Life Cycle Assessment of Linear Alkylbenzene Sulfonate Production: An Adaptation to the Brazilian Context

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Surfactants represent a class of compounds used in large-scale household sanitizers, the Linear Alkylbenzene Sulfonate being the most used. However, there is concern about these compounds' environmental aspects and impacts. This work aims to analyze the life cycle inventory of the production of Linear Alkylbenzene Sulfonate from cradle to gate for the Brazilian context aiming to propose improvements regarding cumulative energy demand and global warming potential. The total energy demand of the base case scenario was 59 MJ-Eq and a carbon footprint of 1.71 kg CO_{2-eq}. A scenario considering the switch in heat and electricity supply to renewable sources was proposed, and a global reduction of Global Warming Potential in 100 years of 15.73% was realized, reducing the carbon footprint of the heat supply chain by 73.07% and the electricity supply chain by 98.90%.
Keywords: Linear Alkylbenzene Sulfonate (LAS). Surfactants. OpenLCA. Life Cycle Assessment (LCA). Material Flow Analysis (MFA).

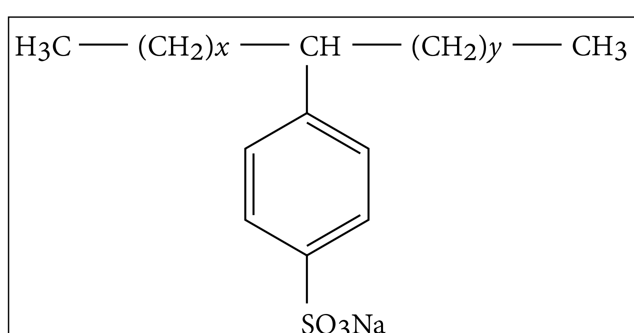
Introduction

Surfactants, or surfactant agents, are chemical compounds widely employed in a solid and liquid state for washing clothes and dishes, mainly for domestic uses but also in several industrial sectors [1]. These compounds represent a class of chemical substances with an affinity for polar or apolar substances. This characteristic is known as amphiphilic and amphipathic, which comes from its molecular structure. Therefore, part of a single surfactant molecule can interact with water, and the other part has a greater tendency to interact with oily substances, for example [2]. This property is responsible for its use in the production of detergents and hygiene products around the world. However, most commercially available compounds are produced from petroleum derivatives [3].

Linear Alkylbenzene Sulfonate, known as LAS (Figure 1), is one of the most widely used surfactants worldwide in the formulation of commercial detergents, the same in 2018 accounted for 84% of the anionic surfactant market [4,5], as it has an excellent acceptance in the market due to its high cleaning potential when compared to that of ordinary soap, the surfactant sodium lauryl ether sulfate (LESS) [6].

Even though it is widely used, this substance, like many others produced by human activities, has a production chain that implies the use of a series of processes involving extraction, manufacturing, and transportation. These processes, when operated, generate impacts on planetary systems, either by releasing carbon dioxide, consuming water, or generating chemical waste.

Figure 1. General chemical structure of Linear Alkylbenzene Sulfonate (LAS).



Source: Sablayrolles and colleagues (2209) [8].

