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A framework for modelling emerging processes' upscaling from an environmental perspective

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Abstract

Upscaling emerging processes is a very uncertain topic due to the lack of information about the impacts of their dissemination in the industrial system and the environment. However, anticipating potential environmental impacts of novel technologies appears to be essential to reach sustainability. In this context, a framework was created in order to help give an insight of these impacts from an early stage, using laboratory data. This article begins with a literature review about upscaling in chemical engineering and Life Cycle Assessment. A framework was then proposed for the upscaling of emerging processes, using laboratory data to anticipate the impacts. A case study is presented in a third section to illustrate the application and results obtainable with the framework to the manufacturing of the surfactant, Alkyl Polyglycosides. Finally, limits and perspectives about this approach are given as conclusions.

Keywords: Upscaling, Emerging processes, Life Cycle Assessment.

Introduction

The University of Grenoble Alps has launched several cross-disciplinary projects [1] aimed to bring together researchers from the various departments of the university and to fund projects on selected scientific topics. One of these projects is Glyco@Alps [2], which is focused on the study of the entire life cycle of glyco-molecules, i.e. sugars, from their synthesis in live organisms to the development of innovations based on them. Sugars are a large family of molecules which includes glucose, cellulose (which is a constituent of wood, therefore paper) or chitin (which can be found in seashells). From the study of these molecules, the development of new materials, products and processes is expected. In this context, the study presented in this article introduces a framework aimed to help to anticipate the impacts of the introduction of these innovations in the industry and in the society by using lab-scale or pilot-scale data to simulate an industrial process.

The main problem to do so is that the impacts of the industrial scale are not directly proportional to those of the lab scale. The answers to this issue encompass researches about upscaling of a process or, in general, of a system. Works on this aspect can be found in the literature and include the consideration of technical, economic and environmental aspects, with high uncertainties. However, no generic methods exist to assist in doing this upscaling.

In this article, the main focus is the environmental impacts of an upscaled process with qualitative technical considerations. The goal of this study was to see how the upscaling of a lab process can be carried out to obtain a satistfying image of what might be the industrial process. To do so, a process engineering software called ProSim [3] was used in order to perform an analysis of the lab process. Then, considering the thermodynamic characteristics obtained with this tool, industrial techniques were added to the process, based on the Best Available Techniques defined in the European regulation [4]. The assumption here is that, if a novel process is to be industrialised, it should comply with the latest regulations. Thus, this

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article will present an application of a framework aimed to help decision making while designing novel technologies based on the upscaling of lab processes in a view to assess their environmental impacts thanks to a Life Cycle Assessment (LCA), and based on current industrial practices, experts' opinion and general trends in the industrial world.

In this article, a literature review will explain the position of the proposed framework compared to existing papers. Then, the framework itself will be presented. Thirdly, a case study in the context of the glyco-industry will highlight its use and the kind of results that can be obtained. Finally, a discussion of the limits of this approach and perspectives for further work will be presented.

1. Literature review

Two main topics have been explored for this study. On the one hand, previous researches about the upscaling of industrial or chemical processes, which constitutes the first sub-section. On the other hand, the assessment of environmental impacts of novel or emerging technologies and the issues related to the lack of data or inconsistencies with existing datasets.

1.1. Upscaling

The issue of upscaling has been studied in the field of process engineering for many years. However, the references found showed that this issue has only been partially solved. The main setback in the literature is the focus on a single technology or process without any clues about patterns which could be applied to other cases. All in all, the literature showed that upscaling is essentially based on experts' opinions, pilot scale plans and experiments, and analogies with existing technologies that are considered as having a similar behaviour.

More in details, a number of recurring issues in upscaling can be identified [5]. The first one is the practice of uncritically applying a scale up factor to the laboratory results to predict those of the industrial scale. Indeed, for chemical processes, using larger quantities can dramatically change the transfer mechanisms and the outcome of a reaction. Therefore, a well-known process at a smaller scale may not work at all, or may have a lower yield after upscaling. Moreover, there is a need to take into account the interactions with the surroundings of a chemical reactor and the potential changes in transfer mechanisms which can be a significant issue. At commercial scale, it is often difficult to reproduce the laboratory conditions due to the lesser isolation of the process and, more generally, because of a higher complexity of the industrial environment. Finally, due to the large quantities and the high temperatures, some physical phenomena can occur and distort the outcome of a reaction.

In other respects, Laird [6] mentioned that because of the large quantities, the operating conditions can become hazardous. This observation implies that safety measures need to be taken to reduce the risks of accidents. Changes in the operating conditions can, as well, eventually lead to changes in physico-chemical parameters. These changes can cause a lower yield or even parasitic reactions which might contaminate the product. This is without mentioning Piccinno et al. [7] who suggested that laboratory data might be incomplete and on top of that, some steps involved might be overlooked, even though at industrial scale, they might become crucial. This article also proposes a framework for continuous processes. On the particular topic of the most important parameter to consider, Sánchez et al. [8], draw the attention on the capacity utilization, which refers to the manufacturing capacity of the firm at any given time.

