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"From measurements to improvements: Life Cycle Analysis as a tool for sustainable analytical development"

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1. Introduction

Analytical laboratories play a crucial role in scientific advancement, but their resource consumption presents a significant environmental challenge. Studies estimate that laboratories consume 5 to 10 times more energy than typical office spaces, utilize 5 times more water, and contribute significantly to the millions of metric tons of plastic waste generated annually [**1**]. Recognizing this impact, laboratories worldwide are increasingly working to minimize their environmental footprint and transition towards a more sustainable model that respects planetary boundaries [**2**]. Data-driven decision-making is essential for this transition, and Life Cycle Analysis (LCA) offers a powerful tool in this endeavor. LCA is a standardized method for evaluating environmental impacts across various categories, providing a multi-criteria and quantified approach for assessing the complete environmental profile of a product or process [**3**]. This functional approach allows for targeted analysis of specific systems to address particular problems within a defined context. In this study, an LCA was conducted on a method commonly used for analyzing natural ingredients. The method employs liquid chromatography (UPLC) coupled with diode array (DAD) and charged aerosol (CAD) detectors, as well as high-resolution mass spectrometry (HRMS). This method was selected due to its frequent application within analytical laboratories, allowing the findings to be potentially extrapolated to a broader range of analytical equipment. The primary objectives of this LCA were to pinpoint environmental hotspots within the method and evaluate strategies for their mitigation and reduction.

2. Materials and Methods

2.1. LCA methodology

This study follows the principles and frameworks of ISO 14040:2006 and ISO 14044:2006 for conducting an LCA.

The life cycle approach allows us to consider all stages of the life cycle of the different elements of the analytical method studied. Life cycle is a standardized, multi-criteria approach that allows for the evaluation of environmental impacts by category throughout the life cycle. The multi-criteria approach makes it possible to determine which elements/stages of the analysis have the greatest impact on a given category. This also helps avoid what are called "impact transfers" in proposed actions.

The LCA methodology comprises four distinct yet interdependent phases, requiring frequent iterations throughout the study. These phases are presented in Figure 1, and described below.

