COMPARISON OF DIFFERENT LIFE CYCLE IMPACT ASSESSMENT (LCIA) METHODS AND SOFTWARE TO EVALUATE IMPROVEMENTS IN CHEMICAL PROCESSES

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ABSTRACT: Two different Life Cycle Impact Assessment methods (Impact 2002+ and ReCiPe) were applied to evaluate two design alternatives for the ammonia's production process: a base case design and a new sustainable design. The methods were applied using two LCA softwares, *GaBi* and *SimaPro*, in order to compare the sensitivity and the behaviour of each method when calculated by the two different software. Both methods and tools were compared in terms of their inventories, characterisation factors and single score values. The results obtained from this analysis pointed out for the requirement of a careful selection of methods and tools applied to comparison of design alternatives.

Keywords: LCIA, Impact 2002+, ReCiPe, GaBi, SimaPro

1 INTRODUCTION

The environmental impact assessment has become an important aspect for companies' global competitiveness [1]. Therefore, several tools were developed in order to assess and quantify the potential environmental impacts of products. The growing concerns regarding this key aspect lead to an increasing number of scientific publications related to environmental assessment, which shows that scientific community has been trying to get a deeper knowledge in this field. The European Commission presents LCA as the best framework for assessing potential environmental impacts and highlighted, as future research, the need of more consistent and consensual data in LCA methodologies [1]. Based on this directive, this work aims to compare different methods and tools, when applied to assess different design alternatives. This work follows up the study developed by Mendes et al. [2] that applied different methods to assess process alternatives from environmental perspective.

Life Cycle Impact Assessment's (LCIA) purpose is to assess the potential environmental impacts, based on a functional unit defined before [3] ISO 14040, 2006]

Its structure is divided in two categories, the obligatory elements and the optional ones. The first category contemplates the selection of impact categories, indicators and characterisation factors, the classification according to the ICL results and the characterisation which basically means to calculate the results of each impact category ISO14040 (2006)) The optional elements are normalization, grouping, weighting and data quality analysis [3], [4], [5].

The main reasons why LCIA is divide in two distinct groups are [4]:

- To clearly define each distinct element;
- To use each method in the LCA objective and scope phase;
- A data quality analysis may be elaborated to the LCIA methods, assumptions and other decisions;
- All the operations of each elements may be transparent to reviews and critical reports;
- The values and the subjectivity related to the choices made in each element, must become transparent to reviews and critical reports.

Impact Categories represent the environmental issues to which the inventory results are related to. The concept of category indicator may be observed in Figure 1:

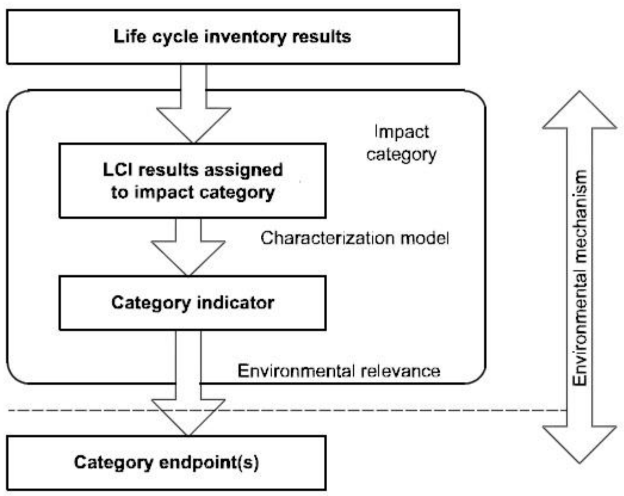

Figure 1 – Category Indicator Concept [6]

The process described in this figure illustrates the environmental mechanism from the inventory results to the category endpoints. First the results are assigned to an impact category. Then, they are related to the category indicator, through characterisation factors established in a model. The environmental relevance of an impact category is given by the proximity of its indicator to the endpoint indicator.