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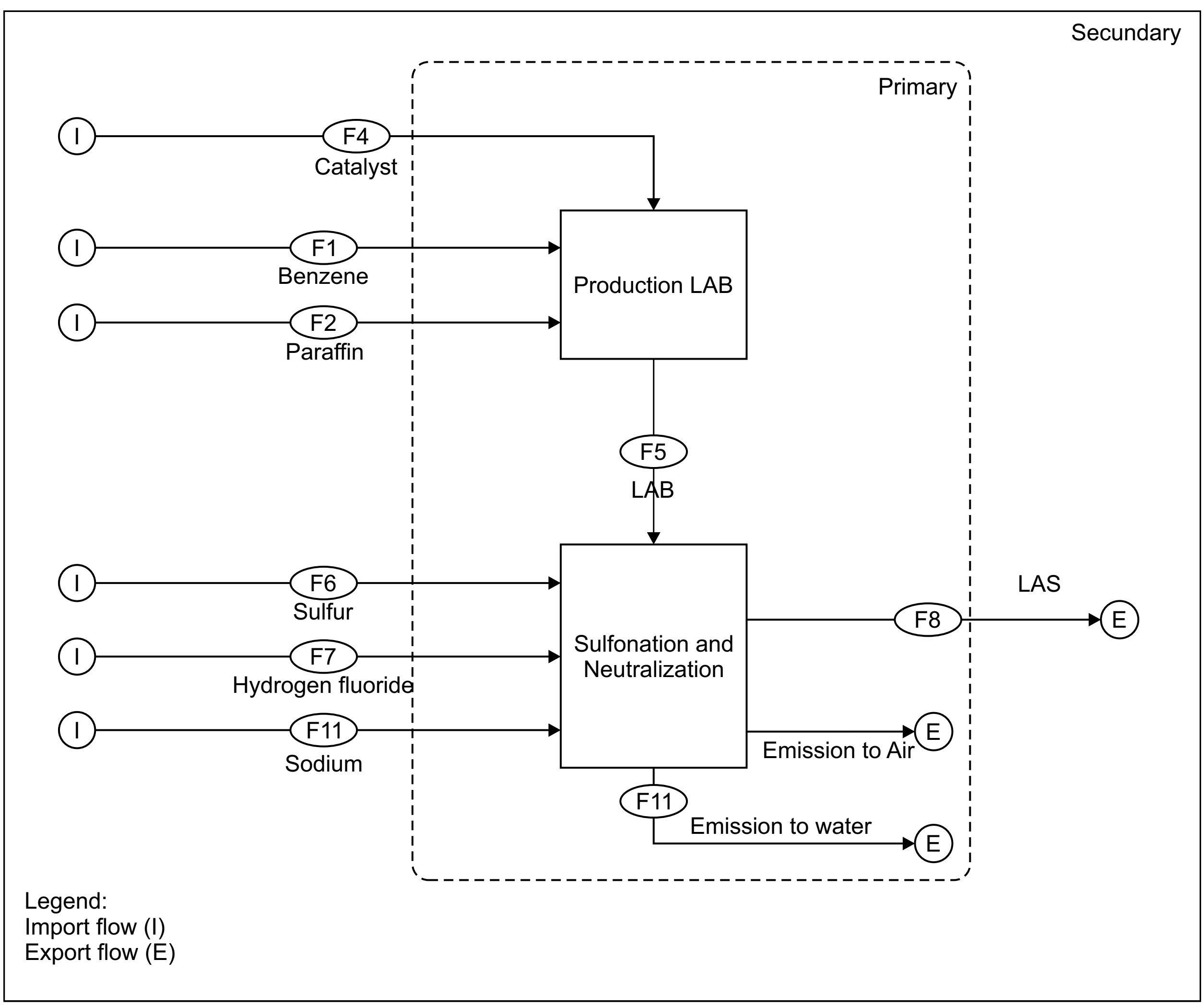
The environmental performance of a product or process throughout its life cycle can be assessed through LCA (Life Cycle Assessment), which consists of analyzing the environmental aspects of a product system in order to understand the impacts generated. The LCA study can use software to support the assessment of impacts [7]. For example, Stan allows the creation of material and energy flow diagrams. In contrast, OpenLCA allows the quantification of aspects and impacts throughout the life cycle in different energy and environmental categories.

In this context, this work aims to perform a life cycle assessment of the production of Linear Alkylbenzene Sulfonate (LAS) from cradle to gate for the Brazilian context to quantify the accumulated energy demand in order to identify opportunities for improving energy and environmental performance.

Materials and Methods

Figure 2 shows the product system considered in this study. Typical production of linear alkylbenzene sulfonate (LAS) is from the sulfonation of linear alkylbenzene (LAB) and neutralization with sodium hydroxide. LAB, in turn, is produced from the alkylation reaction of benzene with mono olefins (obtained from paraffin dehydrogenation) in the presence of the catalysts

Figure 2. Product system of linear alkylbenzene sulfonate production.



aluminum chloride (AlCl3) and hydrofluoric acid (HF) [9,10]. The use of inputs, materials, and energy and the generation of emissions were considered; however, water consumption was not included in the mass balance (Figure 1) performed in the Stan v.2.6 software.