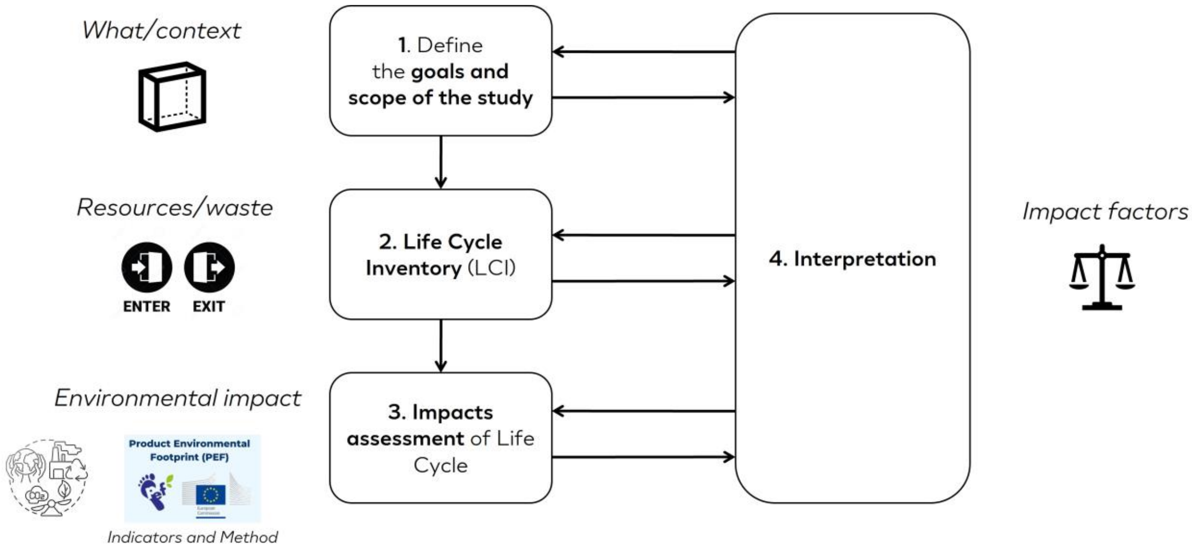

Figure 1: Four interdependent phases of LCA

Phase 1: goal and scope definition. This initial phase sets the foundation for the entire LCA. It defines the specific questions the LCA aims to address, which subsequently guides the methodological choices for the inventory, impact assessment, and interpretation phases. Key aspects include defining the intended application, target audience, product system to be studied, allocation rules, functional unit, system boundaries, data quality requirements, impact categories and indicators, and any assumptions and limitations.

Phase 2: inventory analysis. This phase involves compiling a comprehensive inventory of inputs (ressources, raw materials, energy…) and outputs (emissions and waste) associated with the product system throughout its life cycle. These flows are quantified based on the previously defined functional unit. The data base ecoinvent 3 is used [**4**]. The inventory is analogous to detailed analytical accounting, tracing all relevant flows within the system boundaries. Data collection and processing adhere to the objectives defined in Phase 1, and adjustments to system boundaries or data quality requirements may occur during this phase.

Phase 3: impact assessment. This phase translates the quantified inputs and outputs from the inventory analysis into potential environmental impacts, listed in the following part. Inventory flows are categorized and quantified according to the impact categories they contribute to, and these categories are then characterized using impact indicators. The selection of impact categories and indicators aligns with the study's objectives and the system being studied.

Optional operations, like weighting and normalization, can also be performed depending on the study's goal. The chosen environmental impacts should encompass potential consequences for human health, ecosystems, and resources.

Phase 4: interpretation. The final phase involves analyzing the results and addressing the limitations of the inventory and impact assessment to draw robust conclusions. This includes identifying the strengths and weaknesses of the product system and pinpointing critical parameters and stages within the life cycle. This analysis informs recommendations for corrective actions and impact reduction strategies. Key elements of this phase include sensitivity analysis of assumptions, completeness and consistency checks, and coherence assessment across the life cycle or between different product system options. This interpretation adheres to the ISO 14044 standard for ensuring objectivity and thoroughness.

Limits. LCA evaluates the potential environmental impacts of a product/service across its life cycle, considering both spatial and temporal dimensions. While comprehensive, the LCA uses simplified impact aggregation across locations and time, yielding single impact values per category and not reflecting local environmental sensitivities. Results represent the potential for harm, not actual impacts on specific environments. Indicator robustness varies, with human toxicity and ecotoxicity being particularly uncertain. The ecotoxicity indicator reflects aggregated potential aquatic impacts, not localized pollution. All indicators measure potential, not actual, impacts. The chosen indicators and their calculation methods define the study's assessment methodology.

2.2. Scope of the study

Functional Unit.We considered the analysis of a natural extract by UPLC-DAD/CAD/HRMS, including 20 samples per sequence (with blank, standards, sample) and 2 days of data processing. This represents the typical workload for dereplication of a natural extract at Aulnay-sous-Bois laboratory. The LCA relies on both measured laboratory data and estimated data where direct measurement is not feasible.

Method. 100 mg of the sample is solubilized at 10 mg/L in 1:1 water/ethanol, then filtered with 0.2 µm GHP. UPLC (Ultimate 3000, Thermo Scientific) analysis uses a gradient: 0-1 min: 1% Acetonitrile (ACN); 1-15 min: 1-100% ACN; 15-20 min: 100% ACN; 20.1-25 min: 1% ACN. High-resolution Mass spectrometer (Orbitrap Exploris 240, Thermo Scientific) employs an Electrospray (ESI) source at 400 °C vaporizer, 325 °C transfer tube, -3.4 kV and +3.8 kV spray voltage, 30 (Arbitrary unit, AU) sheath gas, 5 AU auxiliary and 5 AU sweep gas. Mass scanning covers *m/z* 100-1100 with full scan, data dependent MS^2 acquisitions. Data analysis uses Xcalibur 4.4 and Compound Discoverer 3.3 (Thermo Scientific) on an HP Z4 G4 workstation. Analytical set up and operational conditions are described in Figure 2.

