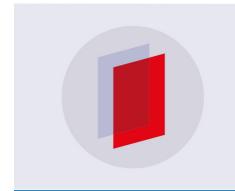
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Sensitivity Analysis of Life Cycle Impacts Distribution Methods Choice Applied to Silica Fume Production

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Abstract. The construction sector is known as an important consumer of natural resources. The use of by-products from different production chains in the sector is encouraged, promoting a reduction in the extraction of natural resources, reducing the need for residues disposal and enhancing circularity. Silica fume is a by-product from the smelting process in the silicon and ferrosilicon industry, commonly used as concrete supplementary cementitious material, which provides chemical and physical effects on concrete microstructure. When LCA evaluation is conducted, different impact distribution models may be applied to assess the potential impact of the by-productss. Although their benefits are recognized, some studies still report them as burden free, having no allocated impacts. Thereby, the aim of this paper is to evaluate the differences in silica fume life cycle impacts by analyzing three scenarios from cradle to gate, considering the modeling procedures described by ISO 14040, the Cut-off model from Ecoinvent version 3.3 and the impact assessment method CML v.4.4, according to the CEN EN 15804 recommended categories. Results enhance the understanding regarding model selection and demonstrate that the selection of the proper distribution model is key, considering that this may lead to important differences in the results.

1. Introduction

The construction sector is recognized by producing numerous environmental impacts due to the high consumption of natural resources, high energy consumption for extraction of the raw material and for the large production of waste. These characteristics set up unsustainable patterns of development and consumption that could potentially lead to resource depletion and the inability to manage the amount of waste produced. Different studies and initiatives make efforts to mitigate this problem by improving materials, constructive techniques and developing new products. In addition, the production chain of the construction industry has enormous potential to increase the volume of materials it recycles, due to the large amount of materials consumed [1]. The use of construction and demolition waste, as well as the waste from other industries in the substitution of natural raw materials, is a sustainable way of handling by-products that would be otherwise disposed of.

There are environmental benefits related to the use of by-products in the construction industry. However, it is essential to quantify such benefits to provide clear information on the advantages or disadvantages related to their use. In this way, Life Cycle Assessment (LCA) is a methodology which allows for the assessment of potential environmental impacts of the use of such materials by

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calculating and evaluating resource consumption and emissions [2]. It is a recognized methodology that provides a structure to develop an environmental assessment of products [3].

LCA models the life cycle of a product through a system product, which is composed of activities that transform inputs to outputs (called 'processes') [3]. Processes that have more than one product as output, are known as multifunctional process [4]. In LCA studies involving multifunctional process(es), ISO 14044:2006 standard recommends firstly, the elementary process division or system expansion. Secondly, it recommends allocation using physical relationships and, thirdly, when a physical relationship cannot be applied, entries should be allocated by functions in a way that reflects other relationships between them such as economic value [5].

Tillman (2000) discussed the relevance of these different methodological choices in an LCA paper of a multifunctional process and its relationship between their goals and applications [6]. This paper distinguished a retrospective LCA, which are commonly known as attributional LCA and a prospective LCA, known as consequential LCA. The paper differentiates between the attributional approach, applied to learn about existing impacts, used to identify improvement possibilities or to make market claims; with the consequential approach, used to investigate the consequences of the changes in product or process design [6]. The ILCD handbook (2010) defines attributional modelling as involving the current or forecasted specific or average supply-chain [4].

Both approaches can be found being applied in LCA of the multifunctional process. Considering the attributional one, Chen et al. (2010) state that the mass allocation procedure has the advantage of being constant with time since the mass proportion between the product and the by-product is not very variable unless there are changes in its production process [7]. Despite being a consolidated method, there are different ways to conduct it. Choices related to the Life Cycle Inventory (LCI) modeling process, such as the different sets of rules that can be applied in the studies, may lead to different results [8]. On the other hand, Saade, Silva and Gomes (2015) mentioned that the conceptual limitations of allocation methods are that they do not look beyond partitioning impacts, and awkward ratios between physical characteristics and market value may distort the results [9]. These authors cited the system expansion approach (which encompasses the whole-system level, redefining the system boundaries to include the function related to the by-product) as their preference due to its capacity to precisely model the studied processes, following a complete and conceptually consistent description which also allows for the consideration of potential improvements at whole-system level. However, they recognize that system expansion application requires alternative data, which can be hard for certain processes [9].

In this regard, different modeling approaches are considered in the Ecoinvent v.3.3 database, giving consistency to studies related to diverse human activities. This database provides the choice among three system models. Two of them are based on the attributional system model - Allocation and Cutoff by classification (Cut-off) and Allocation at the point of substitution (APOS) and the last one is based on the consequential system model and named as Consequential, long-term [10]. It is important to mention that, whenever different alternatives of allocation procedures seem applicable, a sensitivity analysis should be conducted to explain the consequences of replacing the selected approach [5].