The attributional Life Cycle Assessment (LCA) was performed based on ISO 14040 and ISO 14044 [11,12]. The function of the production system was to produce linear alkyl benzene sulfonate, and the Functional Unit (FU) reference flow used was 1.0 kg of LAS produced. The extent of the production system was from cradle to gate of the LAS plant.

The product system was modeled using OpenLCA 1.10.3 software with the Ecoinvent v3.4 database, contained in ecoinv*ent_case_studies_Ceramic_cup_vs_Paper_cup*. From the LAS production inventory (alkylbenzene sulfonate production, linear, petrochemical | alkylbenzene sulfonate, linear, petrochemical | Cutoff, U - RoW) existing in the Ecoinvent v3.4 (cutoff) inventory base.

The data from the foreground process, consisting of LAB and LAS production (Figure 2), were adapted (Figure 3), while those from the suppliers of the background processes were kept the same.

The categories evaluated in this study were Cumulative Energy Demand (CED) from the "Cumulative Energy Demand“ method, given in MJ equivalent, and Global Warming Potential (GWP) from the IPCC 2013 100a v1.03 method, which quantifies the contribution of CO_2 equivalent to global warming potential.

Figure 3 presents the input flow of the foreground inventory for the production of 1 kg of LAS obtained in OpenLCA. Adjustments were made to the heat and power supply of the foreground inventory. The electricity supply (*market group for electricity, medium voltage | electricity, medium voltage | Cutoff, U*) has been changed from RER (European data) to BR (Brazilian data), and the two heat suppliers (*market group for heat, district or industrial, natural gas | heat, district or industrial, natural gas | Cutoff*; and *market group for heat, district or industrial, other than natural gas | heat, district or industrial, other than natural gas | Cutoff, U*) have been changed from RER to GLO (global data).

Figure 4 presents the foreground inventory outputs of the LAS production corresponding to the product and emissions to air and water.

A sensitivity analysis was performed to investigate the effect of replacing the heat and electricity from non-renewable sources (fossil) with renewable sources (wood burning and low voltage photovoltaic panels) for LAS production in the evaluated category. As a result, the heat suppliers presented in Figure 3 were replaced by renewable sources (heat production, wood chips from industry, at furnace 5000kW | heat, district or industrial, other than natural gas | Cutoff, U) from the RoW region (rest of the world data) and electricity supply for also (*the market for electricity, low voltage, label-certified | electricity, low voltage, label-certified | Cutoff, S*) from the Swiss region.

Figure 3. Flow of the foreground inventory input for producing 1kg of Linear Alkylbenzene Sulfonate.

Entradas

Fluxo	Quantidade	Unidade	Provedor padrão	Entrada de qual...
chemical factory, organics	4.00000E-10	Item(s)	P market for chemical factory, organics | chemical factory, organics | Cutoff, U - GLO	(2; 3; 5; 2; 3)
aluminium, cast alloy	0.00320	kg	P market for aluminium, cast alloy | aluminium, cast alloy | Cutoff, U - GLO	(2; 3; 5; 2; 1)
aluminium, wrought alloy	0.00680	kg	P market for aluminium, wrought alloy | aluminium, wrought alloy | Cutoff, U - GLO	(2; 3; 5; 2; 1)
benzene	0.25100	kg	P market for benzene | benzene | Cutoff, U - GLO	(2; 3; 5; 2; 1)
electricity, medium voltage	0.03054	kWh	P market for electricity, medium voltage | electricity, medium voltage | Cutoff, U - BR	(2; 3; 5; 2; 1)
heat, district or industrial, natur...	2.87280	MJ	P market group for heat, district or industrial, natural gas | heat, district or industrial, natural gas | Cutoff, ...	(2; 3; 5; 2; 1)
heat, district or industrial, other...	1.60348	MJ	P market group for heat, district or industrial, other than natural gas | heat, district or industrial, other tha...	(2; 3; 5; 2; 1)
hydrogen fluoride	0.01000	kg	P market for hydrogen fluoride | hydrogen fluoride | Cutoff, U - GLO	(2; 3; 5; 2; 1)
paraffin	0.51600	kg	P market for paraffin | paraffin | Cutoff, U - GLO	(2; 3; 5; 2; 1)
sodium hydroxide, without wat...	0.12700	kg	P market for sodium hydroxide, without water, in 50% solution state | sodium hydroxide, without water, i...	(2; 3; 5; 2; 1)
sulfur	0.10000	kg	P market for sulfur | sulfur | Cutoff, U - GLO	(2; 3; 5; 2; 1)

Figure 4. Flow of the foreground inventory output of 1kg production of Linear Alkylbenzene Sulfonate .