Finally, in the book by Bonem [9] eight factors are identified to help to determine the upscaling strategy for chemical processes, in general: (1) recycling considerations, (2) theoretical considerations, (3) thermal characteristics, (4) equipment related, (5) sustainability, (6) mode related, (7) regulatory requirements, (8) project focus considerations. For this study, only the first four, which are process-related were considered. The other ones and some aspects of the fourth are more system-related and could not be studied at the time of the work.

1.2. Environmental impacts of novel technologies

Environmental impact assessement methods, in particular LCA [10], are meant to be applied after data are avalaible, therefore after a product has been launched on the market. Researches about assessing the environmental impacts in the early stages of product design exist, and the problem considered here is partially similar, except that the focus is on processes and new materials or products whose data may not exist anywhere else than in the lab. Thus, it is possible to simply consider this issue as the application of LCA in the early stages of a design process [11].

On this issue, recent researches defining how to ecodesign an emerging process exist applied to a particular case [12]. Here, the idea is to start with the information available on the basis of the theoretical calculations or measures from the lab or pilot scale in order to improve these results and to compensate the lack of knowledge and experience at industrial scale. Moreover, the matter of the changes in the larger system caused by the release of the new process also has to be answered. When focusing on the factors which influence LCA results of a new technology [13], it is possible to identify intrinsic factors (e.g. change in efficiency or functionality, resource criticity), indirect factors (e.g. rebound effects, impacts of the supply chain), and external factors (e.g. social changes, policies and regulations).

In the particular context of sugar chemistry, the production of cellulose nanocrystal foam, which is an emerging technology was assessed thanks to a combination of LCA and eco-toxicity tests [14]. This article provides an insight about a way to palliate the lack of impact factors for new materials, by resorting to actual ecotoxicity experiment. However, no information is provided about the compatibility of this approach with well-known impact assessment methods such as ILCD [15].

Therefore, similarly to the literature about upscaling there is a distinction between process-related aspects and broader system-related issues which need to be dealt with. However, it appears that generic considerations can more easily be taken on

work about LCA. Another issue to be considered is the availability of data. It seems that process data, although coming from lab experiments, are the most readily available and constitute a proper starting point when addressing the issue of upscaling from the environmental impacts point of view. Thus, the present research has focused of lab chemical processes to see how their upscaling could be simulated. A hypothesis is that it is possible to use chemical process simulation software to obtain the relevant factors, as defined by Bonem [9], and use them in an LCA software to model a factory which would comply to the European regulation.

2. Framework proposition

The proposed framework consists of a sequence of the four steps presented in Figure 1. The general idea was to gather as much information from a lab scale process, then to use them in a process simulation software to get information on thermal and material recycling possibilities, and on the behaviour of the chemical reaction when upscaled. The dimensioning of the upscaling was done using reference documents on the Best Available Techniques accessible from the European Commission [16] to select the equipments and techniques that could be included, mostly as a support to the main reaction into an LCA software. The first step is to obtain data from lab experiments in order to have them in the form of a flow diagram, which is the essential element to have to start studying the process and to carry out an LCA. Alternatively information from the literature can be used. The secondary goal is to have enough information to be able to identify realistic practices about energy and waste management.

Secondly, the collected data are used in a process simulation software, such as ProSim [3] in order to consider more precisely the thermodynamic characteristics of the reaction. Furthermore, a close attention need to be made to the factors found in Bonem's book [9]: the recycle considerations, i.e. the various reactants and other products that can be reused or recycled (e.g. solvants); the theoretical considerations, including the heat and mass transfer mechanisms which may change upon upscaling; thermal characteristics in order to recycle the heat being dissipated at certain steps and for safety considerations ; the equipment to use according to the desired volume or mass of the final product. An interesting module of the software to see the potential for heat recycling is to carry out a pinch analysis. It is a methodology aimed to help to minimise energy consumption of chemical processes by calculating thermodynamically feasible energy targets ; this is done by optimising heat recovery systems, energy supply methods and process operating conditions. Therefore, ProSim is also a support to select lab equipment.

After this, whether an idea of the size of the industrial installation is known or not, Best Available Techniques, as defined in the European directive on Industrial Emissions [4] can be associated with each step of the chemical reaction. Reference documents published by the European Commission provide a precious help to select techniques that could be applied for the simulated factory, according to its industrial sector. This step has been manual so far, but it could be possible to create a database of techniques to be chosen according to a set of criteria.

Fig. 1. Steps of the proposed framework.

