Comparative analysis of the Life Cycle Impact Assessment methods in their application to chemical processes

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Abstract

In the last decades, the recognition of the importance of the sustainable development concept has contributed to the creation of several methods that have allowed various entities to assess the impact of their activity in society. However, it has often been observed that the results of these methods are not consensual when they are obtained for particular cases, turning the final decision-making into a harder task.

The current study compares the results of the implementation of alternative chemical processes in the SimaPro software, in order to decrease the uncertainty regarding the application of some LCIA (Life Cycle Impact Assessment) methods, namely Eco-indicator 99, EPS 2000, EDIP 2003, IMPACT 2002+, ReCiPe, ILCD 2011 Midpoint, and the recent Product Environmental Footprint (PEF). The proposed methodology presents different analyses of the obtained results for a biodiesel production case study. The analyses are mainly related to the single scores of each method and also to the critical impact categories considered by each method. Therefore, it was possible to develop a new methodology called TOP-NORM, which confirms the critical impact categories previously indicated by a Pareto's analysis, showing the importance of the normalisation factors for this nomination. In the end, a new matrix called LCIA-DSM is also presented, which can assist the users in selecting the most adequate LCIA method to employ in an assessment of alternative processes, according to the number of critical impact categories and the end-points coverage (Resources, Human Health and Ecological).

Keywords: LCIA methods, Process design, TOP-NORM, LCIA-DSM

1. Introduction

Over the last decades, different sectors of modern society have shown a growing concern regarding the sustainability of products and services, due in part to the confirmation of the serious consequences registered by the climate changes (Carvalho et al., 2014). Therefore, innovative solutions have been required to assist various entities in controlling their environmental impacts, decreasing them without the need to compromise the current life patterns (Carvalho et al., 2013).

Nowadays, the scientific community provides several methods and tools that allow the quantification of the environmental impacts associated to all the processes included in a product life cycle. However, despite following the same steps (typically; classification, characterisation, normalisation, and weighting), the methods sometimes consider distinctive impact categories with specific nomenclatures and different taxonomies to classify their results, turning their comparison into a harder and unreliable task (Carvalho et al., 2014). So, some questions may arise: Despite their differences, are the most critical impact categories similar in all the methods? How is this importance defined? Considering the different impact categories, and for a given case, is the decision between two alternatives always consensual for all the methods?

Consequently, the existence of different methods makes the choice of the most adequate method to employ in a decision-making harder. Towards this situation, the European Commission expressed the need for more consistent data, as well as a consensus regarding the existent methodologies (Carvalho et al., 2014), proposing a new method called Product Environmental Footprint (PEF).

Therefore, a comparative study of some Life Cycle Impact Assessment methods through their application to alternative chemical processes is proposed here. The results of the quantification of the environmental impacts of each method were provided by the SimaPro software, and allow a conclusion about both the similarities and differences of the analysed methods, as well as the development of new methodologies to support their application.

2. Literature Review

2.1. Life Cycle Assessment (LCA)

The Life Cycle Assessment (LCA) procedure identifies and quantifies the energy and the materials used, as well as the waste and the emission released to the environment. Then, it assesses the impact of these inputs and outputs, which can be defined for a single process or for the complete life cycle, from the raw materials acquisition to the final disposal of the product (Carvalho et al., 2014). This procedure is defined and described in ISO 14040 (2006) and ISO 14044 (2006), consisting in four phases: a) Goal and scope definition, b) Inventory analysis (LCI), c) Impact assessment (LCIA), and d) Interpretation (which influences the change or the improvement of the previous phases).

a) The <u>first phase</u> (Goal and scope definition) specifies the goals and the proposed investigation procedure. This phase includes, for instance, the definition of the system boundary (the set of criteria that specify which processes are included in the system), the functional unit of the system (the quantified performance of a system to be used as a reference unit), and the requirements regarding the data quality.

b) The <u>second phase</u> (Inventory analysis – LCI) includes the realization of the inventory of all the materials needed for the inputs and outputs data, as well as the energy flows, according to the goals defined in the previous phase. The processes included in the analysis should also be defined (depending on the system boundary) – cut-off task.

c) The <u>third phase</u> (Impact assessment – LCIA) refers to the calculation of the potential environmental impacts with effects in the resources availability, as well as the impacts in the human health and nature. These impacts are calculated from the inventory values, which should then be matched to the corresponding impact categories – classification. Then, the inventory values should be converted for a specific unit (a category indicator) through the use of characterisation factors (which depend on the LCIA method that is used) – characterisation.