The environmental evaluation of the by-products used in the construction sector has been much discussed recently. Some of these studies are related to concrete production, one of the most produced materials in the world and with great potential for incorporating wastes/by-products [11]. In the concrete mix, pozzolanic materials have been used to improve properties related to mechanical strength and durability. Silica fume (SF) is one of these by-products, commonly applied due to its pozzolanic characteristics, extreme fineness and high amorphous silicon dioxide content. It is recognized as a pozzolanic admixture that is effective in enhancing concrete mechanical properties [12].

In the environmental assessment context, some SF studies have been developed assessing its environmental impacts as a supplementary cementitious material (SCM). Van Den Heede et al. (2014) compared a cement based concrete slab with a concrete slab with high cement replacement level [13]. By evaluating the impacts adopting an attributional approach, using economic allocation, the authors

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found a reduction when the SF is applied as SCM. Habert et al. (2011) assessing a concrete environmental impact, also applied an attributional approach, finding substantial differences coming from the three SF allocation procedures chosen (no allocation, mass allocation and economic allocation), with mass allocation showing the highest impact [14].

Although, some studies have been developed, the literature still has a lack of studies demonstrating in a clear way the influence of choice of multifuncional modeling procedure on the environmental impacts results. Considering that, and the common use of SF in construction products, the objective of this research is to enhance the understanding of differences in silica fume life cycle impacts by analyzing three scenarios from cradle to gate, considering the multifunctional modeling procedures by ISO 14040, the three distribution Cut-off models from Ecoinvent version 3.3 and the impact assessment method CML v.4.4-2001, according to the CEN EN 15804 recommended categories.

2. Methodological approach

2.1. Goal, scope and inventory analysis

The objective of this LCA is to understand the impacts of choosing a modeling procedure to deal with multifunctionality, as described by ISO 14040, in the LCA of the by-product SF. SF is produced during the silicon metallurgical production process, being collected in very large filters in the baghouse and then made available for use in concrete without further treatment (Figure 1). SF is also produced by the ferrosilicon productive process, but the silicon metallurgical is selected to this evaluation, since it produces higher amounts of proper SF for concrete production [1].

The scope of this LCA considers the production system from cradle to gate. In this way, the impacts related to the material extraction, material production stage, and transportation to the silicon metallurgical factory are evaluated. The use, maintenance phase and end-of-life (recycling and disposal, including transport) are not considered. The functional unit is defined as 1 kg of Silica Fume, produced in Brazil.

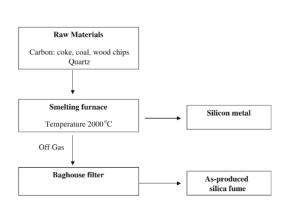
The Ecoinvent database version 3.3 presents the inventory data in three modeling methods to distribute environmental loads [8]. The Cut-off and APOS models are based on attributional approaches and they differ in the approach towards the allocation of recycling and waste treatment products. In the Cut-off model, the product system does not have any previous flows of by-products, waste treatment or recyclable materials since they are burden-free [8]. The APOS model measures all the benefits and impacts of any by-products by means of performing an expansion of the system, and allocation at the point of substitution. It is broader than the Cut-off because it includes all necessary secondary processes, such as treatment, to allow the material to be used as a by-product. Finally, the Consequential model is the broadest system, including the market and the consequences (avoided burden) of the replacement of the raw material by the by-product. And it differs considerably from the attributional system models, depending on the difference of perspective and the modeling principles [8].

Since this paper focuses on the multifunctional modeling procedures, the inventory data used is silicon production, metallurgical grade, location Rest of World (RoW) [15]. Complete data inventory is available on Ecoinvent v.3.3 documentation [15]. The location selected is due to the economic data applied, which are from Brazil. Despite the Ecoinvent v.3.3 having a SF dataset available (in the three models), it is not connected to the silicon production chain and it is reported as material for treatment or recyclable product. Even without this connections, SF is considered as a by-product in this study, and a system expansion and allocation are developed.

The Cut-off system model is selected. The simple cut-off method is the easiest to apply but it does not reflect the full consequences of the outflows and inflows [16]. The cut-off system and APOS system are similar since both models differ mainly in the treatment of recycling materials and wastes [17]. The conflicting criteria are probably part of the explanation as to why it is difficult for the international LCA community to agree on what allocation procedure is the best [16]. Figure 2 shows a silicon production scheme considering the three system models in evaluation.