The combination of the data collected from the previous steps should therefore enable to create a flow diagram for this simulated industrial process, including relevant life cycle inventory datasets and values. The upscaling considerations are here included at every step of the process, supposing that there is no differences in the chain of reactions for both scales. Finally, the chosen way to compare both processes, and to evaluate the performance of the novel process was to compare them through an LCA. In addition to the problem of data availability and possible discrepencies, the goal was to see how far is the simulated industrial process, compared to the performances of the lab which should be worse, since it is not optimised. When possible, comparison with an existing equivalent process would be interesting.

3. Case study: biobased surfactant

The case study used to design the framework was the manufacturing process of a non-ionic surfactant called Alkyl Polyglycosides (APG12). This compound is made from a mixture of

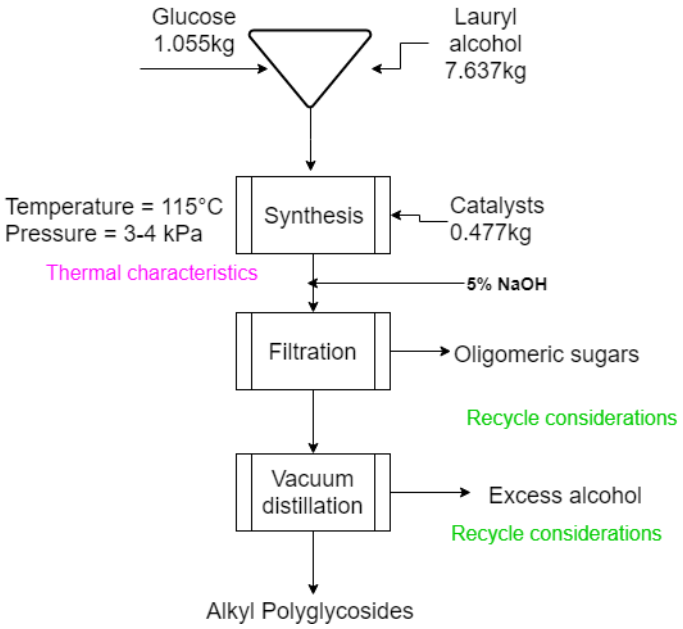

Fig. 2. Steps of the synthesis of APG12.

glucose and lauryl alcohol. A surfactant is a chemical substance that modifies the surface tension between two media; in the case of a detergent it usually is water and grease. The process to model this reaction is described in this section.

3.1. Lab data collection and flow diagram

For this example, data from the literature were used. The processes for extracting glucose from wood chip [17] and for the synthesis of lauryl alcohol [18] were used to construct the manufacturing process, as well as a direct glycosylation [19]. The quantities of the inputs were then extrapolated to produce 1 kg of Alkyl Polyglycosides, according to stoechiometric proportions. The steps of the reaction can thus be summed up as showed in Figure 2. Glucose and Lauryl alcohol are mixed together under at a temperature of 115°C and a pressure of 3 to 4 kPa. Catalysts are also necessary and are considered as not consumed in the reaction. Then, the obtained product is filtered before it is distilled under vacuum and finally extracted thanks to a solvent. Overall, the laboratory process does not have many requirements to meet, and it was considered that there was heat recovery or other energy or material recycling. On these aspects, this lab process can be considered as an extremely inefficient process.

3.2. Industrial considerations

Overall, the process did not differ from lab scale, and in the absence of relevant data, it was considered that the yield was identical. In this study, the creation of the industrial-scale process consisted in the integration of energy optimisation and material recycling. To do so, pinch analysis enabled to identify heat losses which could be recovered. The operation and material recycling equipment choice was based on the manual selection of appropriate Best Available Techniques from the sectoral reference documents available on the European Commission website [16]. This step of the proposed framework is where the four process-related factors for upscaling [9] were used.

In this case, heat recovery potential was assessed though the pinch analysis module in ProSim. Thus a potential of 1,854 kcal/h were found to be recoverable. For the solvents and catalysts, a recycling or reuse rate of 95% was considered, based on experts' opinions on the matter. The remaining 5% were considered as industrial hazardous waste. In an attempt to be more realistic, the energy efficiency was calculated for the scenario process in order to decrease the overall energy consumption of the process.

For material optimisation, such as recycling or emission reduction, reference documents on Best Available Techniques were browsed and hand-picked. Whenever it had been possible, details about the energy and material consumption of these techniques were collected and included. Even though these values may not have been accurate, they enabled to see whether their contribution to the environmental impacts were significant or not; thus implying that further investigations be needed. For example, in section 1.2.3.1. BAT 8.b of the conclusions of the Production of Large Volume Organic Chemicals reference documents [20], in order to decrease the amount of organic waste, the unused raw material and solvents can be recovered through a series of process, such as membrane separation. The choice of the technique used is impacted by the substance to be recovered and only a general idea of this equipment can be integrated in the diagram.

