A CAPE Based Life Cycle Assessment for Evaluating the Environmental Performance of Non-Food Agro-Processes

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With the rise of global warming issues due to the increase of the greenhouse gas emission and more generally with growing importance granted to sustainable development, process system engineering (PSE) has turned to think more and more environmentally. Indeed, the chemical engineer has now taken into account not only the economic criteria of the process, but also its environmental and social performances. To evaluate such non-economic performances is challenging and arduous.
For this purpose, many approaches could be taken into consideration like environmental impact assessment, environmental impact indices, environmental risk assessment, cost-benefit analysis, life cycle assessment (LCA) and Social LCA. Among these approaches, the coupling of PSE and LCA will be investigated here because it is viewed as a good instrument to evaluate the environmental performance of different unitary processes and whole process. The coupling can be of different nature depending on the focus of the study. Either the study is focused on PSE with an associated LCA study (LCA applied to PSE), or LCA study including mass balance and energy balance (PSE applied to LCA). PSE mainly focuses on design, operation, control and optimization of process with the help of computer based methods i.e. Computer Aided Process Engineering (CAPE).
In this study we proceed to an environmental analysis of a non-food agro-process (i.e. biodiesel production from Jatropha) applying our CAPE based LCA proposal. To complement the experimental data the highly impactful unitary processes (i.e. transesterification) is selected for further analysis via simulation. A modelling tool on Microsoft Excel is developed to link LCA and process simulation. For results validation we also implement LCA in a dedicated tool (SIMAPRO) and simulation in a CAPE simulator (ProSim Plus). Furthermore this development of simulation based LCA framework can serve as a step forward for determination of sustainability and eco-efficient designing.

1. Introduction

Jatropha plant is getting an increasing interest these days for its use to extract biodiesel. For the past ten years, a lot of countries or firms have promoted this plant. They consider Jatropha as a profitable commodity and on the same time help to solve the problems of petrol depletion and global warming by producing a biofuel termed as "green fuel". Indeed, Jatropha plant could have a lot of advantages such as growing in lower irrigated and wild areas with lesser soil/field management requirement. As this is a non-edible plant so therefore unfit for human consumption and would not be a threat for the food concurrence in the first place. Actually, Jatropha to produce biodiesel is still under study for commercial production and its environmental consequences are largely concerned by the stalk holders in this field.
Some non-governmental organisations (NGO) blame Jatropha and denounce the social consequences in the countries where it is cultivated. They also denounce the threat on food safety in some developing countries (Koh and Ghazoul, 2008). However, the aviation domain (a sector investigating highly in finding a substitute for kerosene) is still interested by biodiesel produced from Jatropha.

These days scientific community has agreed that life cycle assessment (LCA) is a key methodology for the evaluation of the environmental burdens associated with biofuel production, by identifying energy and materials used as well as waste and emissions released to the environment (Consoli, 1993). Several LCA studies have demonstrated that the use of biomass to produce biofuels from Jatropha curcas that can help in minimizing Resource Depletion (RD) and global warming (Ndong *et al.*, 2009).

An LCA is developed for Jatropha biodiesel production system with standardized norms such as ISO 14041-14044. Scope and limits of our life cycle have to be well defined because our system does not include all the process of biodiesel production with Jatropha Curcas. The system extends from the cultivation of the plant Jatropha Curcas to the biodiesel production, and for all the duration of the plant cultivation, which is approximately 30 years. Crop fields are located in Mali and the refining and transesterification parts take place in Le Havre (France). This system includes the following steps: nursery, transplantation, transport, refining and transesterification. Thus, some steps are not included in this system like harvest, storage and oil pressing.

The functional unit chosen is the MJ of biodiesel, because it is the best unit if other fuels have to be compared with. The inputs are based on an experimental study in Mali and the other data come from Ecoinvent database with the late inclusion of physical properties database used by simulation. In order to develop our inner application, specific substances for Jatropha system have to be identified. Besides, two methods of environmental impacts calculation are selected and implemented: Impact 2002+ and CML2 Baseline 2000.