Saídas

Fluxo	Categoria	Quantida...	Unid...	Custos / re...	Entrada de ...	Descrição
alkylbenzene sulfonate, linear...	**202:Manufacture of other chemical prod...**	**1.00000**	**kg**	**0.80500 E...**		**Linear alkylbenzene sulfonate (LAS) from b...**
Aluminium	Emission to water/surface water	1.06000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Ammonium, ion	Emission to water/surface water	1.59000E-5	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
BOD5, Biological Oxygen Dema...	Emission to water/unspecified	1.72550E-6	kg		(4; 5; 5; 5; 5)	Calculated value. The BOD, COD, TOC and BO...
Carbon dioxide, fossil	Emission to air/high population density	0.00907	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Carbon monoxide, fossil	Emission to air/high population density	4.31000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Chloride	Emission to water/surface water	0.00132	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Chlorine	Emission to air/high population density	7.80000E-8	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Chromium, ion	Emission to water/surface water	4.28000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
COD, Chemical Oxygen Demand	Emission to water/unspecified	1.72550E-6	kg		(4; 5; 5; 5; 5)	Calculated value. The BOD, COD, TOC and BO...
Dissolved solids	Emission to water/surface water	0.00278	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
DOC, Dissolved Organic Carbon	Emission to water/unspecified	5.18273E-7	kg		(4; 5; 5; 5; 5)	Calculated value. The BOD, COD, TOC and BO...
Fluoride	Emission to water/surface water	7.58000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Hydrocarbons, aliphatic, alkane...	Emission to air/high population density	0.00023	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Hydrocarbons, unspecified	Emission to water/surface water	1.49000E-7	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Iron, ion	Emission to water/surface water	2.40000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Lead	Emission to water/surface water	1.30000E-8	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Mercury	Emission to air/high population density	3.20000E-7	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Mercury	Emission to water/surface water	3.00000E-8	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Nickel, ion	Emission to water/surface water	2.08000E-6	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Nitrogen oxides	Emission to air/high population density	0.00010	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Particulates, > 10 um	Emission to air/high population density	1.64000E-5	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Phenol	Emission to water/surface water	5.22000E-7	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Phosphate	Emission to water/surface water	9.81000E-7	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Sulfate	Emission to water/surface water	6.68000E-5	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Sulfide	Emission to water/surface water	0.00011	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Sulfur dioxide	Emission to air/high population density	0.00029	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
Suspended solids, unspecified	Emission to water/surface water	0.00024	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...
TOC, Total Organic Carbon	Emission to water/unspecified	5.18273E-7	kg		(4; 5; 5; 5; 5)	Calculated value. The BOD, COD, TOC and BO...
Zinc, ion	Emission to water/surface water	7.70000E-7	kg		(2; 3; 5; 2; 1)	Literature Value. Process-related emissions ha...

Results and Discussion

Figure 5 presents the Material Flow Analysis for the production of LAS. Again, most of the input is derived from the petroleum products production chain, with the input with the highest mass contribution being paraffin.

Figure 6 shows the energy demand intensity of the different inputs to the product system by energy source. The total energy demand was 59 MJ-Eq, and, notably, the most significant demand is for fossil source energy, and the largest demanders of this energy are the paraffin (28.1 MJ-Eq), and benzene (18.4 MJ-Eq) supply chains, followed by the sulfur (3.0 MJ-Eq) and heat (4.0 MJ-Eq) supply chains.

Changes in the energy supply were suggested; the change of the source of heat and electricity is a feasible strategy for the production of LAS more sustainably (Figure 6) since energy is understood as a transforming resource and, therefore, the source of this energy does not affect the technology of the production process of LAS, in the figure mentioned are shown the energy sources that had higher energy consumption considering the base scenario and the proposed scenario.