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LCA methodology is complex and demands a considerable amount of data because it is based on the life cycle perspective and demands data collection of different flows of energy and materials (input and output). The primary data collection cannot usually be gathered within each specific LCA due to high costs and time limitations [18]. When the primary data is not available, background data may be used as a supplement. The background LCI databases can be considered the backbone of any LCA because they provide the process building structure and the disaggregated unit data [8].



Primary Process
Silicon Production – metallurgical grade

Main product:
Silicon

Cut-off

Slag
Silica-fume

Avoided process:
Cement alternative constituents 6-20%

Silica-fume

X

Product X is replacing Z

Z

System expansion

Figure 1. Schematic diagram of silica fume as produced [12].

Figure 2. Silicon and silica fume production representation with the available multifunctional modeling procedures. No treatment needed to SF [1].

2.2. Scenarios description of sensitivity analysis

Three different scenarios are proposed resulting from the choice of the product system models: (i) Scenario 1- System expansion model; (ii) Scenario 2- System model Cut-off with allocation by physical relationship (mass); (iii) Scenario 3- System model Cut-off with allocation by economic value. The three scenarios are proposed in seeking to expand the discussion about by-product allocation in attributional LCA studies.

Scenario 1 is based on standard ISO 14044:2006 recommendation to divide the elementary process into two or more subprocesses or make a system expansion. In this scenario, a modelling adjustment is needed, because the silicon metallurgical production dataset does not have an output of SF, as a byproduct or waste. In this study, the avoided burden of the SF as a cement replacer is considered [19]. The documents of Ecoinvent 3.3 of silica fume mention it as a replacer of different cement types [20]. The cement production, alternative constituents 6-20% - RoW (CEM II/A) is considered to calculate the avoided burden. This cement type is cited as the greater participation in the market [21].

Scenario 2 is calculated according to Chen et al., (2010) [7] and considers the percentage production as published by Fidjestol (2008) [22]. Scenario 3 is recommended in cases where the byproduct represents more than 1% of the economic value of the product (SF accounts for 6.19% of the total economic value) and added to a share in relation to the total revenue considered low (less than 25%) [23]. The production percentages of SF (SiO2 %) from silicon metallurgical production data were provided by a manufacturer [22], given as 40-50% (in mass) of SF. In this paper, a midpoint of 45% is used. Table 1 presents the values used in the allocation of SF.

2.3. Impact assessment

The support platform used for performing the LCA was OpenLCA 1.6.3, and the potential environmental impact evaluation is based only on the impact categories mentioned in CEN EN 15804 (2013): (i) Climate change – GWP-100 – kg de CO2-Eq. (100a); (ii) Acidification potential – AP – kg

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SO2-Eq. (average Europe); (iii) Eutrophication – generic EP – kg PO4-Eq. (generic); (iv) Photochemical oxidation -POCP – kg etileno-Eq. (high Nox); (v) Ozone layer depletion – ODP – kg CFC-11-Eq. (steady state); (vi) Depletion of abiotic resources – not fossil – ADPN – kg antimônio-Eq. (ultimate reserves); (vii) Depletion of abiotic resources – fossil – ADPF – MJ-Eq. (fossil fuels),; all from CML v. 4.4 baseline (2015) [24].

Table 1. Silica fume allocation percentages by mass and by economic value [7].

	Production (tons)	Market price (1 ton)	Allocation by mass	Allocation by economic value
Silicon	1,00 t	US\$ 3145 a,b	-	-
Silica fume	0, 45 t	US\$ 354 a,b	4,8%	31,0%

^a Morales et al. (2016).

3. Results and discussion

Table 2 presents the impacts of the three available multifunctional modeling procedures by ISO 14040. Comparing the results, Scenario 2 (allocation by mass) shows higher numbers than the others followed by Scenario 3 (allocation by economic value).

Table 2. LCA impacts of 1kg of SF considering three available multifunctional modeling procedures by ISO 14040. Values (in %) represent the comparison between SF and the avoided product impacts.

		Avoided product ^a					
				Scenario 3 -			
	Scenario 1 -	Scenario 2 -		Allocation by		Cement CEM	
Impacts	System expansion	Allocation by mass	%	economic value	%	II/A	%
GWP-100	-8,56E-01	9,38E+00	1095%	1,46E+00	170%	8,56E-01	100
AP	-1,78E-03	4,81E-02	2697%	7,46E-03	419%	1,78E-03	100
EP	-4,32E-04	1,46E-02	3384%	2,27E-03	525%	4,32E-04	100
POCP	-6,98E-05	3,30E-03	4724%	5,12E-04	733%	6,98E-05	100
ODP	-2,13E-08	4,31E-07	2023%	6,69E-08	314%	2,13E-08	100
ADPN	-3,00E-07	2,40E-06	800%	3,73E-07	124%	3,00E-07	100
ADPF	-3,13E+00	8,07E+01	2577%	1,25E+01	400%	3,13E+00	100

^a Silica fume is cement replacement.