2. Material and methods

CAPE methods and tools permit us to simulate the whole process, a part or a unit operation. In our study, we use CAPE to model and simulate the transesterification, one part of our development process of the biodiesel production for its life cycle assessment. One core objective is so the implementation of an application which simulates the transesterification sub process of Jatropha Curcas oil. This process simulator is linked with the Life Cycle Assessment (LCA) of the global production process. Figure 1 shows the basic structure of our framework (called "simLCA") that allows a "simulated LCA" applied to the Jatropha biodiesel production.

Figure 1: Basic structure of simLCA tool
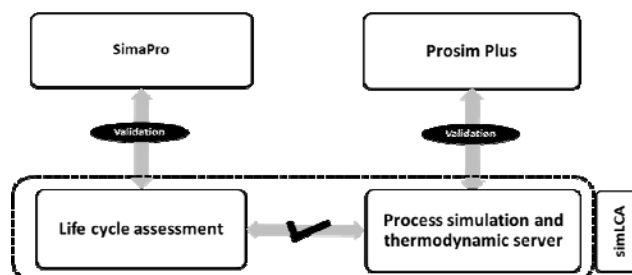
The direct coupling between the well-known commercial applications (i.e. SIMAPRO for LCA and ProSim Plus for CAPE) is arduous not only for the whole production system but also for the transesterification unitary process. The tool simLCA is developed in Visual Basic supported by the Microsoft Excel framework. On the one hand, it was thought out similar to SIMAPRO calculation process. On the other hand, the unitary chemical process under consideration is simulated through a dedicated simulator relied on the Simulis thermodynamic server. At first, to create the simulator, studies from literature were reviewed in order to acquire the information about the transesterification process. Then a process flowsheet was considered to focus on the hypothesis of work and its global calculations. At the end of this task the application was structured to make it user-friendly and efficient. That is why it was decided to create one main sheet (user interface) in which any user is able to configure all the process and LCA parameters before running simLCA.

2.1 Jatropha biodiesel production

The aim was to better understand the production process of biodiesel from Jatropha and their respective environmental impacts it generates. Thus, this study includes the construction of our frame according to two dimensions, LCA and CAPE, dedicated to the analysis of the life cycle for a non-food agro-process. The first was to implement simLCA for life cycle analysis. The second aim was to validate the whole project by comparing with SIMAPRO. The target of our tool is obviously not to model the entire scheme of SIMAPRO. It is dedicated to the environmental assessment for non-food agro process domain and eases

the integration of CAPE in order to improve such analysis. From a first shot based on a pure LCA study, it was revealed that the most impactful part of biodiesel production global chain is the transesterification sub-process (Gillani *et al.*, 2011). In order to have a better understanding of the reaction of transesterification, it is necessary to be aware of its role in the complete process which permits to turns oils or fats to biodiesel. For a good conversion rate, we study the influence of different parameters on the reaction of transesterification such as side reactions (saponification and hydrolysis), thermodynamic model and kinetics of transesterification.

2.2 Limits and definition of system

The system extends the culture of Jatropha production to biodiesel production, for a life cycle of 30 years. Crop fields are located in Mali and processing took place in Havre, France. Our system includes the steps of cultivation of Jatropha plants for one year, planting in the fields, culture in the second year, culture in the third year, culture in years 4-30, (where the whole operating conditions are considered to be the same for all these years), transport of oil from field to refinery units and further for transesterification (we considered that oil is transported by truck for 32 km to the field station Teriya Bugu, for 564 km from the station and transported by boat during 6528 km of Mali to Havre), refining and transesterification step. However, the following steps are not taken into account: i) Harvesting of seeds; ii) Transport of oil to refining and transesterification units; iii) Transport and storage of biodiesel consumption points.

2.3 Functional unit and inventory data

The functional unit is a measure of the performance of the functional outputs of the product system. The ISO 14040 standards demand that functional units are clearly defined, measurable, and relevant to input and output processes. So for Jatropha LCA the functional unit is set to be 1 MJ release to an engine fuelled by Jatropha biodiesel. There is also a reference flow which initiate and inventory to be made for system inputs and outputs. Here it is the quantity (in kg) of Jatropha seed required to fulfil the functional unit.

For Jatropha biodiesel production there is a continuous run of matters, energy through the system boundaries which is quantitatively well described by this inventory phase. Many field emissions to air, soil and water were included accordingly due to land application. The back ground data for these emissions were extracted from Ecoinvent database.