According to ISO 14040 (2006), the previous operations are mandatory. However, it can also be considered the normalisation operation (obtainment of the results in relation to a reference value – normalisation factor – for instance, the annual output of a defined geographical area or the annual average contribution of a person) and the weighting operation (with the aim of obtaining a single score, based on value judgements given about the relative importance of the considered impact categories) (Pinheiro, 2014). This phase of the LCA study (Figure 1) is often performed with the support of a specialized software such as the SimaPro software, facilitating the calculations required.

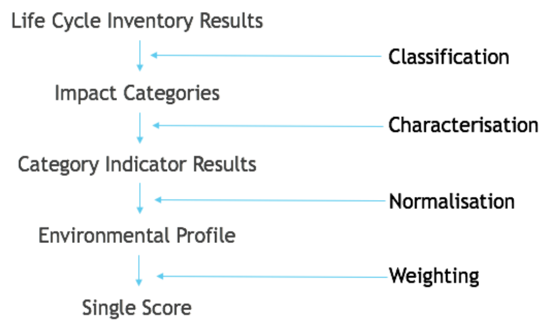

Figure 1 – Steps in the environmental impact assessment procedure (Pinheiro, 2014).

d) In the <u>fourth phase</u> (Interpretation), the LCI and/or LCIA results are verified and assessed, in order to confirm their consistency with the defined goal and scope of the study.

2.2. LCIA Methods

For the application of the third phase (Impact assessment – LCIA) previously mentioned, it is necessary to define the method which is used for the calculations of the characterisation and normalisation operations. The different methods that quantify the impacts in the LCA context are called Life Cycle Impact Assessment (LCIA) methods.

According to Mimoso et al. (2015), the best approach to assess the environmental impacts of chemical processes is the one that reaches a single score, so the following seven methods were applied in the current study: Eco-indicator 99 (Goedkoop and Spriensma, 2001), EPS 2000 (Steen, 1999), IMPACT 2002+ (Jolliet et al., 2003), EDIP 2003 (Hauschild and Potting, 2005), ReCiPe (Goedkoop et al., 2009), ILCD 2011 Midpoint (including normalisation and weighting) (European Commission, 2011), and PEF (according to the information available in European Commission (2013)).

3. Proposed Methodology

The current study consists of the application and comparison of some LCIA methods previously mentioned in the context of a case study in the chemical industry. For that, an investigation methodology is proposed, which includes the following steps.

3.1. Step 1: Characterisation of the case study

In this first step, the chosen case study was characterised. It was selected after a research in the *ScienceDirect* platform, providing the mass and energy balances that were implemented in the SimaPro software (the values will be shown in Step 2 of this methodology), as well as the system boundary and the functional unit that were also defined for the two alternatives considered in a biodiesel production case, based on the work of Farrell and Cavanagh (2014).

This cradle-to-grave case study intends to compare the environmental impacts of the production and final usage of two fuels: biodiesel from new vegetable oil (NVO) and biodiesel from waste vegetable oil (WVO). The system boundaries for both processes include the production and the final usage of the fuels. The NVO biodiesel production (alternative A) involves rapeseed oil production, transportation, oil extraction, and the process of transesterification. The WVO biodiesel production (alternative B) involves salvaging waste vegetable oil, which eliminates the raw material production observed in the other process. Glycerine is considered a sub-product of the transesterification reaction, and the combustion in a generator is considered the final usage of each fuel. The functional unit is 1 kg of biodiesel.

