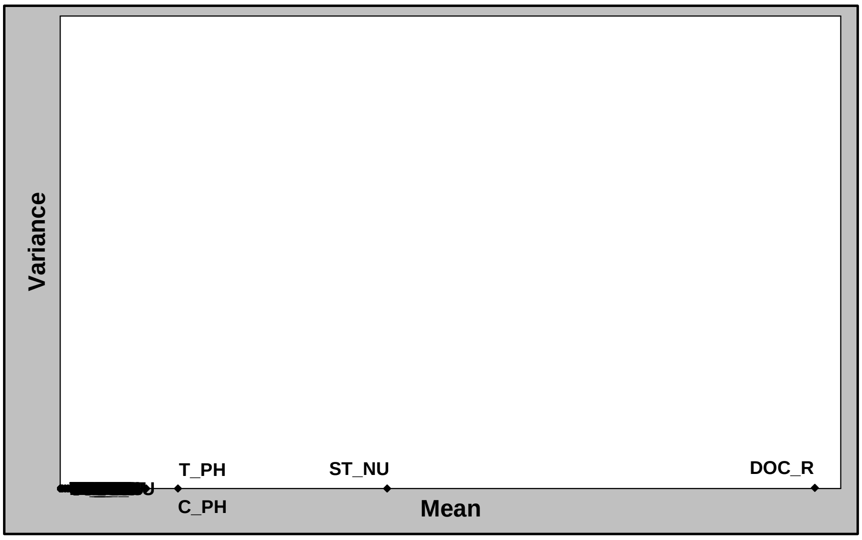

Fig.3: Morris graph for the result "Resources"

The Morris graph (Fig.3) shows that only 4 parameters have a significant influence on the results compared to the others. But all of them have a quite linear influence. A bar graph (Fig.4) represents only the mean of the elementary effects.

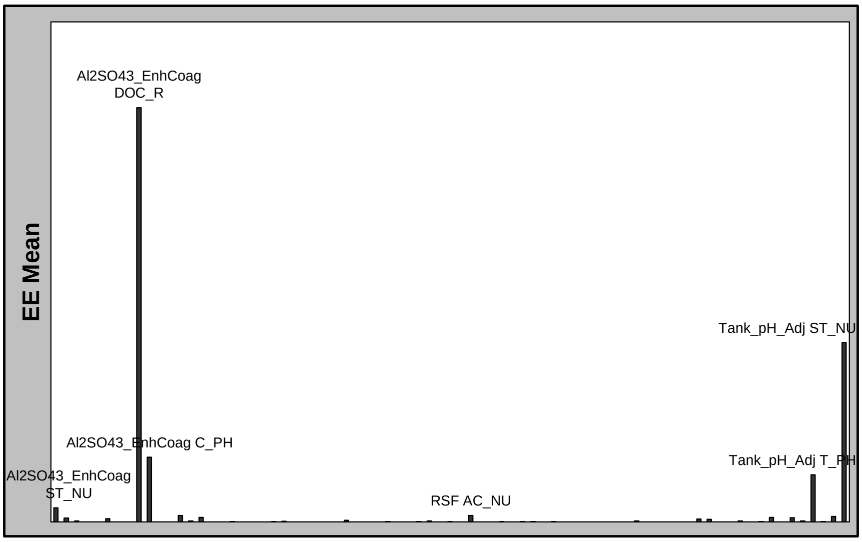

Fig.4: Mean of the elementary effects on the result "Resources"

The most influent parameter (i.e "DOC_R") is a coagulation process objective (dissolved organic carbon removal). This parameter affects the coagulant dose required to reach the treatment objective while the coagulant consumption is a major source of environmental impacts. The result is evident but the added value of sensitivity analysis is the capability of comparison between the numerous parameters.

6 Discussions

The EVALEAU tool is applied to existing plants in order to validate the modelling approach. More unit processes need to be modelled and implemented in the module library to get a complete set of drinking water treatment processes. The numerous potential uses as well as innovative methodologies developed make this tool quite promising.
Such detailed modelling makes the connection between technical changes at process level, resource variability and improvements of environmental impacts at project level. This connection between different issues is a recommendation of the LCA community [4] and it is a significant enhancement of LCA. First and foremost, decision-makers need to believe in the technical feasibility before they get interested in LCA results. This objective led the modelling approach during the project. LCA is an efficient aid for eco-design only if it is predictive and realistic. So, predictive LCI is the first requirement for eco-design based on LCA. High parameterization is a good option to take into consideration industrial issues. In addition, linking LCA software tools with other well-known and specific tools (like PHREEC) makes it possible to integrate complementary knowledge. These concepts make the predictive LCI and the LCA results more reliable for industry managers.
The conclusions of a process parameter sensitivity analysis could have an actual meaning for the plant operators and it could be a useful help to minimize environmental impacts. More efforts are required to confirm the consistency of such methodology. More mathematical methods could be coded if needed, for example to get quantified results.

7 References

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