3. Proposal for coupling CAPE and LCA

LCA as an efficient method for environmental quantification has been studied recently for designing a sustainable chemical process (Gillani *et al.*, 2010). In addition the economic criterion can be integrated in the analysis such as (Cavalettlf *et al.*, 2011) for bioethanol production. We study only the environmental side in this paper. We identify two approaches; either embedding process dimension in LCA work or embedding LCA dimension in process design. (Morales-Mendoza *et al.*, 2012) introduce a frame which is chemical engineering oriented and is therefore based on the LCA embedded CAPE approach. Our frame complies with the former approach as the primary purpose is to improve the present environmental assessment of biodiesel production global chain.

In figure 2 we provide an overview of the proposed framework. This whole concept has been divided in three phases which start with an ISO 14040-14044 framework for LCA (Phase-I) with the help of experimental data and Ecoinvent. Then it expends to global production chain (Phase-II) of non-agro food through evaluation of its impact assessment. In our case the CAPE simulation of global production chain in a whole is a rare possibility so a sub process of transesterification (Phase-III) is chosen which is termed as the most impactful category in the light of previous studies. Further this transesterification is simulated through the inclusion of its kinetic model, thermodynamic model and other parameters. This simulator provided by this whole phenomenon could then be integrated in LCA in order to achieve simLCA at the end. In this whole phenomenon there is a continuous flow of information which has been represented by numbered arrows. First is the information flow for field data (1) from inventory analysis followed by impacts of sub processes and operating data (2) from global production chain to sub process for simulation. Then there is a flow of information in upward direction related to mass, energy and enthalpy balances along with design parameters (3). In the last flow we can then indicate potential key parameters (4) for the improvement of whole system. There is always a supposition of internal loops in-between two phases or even for the whole system. In our case this iterative workflow is two tier between phase I & II and single tier between II & III. In the light of this proposed concept we can now provide a simulation based LCA which we termed as simLCA. Where there is always a chance of improvement through the information flow down and upward direction.