3.2. Step 2: Implementation in the SimaPro software

This step consists of the implementation of the case study in the SimaPro software. Firstly, only the production processes for each fuel were created. Tables 1 and 2 indicate the input/output data that were implemented in the SimaPro software for the assessment of the production processes for both alternatives A and B, respectively.

Table 1 – Input/output data implemented in the software for the NVO biodiesel production process (alternative A).

Type of *input/ output*	Name defined in the SimaPro software	Quantity	Unit
Product	Biodiesel - A	0,868	kg
Avoided Product	Glycerine $\{US\}$| esterification of soybean oil |Alloc Def, S	0,095	kg
Inputs of materials/ fuel	Rape seed oil, in supermarket	0,900	kg
	Methanol, at plant/RNA	0,158	kg
	Sodium hydroxide, without water, in 50% solution state $\{GLO\}$| market for |Alloc Def, S	0,007	kg
	Tap water, at user $\{RoW\}$| market for |Alloc Def, S	1500	g
Inputs of electricity/ heat	Electricity, medium voltage $\{WECC, US\ only\}$| market for |Alloc Def, S	0,316	kWh
Waste and emissions	Waste water – untreated, EU-27S	1598	g

Table 2 - Input/output data implemented in the software for the WVO biodiesel production process (alternative B).

Type of *input/output*	Name defined in the SimaPro software	Quantity	Unit
Product	Biodiesel - B	0,862	kg
Avoided Product	Glycerine $\{US\}$| esterification of soybean oil |Alloc Def, S	0,094	kg
Inputs of raw materials	Water, cooling, drinking	1500	g
Inputs of materials/ fuels	Used vegetable cooking oil $\{GLO\}$| market for |Conseq, S	0,894	kg
	Methanol, at plant/RNA	0,158	kg
	Sodium hydroxide, without water, in 50% solution state $\{GLO\}$| market for |Alloc Def, S	0,007	kg
Inputs of electricity/ heat	Electricity, medium voltage $\{WECC, US\ only\}$| market for |Alloc Def, S	0,316	kWh
Waste and emissions	Waste water – untreated, EU-27S	1599	g

Then, another implementation was performed in the software, considering the inventory data related to the fuel production and the emissions released during combustion, which can be found in Tables 3 and 4 for the production and final usage processes of both alternatives A and B, respectively.

Table 3 – Input/output data implemented in the software for the NVO biodiesel production and final usage processes (alternative A).

Type of *input/output*	Name defined in the SimaPro software	Quantity	Unit
Product	Biodiesel final - A	1	kg
Inputs of materials / fuels	Biodiesel - A	1	kg
Emissions to air	Carbon monoxide, biogenic	4,97E-3	kg
	Carbon dioxide, biogenic	1,7	kg
	Nitrogen oxides	4,49E-3	kg

Table 4 - Input/output data implemented in the software for the WVO biodiesel production and final usage processes (alternative B).

Type of *input/output*	Name defined in the SimaPro software	Quantity	Unit
Product	Biodiesel final - B	1	kg
Inputs of materials / fuels	Biodiesel - B	1	kg
Emissions to air	Carbon monoxide, biogenic	4,98E-3	kg
	Carbon dioxide, biogenic	1,68	kg
	Nitrogen oxides	4,47E-3	kg

In order to apply the PEF method in the SimaPro software, a methodology according to the information available in the guide of the method (European Commission, 2013) was developed. It consists of the application of the most adequate method available in the SimaPro software for each impact category considered, since the PEF method covers numerous methods. So, the software automatically shows the characterised results for each impact category, according to the chosen method, as is indicated in Table 5.

After the obtainment of the characterised results, the normalisation operation followed, which is optional according to the PEF guide (European Commission, 2013). However, since the comparison of the single scores of all chosen methods was proposed, the calculation needed for this phase was performed. So, the characterised results were divided by the normalisation factors provided by Benini et al. (2014). Finally, a single score was obtained after the weighting phase (which is also optional according to the PEF guide). The weighting factors had the value of 1 for all the categories, so by multiplying this value by the normalisation results and after adding all up in the end, a single score (in Pt) was obtained.