In this article, two LCIA methods are considered, Impact 2002+ and ReCiPe. Impact 2002+ is a midpoint/endpoint approach. This is a method that considers 14 midpoints and 4 endpoints. This method considers the use of normalisation and weighting elements, but this last one is yet not developed for this method [7]. The ReCiPe has as objective to combine in a consistent way, the midpoint and the endpoint approach. In this methodology the characterisation factors are obtained in a consistent cause-effect chain. It considers 17 midpoints and 3 endpoints as well as normalization and weighting. [8]

In literature, some comparisons between methods are made, such as the work of Bovea & Gallardo (2006) [9] and Buchgeister (2012) [10]. Literature review shows however that there is a gap in the comparison of alternative processes, or just processes itself, since the studies made are more focused on the final product.

This paper intends not only to compare the two process alternatives for the ammonia case study, but also to check the differences between SimaPro and Gabi softwares.

2 CASE STUDY

In this study, the ammonia case study [11] - Carvalho, A., Matos, H.A., Gani, R., (2010)] has been selected as the basis for this analysis. In the current process, ammonia is obtained from catalytic reactions of a feed of natural gas containing also nitrogen, hydrogen and impurities (argon and methane).

Only for the production of ammonia there are 4 licenses, in this paper the Kellogg method will be considered. This methodology presents 4 stages, 57 streams, 42 operational units and 14 compounds, all represented in Figure 3 [11].

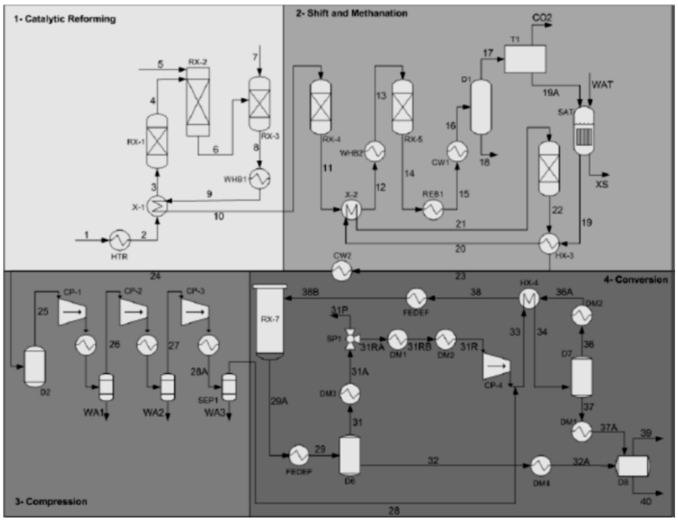

Figure 2 - Systematized Ammonia production [11]

The following tables (1,2 and 3) present the mass and energy balance of this production for boss base case and alternative case.

Table 1 - Ammonia's input masses [11]

In (kg/h)	Base Case	New Case
Water	8171.5	8171.5
Argon	173.5	173.5
Nitrogen	9996.2	9996.2
Natural Gas	6065.1	6065.1
Oxigen	3072.3	3072.3
Vapour	32299.7	8910.2

Table 2 - Ammonia's output masses [11]

Out (kg/h)	Base Case	New Case	Status
Water	31709.1	135.5	Líquido
Ammonia	302.4	302.4	Ar
Argon	163.2	163.2	Ar
Nitrogen	245.6	245.6	Ar
Carbon Dio-xide	15316.1	15316.1	Ar
Hidrogen	55.9	55.9	Ar
Methan	98.9	98.9	Ar

Table 3- Ammonia's Energetical needs [11]

Energia	Base Case	New Case	Unit
Arrefecimento	202.5	129.4	GJ/h
Aquecimento	85.6	85.6	GJ/h
Eletricidade	247.4	720.4	kWh

3 METHODOLOGY

The comparison of the different methods and software follows the methodology described in Figure 1. On the first step the inputs of each tool are compared. On step 2 the main differences of the software's inventories are pointed out. The characterisation phase is presented on the third step, where the most important factors of each method and software are highlighted. Finally, on the forth step the single score results are compared.

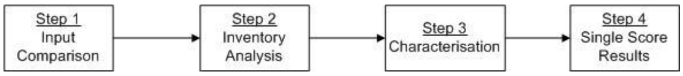

Figure 3 - Methodology for methods and software's comparison.