3.3. Simulated industrial process

The combination of the lab-scale process, the pinch analysis and selection of Best Available Techniques enabled to draft a flow diagram for the simulated industrial process and to gather data for a life cycle inventory to be used in the following step.

3.4. Comparison through LCA screening

In this case, it was decided to study a functional unit corresponding to the synthesis of 1 kg of APG. In order to have a baseline comparison, industrial data from Chalmers were used [21]. The LCA software used was SimaPro 8, with EcoInvent 3. The inventories for both scales can be found in the references [17–19,22–24].

Table 1 shows that the environmental impacts of the production of 1kg of APG12, calculated with the ILCD method, are the highest for the simulated industrial process. However, important variations occur, and globally the petrochemical APG has the lowest impacts. Chalmers' process is intermediate in most cases. All in all, conclusions are difficult to draw about the relevance of the framework. Nevertheless, this study raised interesting questions that are stated in the following section. The main processes which contribute most to the differences of the impacts cannot always be explained. The most clearly identifiable causes are due to the energy mixes or hazardous waste scenario treatments which may not appear in the reference in-

dustrial process or happens in more or less sensible locations. The detailed analysis of theses causes will be the subject of a future research.

Besides, an allocation problem may also come into play. Indeed, the simulated industrial process does not consider whether the installation is supposed to produce only the functional unit, or is part of a larger plant whose general impacts would be allocated amond its multiple outputs.

Table 1. Characterisation results of LCA of 1kg of the simulated industrial process, petrochemical APG from EcoInvent and Chalmers' dataset.

Impact category	Simulated industrial process	Petrochemical APG	Chalmers'
Climate change	100.00%	14.13%	13.13%
Ozone depletion	100.00%	4.29%	2.95%
Human toxicity, non-cancer effects	100.00%	8,01%	21.73%
Human toxicity, cancer effects	100.00%	8.14%	10.44%
Particulate matter	100.00%	9.73%	8.21%
Ionizing radiation HH	100.00%	1.26%	9.53%
Ionizing radiation E (interim)	100.00%	2.11%	16.30%
Photochemical ozone formation	100.00%	12.10%	10.13%
Acidification	100.00%	5.59%	14.21%
Terrestrial eutrophication	100.00%	5.99%	30.24%
Freshwater eutrophication	100,00%	7.11%	7.07%
Marine eutrophication	100.00%	5.76%	45.02%
Freshwater ecotoxicity	100.00%	5.71%	23.94%
Land use	100.00%	3.61%	29.56%
Water resource depletion	100.00%	-1.18%	23.44%
Mineral, fossil & ren resource depletion	100.00%	4.47%	4.64%

However, for other causes, it seems that they might be due to differences of boundaries or an aggregation of the datasets which prevent to further analyse the origin of the differences. For example, the lab process considered the market products as inputs, whereas the petrochemical APG used other mixes or elementary flows as its reactants.

4. Discussion and perspectives

The main limit to this approach is the impossibility to consider the differences of yield that can be expected to be found between the lab and industrial scales. Therefore, the integration of this aspect would be the next step. The difficulty on this is the dependency of this factor to the intrinsic characteristics of the reaction. Indeed, it seems that the prediction of the yield, either higher or lower, when upscaling may greatly vary from one case to another. More generally, the current approach to create a factory showed important differences with industrial data. However, the causes may be boundaries discrepancies or related to uncertainties on the models and data. Consequently, these would also need to be investigated in future researches to ensure consistency in data sources and accuracy, especially about localisation of processes or their age.

An idea to consider a more realistic behaviour of the simulated installation would be to include in the framework, a connection to open databases, either European [25] or local [26], to formalise the selection of techniques and to associate emission and consumption levels to the simulated industrial process. These data could be processed thanks to data mining and machine learning methods, such as the ones used in previous researches about Best Available Techniques [27].

On issues related to LCA applied to novel technologies, it would also be essential to find ways to take into account rebound effects caused by their launch and diffusion into the society. Finally, this study has showed that it may be possible and relevant to create an interface between process simulation and LCA programmes, in the case of the design of new chemical processes.

5. Conclusion

The proposed framework is an attempt to anticipate the environmental impacts of a novel chemical product. So far, it only considers the synthesis process with consideration of energy and material recycling at every of its steps. The integration of data from the Best Available Techniques reference documents enables to add some realism to a simulated installation. However, the consistency of the system boundaries still needs to be investigated. Applications to other processes will be undergone, considering either novel processes for novel usages, novel processes for well-known usages or well-known processes for well-known usages. The latter will be the best way to be able to compare the simulated system with the content of current LCA databases and ensure that geographical and temporal information is considered. The key characteristics of the applicability of the framework also need to be identified in terms of industrial sectors and type of process. To avoid repeating similar actions in process simulation software and LCA software, the feasibility of interfacing each other should be also studied.

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