Table 5 – Impact categories considered for the PEF method and the corresponding methods that were applied in the software (European Commission, 2013).

Impact category	Method applied in the software
Climate change	IPCC 2007 GWP 100a V1.02
Photochemical ozone formation	ReCiPe Midpoint (H) V1.08 / Europe ReCiPe H
Acidification	ILCD 2011 Midpoint V1.02
Resource depletion – mineral, fossil & renewable	ILCD 2011 Midpoint V1.02
Eutrophication - aquatic (freshwater)	ReCiPe Midpoint (H) V1.08 / Europe ReCiPe H
Eutrophication - aquatic (marine)	ReCiPe Midpoint (H) V1.08 / Europe ReCiPe H
Human toxicity, cancer effects	USEtox (sensitivity) V1.02 / Europe 2004
Human toxicity, non-cancer effects	USEtox (sensitivity) V1.02 / Europe 2004
Ecotoxicity for aquatic fresh water	USEtox (sensitivity) V1.02 / Europe 2004
Particulate matter	ILCD 2011 Midpoint V1.02
Land use (land transformation)	ILCD 2011 Midpoint V1.02
Ozone depletion	EDIP 2003 V1.04 / Default
Resource depletion - water	Pfister et al. 2009 (Water Scarcity) V1.00

Thus, it was possible to apply all the selected methods, including the PEF method, using the SimaPro 8 software. In this software the methods sometimes present more than one version. Table 6 shows the names defined by the software of the version used for each method that was applied.

Table 6 - Names defined by the SimaPro software for each method that was applied.

Method	Name of the version in the SimaPro software
Eco-indicator 99	Eco-indicator 99 (H) LCA Food V2.03 / Europe EI 99 H/H
EPS 2000	EPS 2000 V2.07 / EPS
IMPACT 2002+	IMPACT 2002+ V2.11 / IMPACT 2002+
EDIP 2003	EDIP 2003 V1.04 / Default
ReCiPe	ReCiPe Endpoint (H) V1.08 / Europe ReCiPe H/H
ILCD 2011 Midpoint	ILCD 2011 Midpoint V1.02

3.3. Step 3: Results analysis

In this step, several analyses were performed from the results obtained in the SimaPro software, namely:

1. First, the single scores of all the methods were compared, which allowed the identification of the most sustainable alternative considered by each method (with the lowest value in Pt), from a quantitative perspective.

2. Next, considering the single scores presented, the ratios of the results of one alternative related to another were calculated for all the methods, in order to better confirm in which alternative there was an improvement. So, for instance, for the X method and for the alternatives A and B, the ratio was calculated through the Equation (1).

$$Ratio\ for\ the\ X\ method = (SS_A - SS_B)/SS_A \quad (1)$$

Where SS_A and SS_B are the single scores for the alternatives A and B, respectively.

Since one of the goals of the current study was the application of the PEF method (considered the most recent method of the environmental impact assessment in the LCA context), it became relevant to know the difference between the PEF ratios and the other methods' ratios. Thus, for instance, the ratio obtained for the X method was divided by the ratio obtained for the PEF method. This analysis allowed the understanding of the exigency level of each method regarding the established improvement between both alternatives, based on what was defined by the PEF method.

3. Afterwards, a Pareto's analysis was performed to obtain the most critical impact categories considered by each method for both alternatives. First, considering the single scores (in Pt) for each method and for each alternative, the values obtained from each impact category were divided by the total impact value. Next, these quotients (in %) were sorted, and the highest results were totalled until 80% (this value was exceeded when necessary). So, for each method, the most critical impact categories were the ones that had the highest quotients included in the sum.

4. Finally, the most critical impact categories obtained by Pareto's analysis were analysed. These categories were classified into end-points, according to the similarities between them, as was proposed by Carvalho et al. (2014). This way, a growing coverage of levels (impact category < end-point) could be observed, which allowed a better interpretation of the results.