4 RESULTS

The methodology of Figure 1 was applied to Impact 2002+ and ReCiPe methods using the LCA software *GaBi* 5 (education license) and *SimaPro* 7.3.

4.1 *INPUTS*

GaBi and *SimaPro* are two different tools for the same purpose, which is the application of LCIA methods. From this study, it is plausible to say that the input methodology of *SimaPro* is more intuitive than *GaBi's*. *SimaPro* divides the inputs by origin (or destination in the case of emissions), which allows the user to easily systematise its process. This *Si-*

maPro's layout makes the search of emissions in the database easier and more accurate, since it is easier to keep track on all the inputs. In *GaBi* this procedure is not so intuitively. It is very important to point out though, that the version of *GaBi* in question is an educational one. This means that the number of databases and the databases themselves are limited. Moreover, the full set of features of this software is not available.

4.2 *INVENTORY*

The resulting inventory from both tools is clearly different. Taking as an example the inventories regarding flows of material, *SimaPro* considers 208 more components than *GaBi*. However the final characterisation results are not that different. Even with different amounts of compounds considered, both software distinguish used water and air as main components of the inventory. In order to see that differences are not that relevant, we point out the example of carbon dioxide, the third component in the contribution ranking, which only presents a difference of 0.89 kg between the two software inventories. The differences in the inventory analysis and in the following steps come as no surprise since an educational version of *GaBi* is being used, and it was not possible to assure that the databases used were the same in both software. Despite that, all the analyses made in this study are valid since the main objective is to check if both tools tend to deliver the same result when applied to compare more than one process design alternative.

4.3 *CHARACTERISATION*

The characterisation analysis is presented in Table 4 for Impact 2002+ and in Table 5 for ReCiPe. In both cases, the top 5 categories were selected according to their contribution to the final single score. Both software present as output 15 impact categories for Impact 2002+ application, but they are not all the same. While *SimaPro* divides the respiratory effects into organics and inorganics and does not consider photochemical oxidation, *GaBi* considers the latter and does not divide the respiratory effects. Regarding ReCiPe method, *SimaPro* considers 3 more categories than *GaBi,* which are agricultural land occupation, natural land transformation and urban land occupation. The remaining 14 categories are the same.

Table 4 - Main Impact 2002+ Impact Categories for the characterisation

	Impact category	**Unit**	**SimaPro**			**GaBi**		
			Base Case	**New Case**	**% ∆rel.**	**Base Case**	**New Case**	**%∆rel**
Impact 2002+	Non-renewable energy	MJ Primary	46.37	41.50	-12%	18.03	12.65	-42%
	Global warming	Kg CO_2 eq.	2.50	2.22	-13%	2.41	2.10	-15%
	Aquatic ecotoxicity	kg TEG Water	0.98	2.55	62%	1.97	1.45	-36%
	Terrestrial ecotoxicity	kg TEG Soil	0.55	0.98	44%	0.39	0.38	-0.4%
	Terrestrial acid./nutri.	kg SO_2 eq.	0.39	0.39	0%	0.33	0.32	-2%

Table 5 - Main ReCiPe Impact categories

	Impact category	**Unit**	**SimaPro**			**GaBi**		
			Base Case	**New Case**	**%∆rel**	**Base Case**	**New Case**	**%∆rel**
ReCiPe	Fossil depletion	$	$1.8x10^{+01}$	$1.6x10^{+01}$	12%	$7.6x10^{00}$	$5.4x10^{00}$	-42%
	Metal depletion	$	$2.3x10^{-05}$	$2.6x10^{-05}$	11%	$3.7x10^{-05}$	$2.9x10^{-05}$	-26%
	Climate change Human Health	DALY	$3.9x10^{-06}$	$3.5x10^{-06}$	12%	$3.8x10^{-06}$	$3.3x10^{-06}$	-15%
	Particulate matter formation	DALY	$2.3x10^{-06}$	$2.3x10^{-06}$	-1%	$2.2 x10^{-06}$	$2.2x10^{-06}$	-1%
	Climate change Ecosystems	Species.yr	$2.2 x10^{-08}$	$2.0x10^{-08}$	-12%	$2.1x10^{-08}$	$1.9x10^{-08}$	-15%

It is plausible to say that the new case presents better overall environmental performance. In fact, that was the result for the studied methods.