Figure 2: Overview of the framework
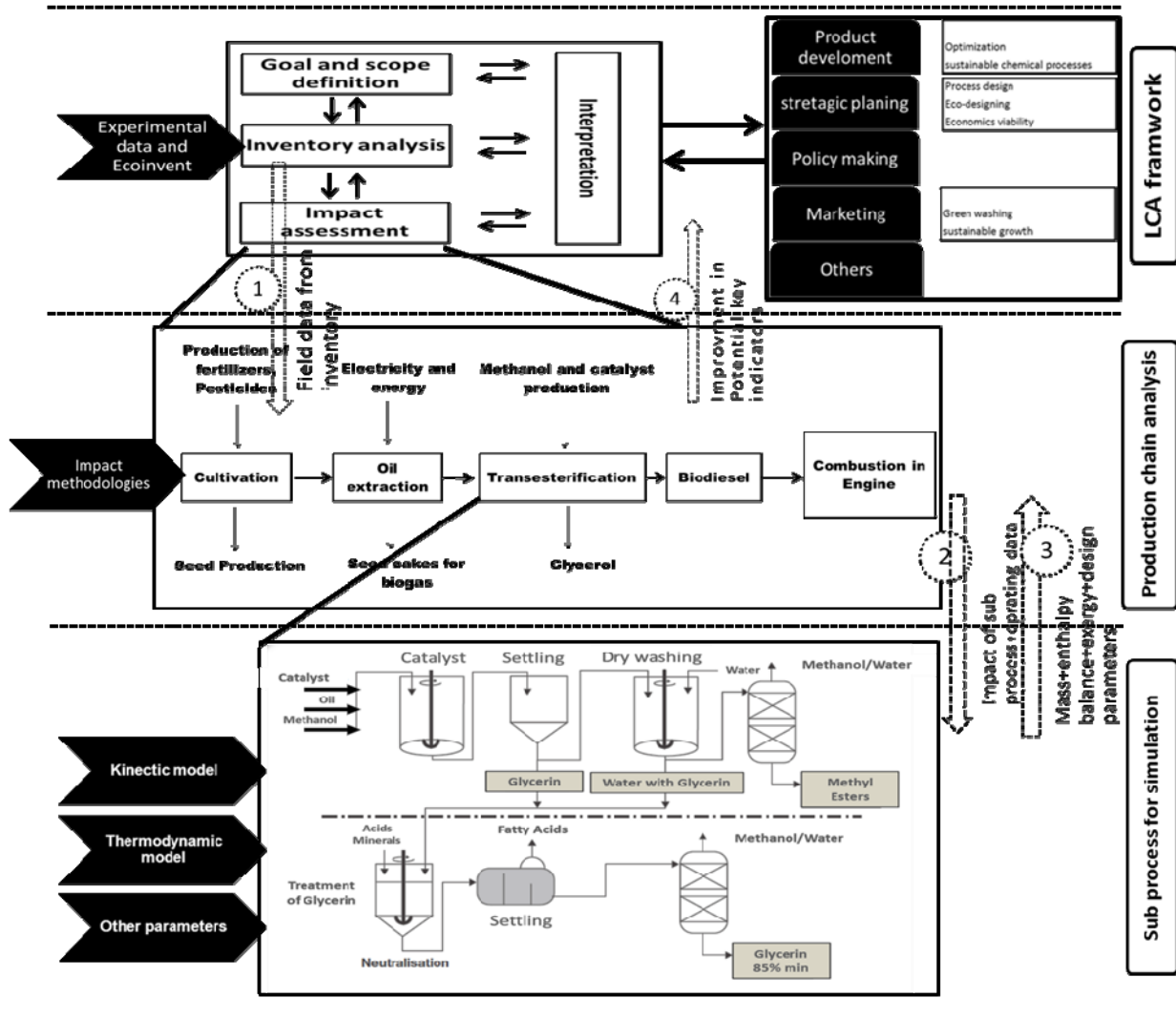

4. Results and discussions

4.1 SimLCA application

Results from the process simulator of transesterification indicate high level of similarities with that of ProSim in global mass and enthalpy balances. There are some differences concerning the distillation column but they are negligible. So we have solid background set for linking this process simulator with LCA and can get the acquired results/impacts through our own excel base framework. There are different impact methodology consists of several impact categories. For this study, only the most significant impacts have been preserved after normalization. Concerning the method CML 2 Baseline 2000 Ozone layer depletion impact has not been taken into account. On the other hand for Impact 2002+ method impact categories such as ionizing radiation, ozone layer depletion, respiratory organics, aquatic ecotoxicity, land occupation, aquatic acidification, aquatic eutrophication and mineral extraction were not taken into account. Indeed, only 8 impacts are relevant in the context of our life cycle for Impact 2000 + methodology. In addition, we have not considered the impact like "land occupation" because of a lack of data.

The screen shot below (figure.3) provide an outlook for a complete simulation based LCA, Where the calculation is performed for each category in two steps. The first step is to create a table for same dimension which use a directory for emissions caused by respective inputs. The second step is to create a second table, once for each unitary process, which includes for gross input value of each impact category. Other tables are then used to compile the results, and then normalize and combine them into end point evaluation with the help of Impact 2002 + methodology. The process simulator in simLCA application is

being integrated with the help of Simulis with its physical properties, thermodynamic, kinetics and other models taken into account.

Figure 3: Screen shot of simLCA
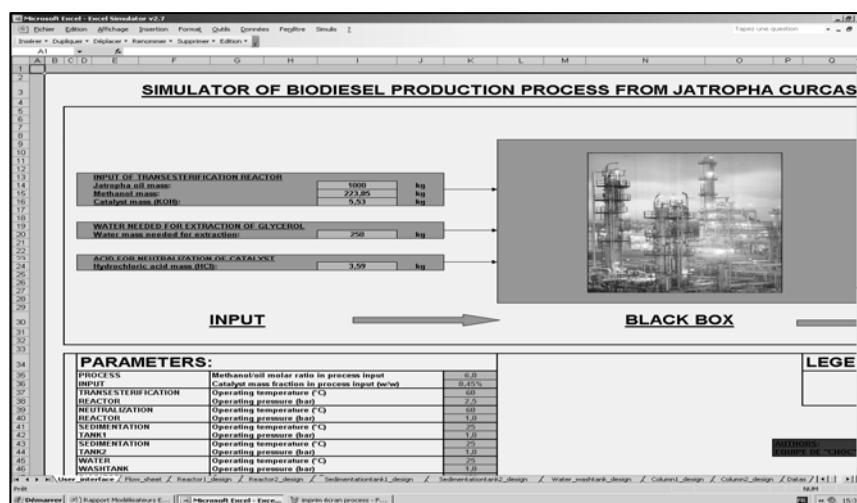
Our simulation based LCA application cannot be useful if it provides results which are not close enough to that of SIMAPRO. So we validate our results first for process simulator with ProSim and then the results obtained from simulation based LCA with SIMAPRO. The results appear almost identical. SIMAPRO values are sometimes slightly larger because it takes into account all substances. For example in non-renewable energy SIMAPRO gives a value of 3.07 MJ while our LCA application gives 3.06 MJ (same is the case for other impacts with negligible variations). Here results in total are not discussed in detail. Instead we provide an insight of how these impacts has been calculated through simLCA. In any case, the results between the two tools are similar enough to allow the same conclusions on an analysis of the life cycle which must nevertheless be specific to the production of biodiesel from Jatropha. After this validation we have a solid background to put forward a new integrated approach by combining process simulation and LCA for an eco-efficient design in chemical engineering. In other words this study can serve as an opening to systematic process engineering and eco-designing which leads to optimization.