3.4. Step 4: Development of the TOP-NORM methodology

From the analysis of the critical impact categories, it was possible to develop a new methodology called TOP-NORM, which confirms the critical impact categories indicated by Pareto's analysis for each method, showing the importance of the normalisation factors for this nomination.

3.5. Step 5: Creation of the LCIA-DSM matrix

The analysis of the critical impact categories contributed to the creation of a new matrix called LCIA-DSM (Decision Support Matrix for the application of the LCIA methods), which can assist the users in selecting the most adequate LCIA method to employ in an assessment of alternative processes, according to the number of critical impact categories and the end-points coverage (Resources, Human Health and Ecological).

4. Results and Discussion

4.1. Single Scores

The results of the different methods demonstrate that, for the chosen case study, there is no consensus regarding the choice of the most sustainable alternative. This can also be verified through the analysis of Figure 2 which presents the ratios calculated for each method, based on the ratios of the PEF method, showing that some values are positive and others are negative. This means that the ReCiPe, EDIP 2003 and IMPACT 2002+ methods demonstrate that the most sustainable alternative is the one that uses waste vegetable oil, while the other methods demonstrate that it is the one that uses new vegetable oil. So, the choice of the method to be used can influence the decision about the most sustainable alternative in a given case, when it is not the same for all the methods, proving also that the methods have different exigency levels of the considered improvement between alternatives, and the PEF method can be considered the most demanding one.

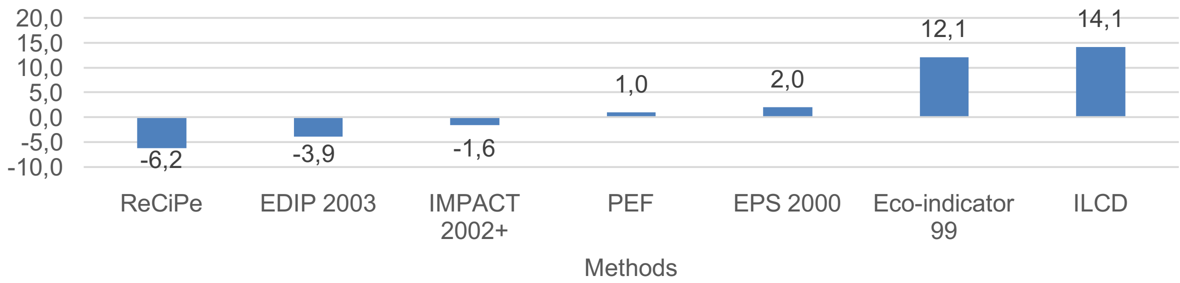

Figure 2 – Difference between the methods' ratios for the biodiesel production case study.

4.2. Analysis of the critical impact categories obtained by a Pareto's analysis

The most critical impact categories for each method and for both alternatives A and B can be seen in Figures 3 and 4, respectively. In these figures, the contribution of each category to the total impact can also be observed. Through the analysis of Figure 3, it can be verified that:

- The PEF and ILCD methods have in common the *Eutrophication – aquatic (marine)* and *Land use* categories;
- The EDIP 2003 method has one category in common with the PEF and ILCD methods (*Eutrophication – aquatic (marine)*), and another category in common with the PEF method (*Acidification*);
- The Eco-indicator 99 method has one category in common with the PEF and ILCD methods (*Land use*).

On the other hand, through the analysis of Figure 4, it can be verified that:

- The PEF and ILCD methods have in common the *Land* use and *Resource depletion – water* categories;
- The ReCiPe method has one category in common with the IMPACT 2002+ method (*Terrestrial ecotoxicity*).