We showed that the total CO_2 equivalent was 1.71 kg (Figure 7). The most significant $CO_{2\text{-eq}}$ emissions come from the petroleum chain (benzene and paraffin), which represent 0.92 kg. It can also be noted that the sum of the heat supply chains is 0.34 kg $CO_{2\text{-eq}}$. The sodium hydroxide and aluminum forging supply chains also present significant values.

In the proposed scenario (Figure 7), even with the total increase in energy demand for the system, there were reductions in GWP100a impacts in both the electricity and heat supply chains. The total contribution of the 100-year Global Warming Potential to this scenario was approximately 1.44 kg $CO_{2\text{-eq}}$, which represents a reduction of 15.73%.

Figure 5. Mass Balance of 1kg Linear Alkylbenzene Sulfonate Production with reconciled data.

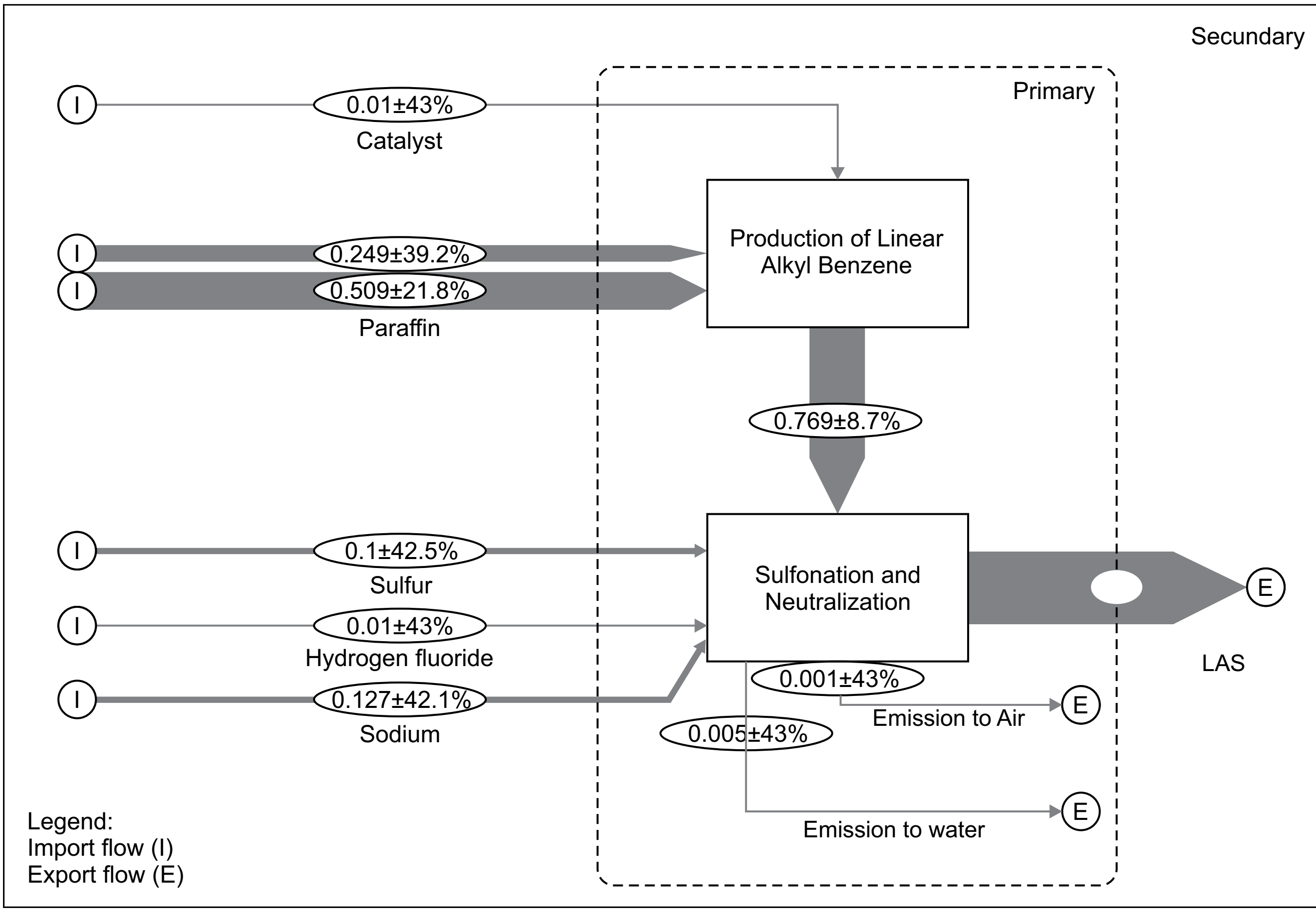


Figure 6. Cumulative Energy Demand for 1 kg of Linear Alkylbenzene production in the baseline scenario and the proposed scenario with renewable heat and electricity sources.

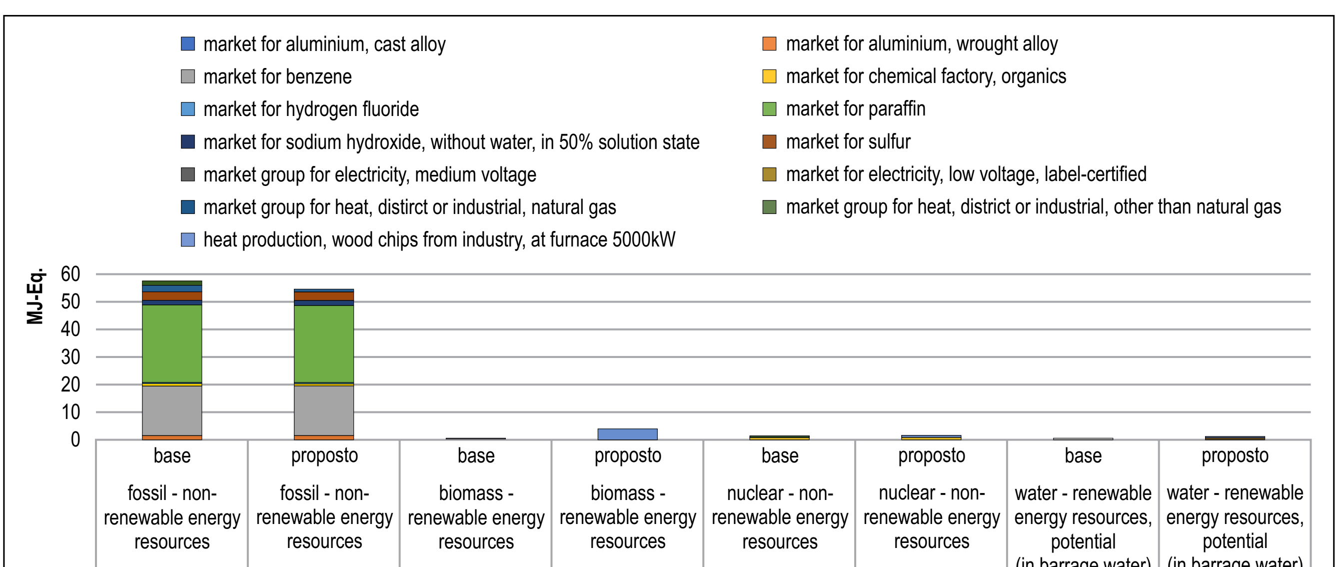
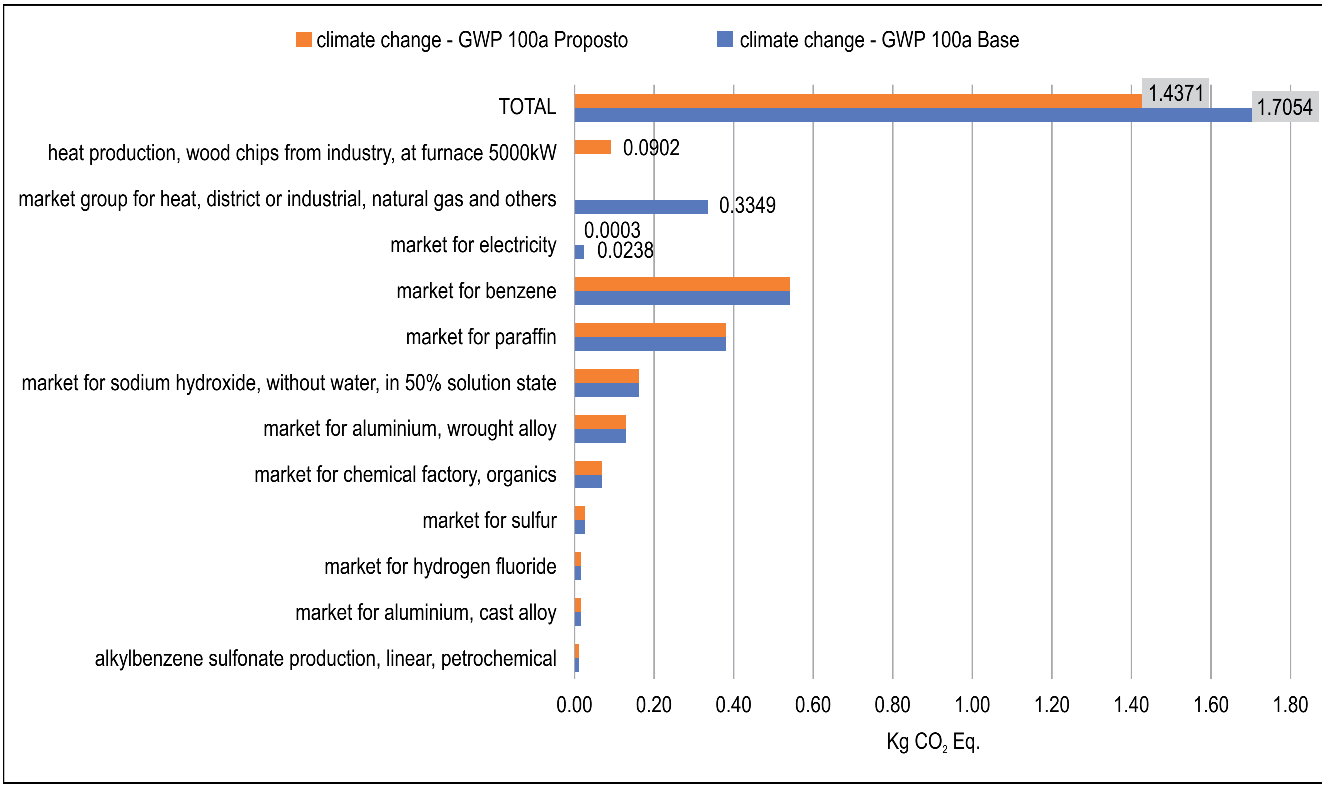