This analysis shows that the categories with greater contribution to the final single score in both methods and software are the same. It also shows that relative improvement of each category is similar to the correspondent in both software. Despite this fact, not all tend to the same result. In the case of Impact 2002+, while *GaBi* reveals that the new case represents an improvement at all levels, *SimaPro* results show that only 2 of those 5 categories represent an improvement when the alternative process is applied. With ReCiPe, only metal depletion with *SimaPro* indicates a lower performance of the new case scenario. It is also shown that the results' order of magnitude is similar, which reveals that the analyses made are coherent, as stated before, even using different databases.

4.4 *NORMALISATION*

The Normalisation phase does not interfere, as expected, in the relative variation between alternatives. In this element of LCIA is the absolute value of each category that it's important to point out. In this case study, the normalisation confirms the new alternative as the best environmental choice. However different, both methods point out similar categories with bigger environmental impacts. While ReCiPe indicates the fossil depletion, Impact 2002+ indicates non-renewable energies as the most problematic. This study allows to take some conclusions, that both methods are similar in the normalized evaluation, since they both point out to the same result (better performance of the new case) and with comparable categories with the greater impact. It is important that some methods show up close results in such important LCIA elements as normalisation that is very dependent of subjective assumptions and dependent on pre-established criteria.

4.5 *SINGLE SCORE*

Table 6 shows the single score values for both alternatives of the ammonia process, for each method and for each software. It is possible to conclude that the new case scenario is environmentally better than the base case, since its single score is always lower. Table 3 also shows that both software deliver a relative improvement with the same order of magnitude. This means that they are equally sensitive, even with different values provided by different databases.

Table 6: Single score values for each alternative process obtained by using the two LCIA methods and the two LCA softwares.

Table 6 - Ammonia Single Score Results

	Simapro			**Gabi**		
	Base Case	**New Case**	**∆rel**	**Base Case**	**New Case**	**∆rel**
ReCiPe	3.42×10^{-01}	3.09×10^{-01}	-11%	2.24×10^{-01}	1.85×10^{-01}	-21%
Impact 2002+	9.29×10^{-04}	8.65×10^{-04}	-7%	7.19×10^{-04}	6.46×10^{-04}	-11%

Single Score is a LCIA element that should be considered and taken into account since it allows the decision maker to choose directly between two methods. However, the results, just as in the case of normalisation, are subjective and dependent on the criteria that are pre-established.

5 CONCLUSIONS AND FURTHER WORK

In a world looking for sustainability there is a growing need and investment in more lucrative and social and environmentally aware solutions.

Many environmental tools appeared in order to satisfy such need but, the one chose by the European Union to assess Life Cycle Impacts is the LCIA. This i sone of the mais reasons that led to a numberless amount of LCIA methods, developed by different entities, with different purposes and different criteria.

This work tries to categorize and systematize the study of two of those methods, applying them to a case study where two alternative processes are taken into account, comparing 3 LCIA elements.

Results show that the new process is environmentally better than the base case. These results are consistent in the 3 elements considered for both methods studied. It was also shown that, these are two close methodologies that, even when the category is not exactly the same, it's at least related to the same impact.

There some differences regarding the LCIA softwares mentioned in this paper. Beside showing the same result for both methods in all elements, the results are not always consistent, showing different orders of magnitude for example.

For the decision makers, it is fundamental to know all these differences in advance. When an ACV is needed, it matters to know how will a certain method react, which factor is associated to which element in which method etc. and that different softwares may mean different results even considering the same methods for the assessment.

The future work proposed is to try to aggregate the LCIA methods, in order to achieve an universal and standardized way to assess life cycles, with clear impact categories and globally accepted normalization and weighting factors. It is also suggested that the main data bases are reviewed, since the software tools are not responding the same way to the same case study, regarding the inventory, making it important to understand its importance in the final score.

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