Then, the critical impact categories were classified in three end-points (Resources, Ecological and Human Health), which are presented in Figure 5 for each method and for each alternative, and it can be verified that:

- Comparing both alternatives, the same end-points are observed for the EPS

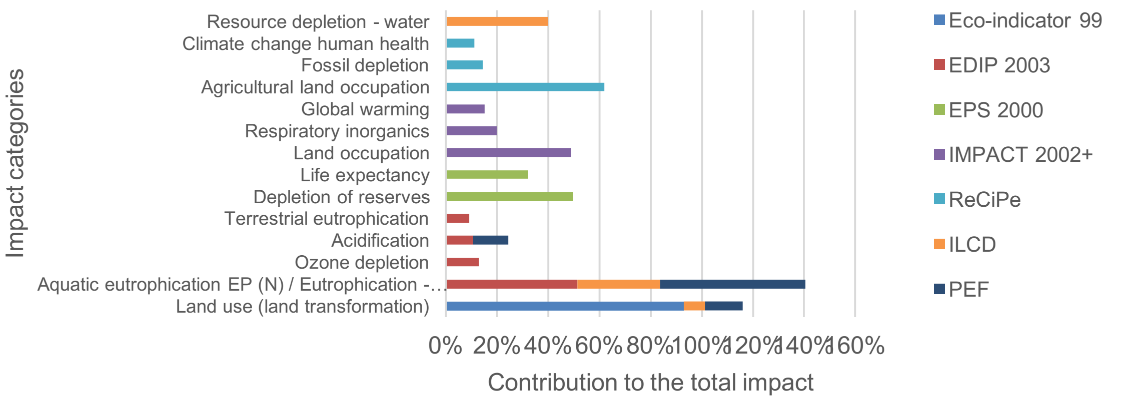

Figure 3 – Critical impact categories considered by each method for the NVO biodiesel production (alternative A).

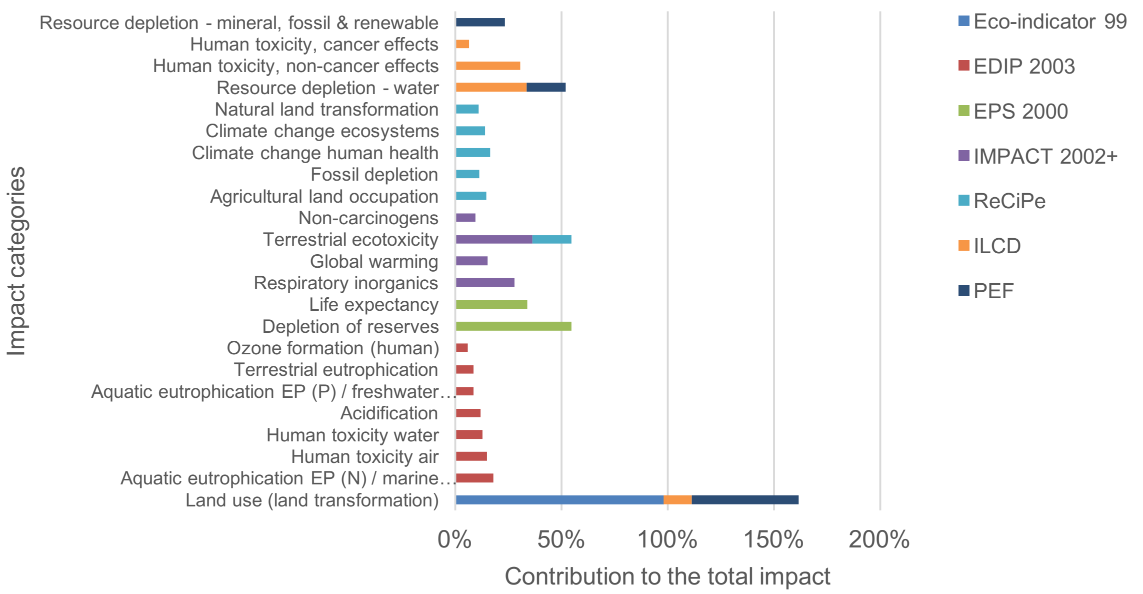

Figure 4 - Critical impact categories considered by each method for the WVO biodiesel production (alternative B).