4.2 Discussion

There are more than one objectives linked with the integration of transesterification process simulator within LCA of Jatropha biodiesel in order to have a simLCA application. First we start with phase-I which drives us to LCA of global chain production in phase-II. Then simulation of the given chemical process of transesterification in phase-III by doing the pre-analysis and identification of chemical components and properties with the help of process inputs and outputs. There is always a top-down and bottom up flow takes place between each phases. From phase-I to phase-II we have a flow of field data coming from inventory then the second work flow for impact of sub processes and operating data has a top down influence. Further we have the bottom up flow related to mass balance and enthalpy balances through thermodynamic and kinetic model for transesterification. Likewise study of(Vlysidis *et al.*, 2011) shows the utilisation of crude glycerol in transesterification can enhance the sustainability of bio-refineries. The coupling of this simulator with LCA of Jatropha biodiesel enables a direct automation of information flow between different phases. The interest here was to open a gateway for proposed eco-efficient process design. That has been used for sustainable production but they are not very up to the task in industrial practices.

It is now therefore possible to direct the user in order to modify these set of tools according to their own operating condition for a whole process. In our case for the process of transesterification we study the whole model and its impact on the entire production process. This simulation based LCA can now be very helpful to develop a more generic eco-efficient approach that can be used in the primary stage of production design. Another key interest here is that we can choose the best operating parameters by evaluating and finding different set of configurations. The approach presented here is used for analysis of specific process and can be applied to any process in the production chain of Jatropha biodiesel but the main hurdle here is the coherence of primary field data with operating data for simulation. Since our simLCA application gives results similar to that of SIMAPRO hence we can say that this study could further

leads us to social economic and (as in our case) environmental aspects which are the three main pillars of sustainability (Azapagic *et al.*, 2006). In addition, the implementation of such a tool involves many assumptions that may significantly affect the LCA. The user must therefore ensure to take into account these assumptions and change if possible. The structure and process of construction of this simLCA and associated iterative work flow can also be used for other environmental studies of non-food agro-processes.

5. Conclusion

We suggest a frame for a CAPE based environmental analysis and the study and influence of process parameters can be obtained on the sustainability matrices. To integrate such LCA methodology in the presence of CAPE allows (i) on the industrial side, an eco-designing process optimization and (ii) on the society and end-users side, a process environmental performances dashboard. Through this study we highlight the need of further assimilation of CAPE with LCA and social LCA methodologies in order to serve the society and process industry to become more eco-friendly. We worked on an actual case study of Jatropha biodiesel production system. Then we pick the most impactful unitary process for simulation which at the end coupled with LCA for Jatropha to develop a new CAPE based LCA framework. In parallel, the LCA of whole production system of biodiesel was also performed. This whole study has been a way forward to future for CAPE based environmental analysis of agro components since it allowed us to highlight process engineering and sustainability engineering. The coupling within one application (simLCA) allows an automatic updating sequence of results whenever there is a modification in the operating condition (conversion rate of the transesterification reaction, for example), and thus to deepen and refine the LCA which we termed as CAPE embedded LCA. The structure and associated workflow of simLCA carry out the evaluation of environmental performance of non-food agro-processes. The future steps are especially important to integrate economic and social variables to current framework and to open the optimization option in sustainability.

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