Figure 7. Impact of Global Warming Potential over a 100-year horizon for production of 1 kg of Linear Alkylbenzene with renewable heat and electricity sources.



The sum of the heat sources used for the reference flow (Figure 7) is 0.09 kg $CO_{2\text{-eq}}$, reducing 0.24 kg or 73.07% from the previous scenario concerning heat supply. On the other hand, electricity supply represented a reduction of 0.02 kg or 98.90% $CO_{2\text{-eq}}$ in 100 years.

Conclusion

A life cycle assessment of the production of Linear Alkylbenzene Sulfonate from cradle to the gate was performed. It was observed that the production of paraffin and benzene inputs are the most significant contributors to the accumulated energy demand.

As a proposal for reducing the accumulated energy demand without affecting the production technology of LAS, a sensitivity analysis was considered to affect the exchange in the supply of heat and electricity, replacing them with renewable sources, the heat supply was by burning biomass in boilers and the electricity supply with the use of low voltage photovoltaic plates certified by the distribution network by overhead line cables (CH), being observed a reduction of fossil energy sources. As a proposal to reduce the environmental impacts without affecting the LAS production technology, it was considered the exchange in the supply of heat and electricity to the system, replacing them with renewable sources, The heat supply was given by burning biomass in boilers, and the electricity supply with the use of low voltage photovoltaic panels and it was possible to observe a reduction of fossil energy sources in detriment of the use of biomass for energy generation and overall reduction of Global Warming Potential (GWP) in 100 years of 15.73%, reducing the heat supply chain by 73.07% and the electricity supply chain by 98.90%.

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