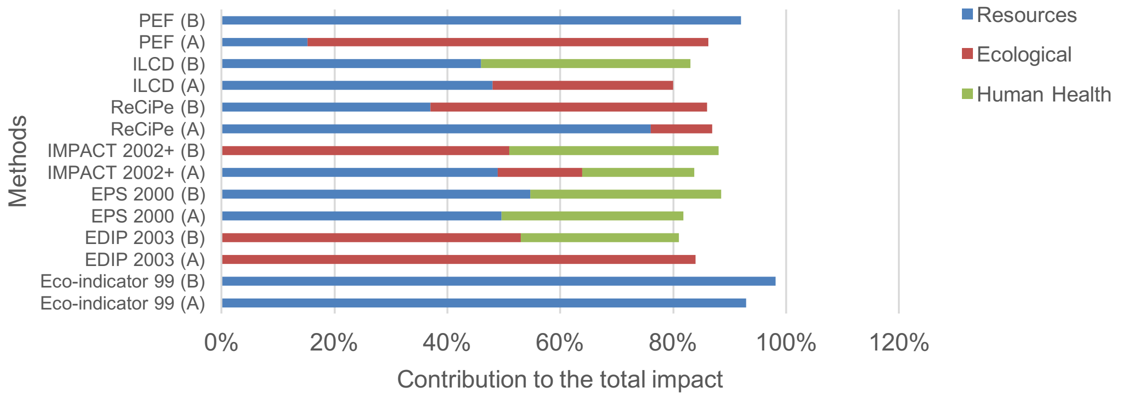

Figure 5 – End-points for each method and for both alternatives of the biodiesel production case study.

2000 and Eco-indicator 99 methods;

- For alternative A, the PEF method considers a higher weight to the *Ecological* end-point but it also considers the *Resources* end-point, which has an exclusive relevance for alternative B;
- The difference between PEF and ILCD methods occurs for alternative B, since the ILCD method also considers the *Human Health* end-point;
- The Eco-indicator 99 method considers an exclusive relevance for the *Resources* end-point;
- The IMPACT 2002+ method considers the three end-points for alternative A, while it only considers the *Ecological* and *Human Health* end-points for alternative B;
- For alternative A, the EDIP 2003 method considers an exclusive importance for the *Ecological* end-point, while it only considers the *Human Health* end-point for alternative B;
- For both alternatives, the ReCiPe method only considers the *Resources* and *Ecological* end-points;
- For both alternatives, the EPS 2000 method only considers the *Resources* and *Human Health* end-points.

4.3. The new TOP-NORM methodology

As a consequence of the analysis that was previously presented, there was an attempt to understand and justify the reason behind the relevance that was demonstrated by some categories when a given method was applied. In fact, the LCIA methods can differ in terms of the characterisation, normalisation and weighting factors that are used, and they affect the obtained results.

Therefore, the relation that exists between the characterised results and the normalisation factors (or reference values) was tested. So, choosing one method, the ratio for each impact category was calculated through Equation (2), and the normalisation factor was firstly calculated through Equation (3).

$$Ratio_{imp.cat.} = \frac{Characterised\ results - Normalisation\ factor}{Normalisation\ factor} \quad (2)$$

$$Norm.Factor = Charact.Results / Norm.Results \quad (3)$$

From the ratios obtained, similar conclusions were verified for the different methods, allowing the development of a new methodology that confirms the nomination of the most critical impact categories (TOP categories) previously indicated by the Pareto's analysis. This new methodology called TOP-NORM is represented in Figure 6, and proves that the normalisation factors contribute to the relevance assigned to a given impact category.

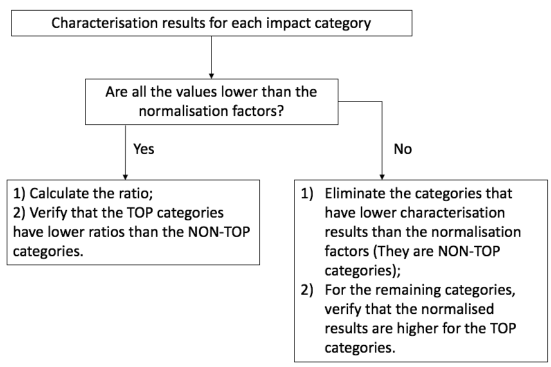

Figure 6 – TOP-NORM methodology.