GWP-100 - Climate change (kg de CO2-Eq. 100a); AP - Acidification potential (kg SO2-Eq.); EP - Eutrophication Potential (kg PO4-Eq.); POCP - Photochemical oxidation (kg etileno-Eq.); ODP - Ozone layer depletion (kg CFC-11-Eq.); ADPN - Depletion of abiotic resources - non fossil (kg antimônio-Eq.); ADPF - Depletion of abiotic resources - fossil (MJ-Eq.).

The Scenario 1 system expansion approach assume that 1 kg of SF could be applied in concrete production as an equivalent replacement of 1 kg cement CMII/A show negative results related to the avoided burden. This result is coherent since it is related to other markets. However, special attention should be given to issues regarding the availability of the by-product, because when we replace the main product (cement) with the by-product (SF), we assume "infinite" availability of the by-product, which does not occur because it belongs to a restricted production market. The worldwide generation of SF is estimated at 1.5 million tons, but today some of these materials are still not captured [22]. In an optimistic scenario assuming the capture of 70% of the generated SF (currently does not occur), the SF production would be 1.05 million tons [22]. This production represents approximately 0.13% of the world's cement production, which reached 818 million tons in 2016 [25]. This fact demonstrates that the market for SF production is restricted, and that it is therefore not appropriate to consider high

^b Considering that US\$ 1,00= R\$ 3,82 (price of the currency in march/2019).

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cement replacement rates for this material because of its low availability in comparison to the large size of the cement market. Besides this, SF efficiency in concrete is not constant at all percentages of replacement [12].

The system boundaries of the LCA of multifunctional processes can be relevant in the results. In Scenario 2, allocation by mass value, the amount of by-product generated increases the percentage of impacts related to SF. These results prove the importance of the allocation method selection. In Scenario 3, allocation by economic value, the low sales value of SF in the generation point results in lower shareholdings (Table 1). The different allocation approaches can lead to significant result variability when economic parameters are applied. In contrast, mass relationships are controlled by the production process, which is tied to the main product's production process [7]. It is therefore quite straightforward and the mass ratios are mainly constant in time [9]. However, it is important to consider that allocation by mass induces large impacts on by-products that are used in the cement industry [7]. Hence, it could increase the impacts, influencing the interest to apply by-products as replacement. In this sense, the choice of system boundaries is closely related to the objective, including the activities relevant to the purpose of the study [26].

The use of pozzolanic material as SF in SCM has been consolidated. However, special attention should be given when the system expansion multifunctional modeling procedures are applied, because the avoided product functions can be equivalent to it but not equal. According to ASTM C 618 (1978) and NBR 12653 (ABNT, 1992), pozzolanic material is defined as a siliceous or silico-aluminous material which by itself has little or no cementitious property but when finely divided and in the presence of moisture, reacts with the calcium hydroxide at room temperature to form compounds with cementitious properties [1]. In this sense, SF may only partially substitute cement, in specific rates.

Despite the concern to reduce the environmental impact by replacing raw materials with by-products or residues, it is fundamental to guarantee the quality of the new product produced without causing losses in the durability and resistance [1]. In this way, the addition of SF to concrete protects the embedded steel from corrosion and improves the durability of concrete through reduction in the permeability and refined pore structure. This leads to a reduction in the diffusion of harmful ions and reduces calcium hydroxide content which results in a higher resistance to sulfate attack [12].

The lack of data affects the quality of the LCA application and emphasizes the importance of the quality of the available data of the unitary processes provided by the database, as well as its relation between the different productive chains.

4. Final remarks

The results enhance that the selection and understanding of the proper distribution model is key, due to their great influence on the results obtained. In addition, the evaluation of modeling choices and allocation systems is decisive, since they may influence the decision-making process. When the byproduct allocation is not considered, an increase in fluxes in the main product is observed. In the system expansion, the avoided burden of by-product (in this case SF) replacing a virgin raw material, (in this case cement) with a by-product (in this case the SF) contains the assumption that the byproduct is available for the entire world market. This inference may not be real, in this particular case, as the demand for clinker is considerably greater than the SF production, it seems like the system expansion is not suitable.

Finally, the importance of the modelling choice and its understanding must be highlighted, especially in product systems that deal with multifunctionality, to promote results that properly represent the evaluated products.

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