4.4. The new LCIA-DSM matrix

Other analyses to the critical impact categories were performed for other case studies in the chemical industry, similarly to what was done for the biodiesel production case study that was presented here. So, from these analyses, it was possible to create a new matrix called LCIA-DSM, which is represented in Figure 7.

This matrix can assist the users in selecting the most adequate LCIA method to employ in an assessment of alternative processes, according to two possible criteria:

1. The end-points covered by the method (*Resources - R*, *Human Health - HH* and/or *Ecological - E*);
2. The number of critical impact categories considered by a method compared to the total number of impact categories that are available for that method.

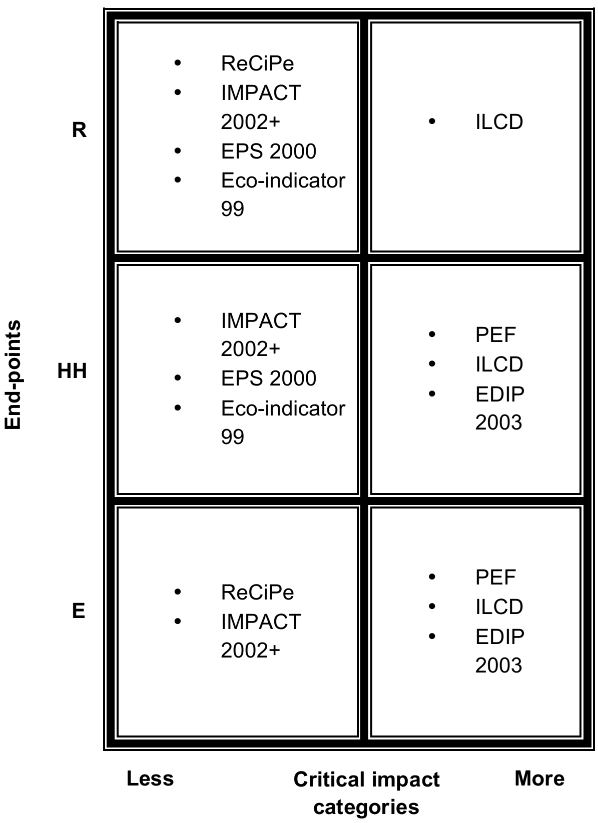

Figure 7 – LCIA-DSM matrix.

5. Conclusions

This study reveals that the LCIA methods are useful tools to quantify the environmental impacts. However, a proliferation of these methods has been verified, which has originated a disagreement regarding the impacts assessment procedure.

Therefore, a comparative analysis of seven LCIA methods was proposed: Eco-indicator 99, EPS 2000, EDIP 2003, IMPACT 2002+, ReCiPe, ILCD 2011 Midpoint, and Product Environmental Footprint (PEF). These methods were applied to a case study, so two alternative processes for biodiesel production were implemented in the SimaPro software. The results demonstrated that there is no consensus regarding the choice of the most sustainable alternative, which means that the final decision about an environmental impact assessment is influenced by the method that is applied. Furthermore, the methods demonstrate different exigency levels about the improvement considered between alternatives, so a future work to understand how the exigency of each method is determined is suggested. Besides, some methods present common critical categories and some methods sometimes present the same critical categories for both alternatives, while other methods present different categories, so a future work to explain the reason for that is also suggested. Moreover, it has been proven that the normalisation factors influence the weights that are assigned to each impact category, and consequently to each end-point. Therefore, the TOP-NORM methodology was developed, which confirms the nomination of the critical impact categories indicated by a Pareto's analysis. Finally, it was possible to create the new LCIA-DSM matrix, in which the methods are disposed according to the number of critical impact categories and the end-points coverage.

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