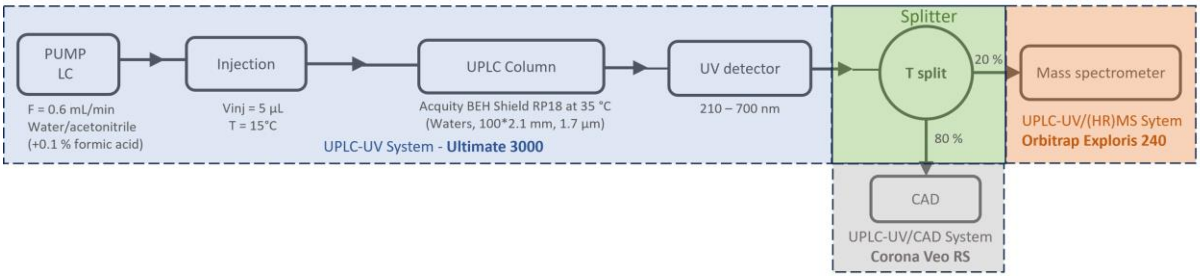

Figure 2: Analytical system studied.

The LCA considers consumables (vials, filters, columns), chemicals and solvents (water, ethanol, acetonitrile), energy consumption of equipment, sample transportation (Toulouse to Aulnay-sous-Bois), and equipment depreciation (UPLC, workstation).

List of Impact Categories Studied. The 16 indicators used are those developed by the European Commission's Product Environmental Footprint (PEF 3.0) method [**5**].

- **Air:**
  - Climate change (CO_2): represents modifications to the global climate, expressed in CO_2 equivalents.
  - Particulate matter: addresses the health effects of fine particles entering organisms, primarily through the lungs.
  - Ozone depletion: quantifies the thinning of the protective ozone layer, increasing exposure to harmful UV radiation.
  - Photochemical ozone formation: represents air quality degradation due to smog formation, with negative health consequences.
  - Acidification: reflects the ecosystem impacts of chemical emissions deposited from the atmosphere (e.g., acid rain).
- **Water:**
  - Water depletion: measures water consumption, considering regional water scarcity.
  - Marine eutrophication: quantifies the excessive nutrient enrichment in marine environments, leading to oxygen depletion and dead zones.
  - Freshwater eutrophication: similar to marine eutrophication, but focuses on freshwater ecosystems like rivers and lakes.
- **Soil:**
  - Terrestrial eutrophication: addresses the imbalance and ecosystem degradation caused by excessive nutrient enrichment in soil, particularly in agricultural lands.
  - Land use: reflects the impact of land use change (e.g., deforestation, urbanization) on biodiversity, compared to a natural state.
  - Fossil resource depletion: represents the depletion of non-renewable energy sources (coal, gas, oil, uranium).
  - Mineral resource depletion: quantifies the depletion of non-renewable mineral resources (copper, potash, rare earth elements, sand).
- **Air, water, and soil:**
  - Ionizing radiation: represents the impacts of radioactivity, specifically from nuclear electricity production waste.
  - Toxicities (3 types): includes freshwater ecotoxicity, human carcinogenic and non-carcinogenic toxicity, indicating toxicity via environmental contamination. These indicators are currently less robust.

By using these PEF indicators, LCA results can be more easily compared to other studies and can help demonstrate compliance with emerging environmental regulations.

3. Results

3.1. Contribution analysis

First, the contributions of different elements within the analysis to the overall environmental impact were assessed. These elements included electricity consumption by analytical equipment, equipment depreciation (based on lifespan), consumables, chemical/solvent use, and sample transport equivalent to a round trip between Aulnay-sous-Bois (France) and Toulouse (France) via medium-sized truck (Figure 3).

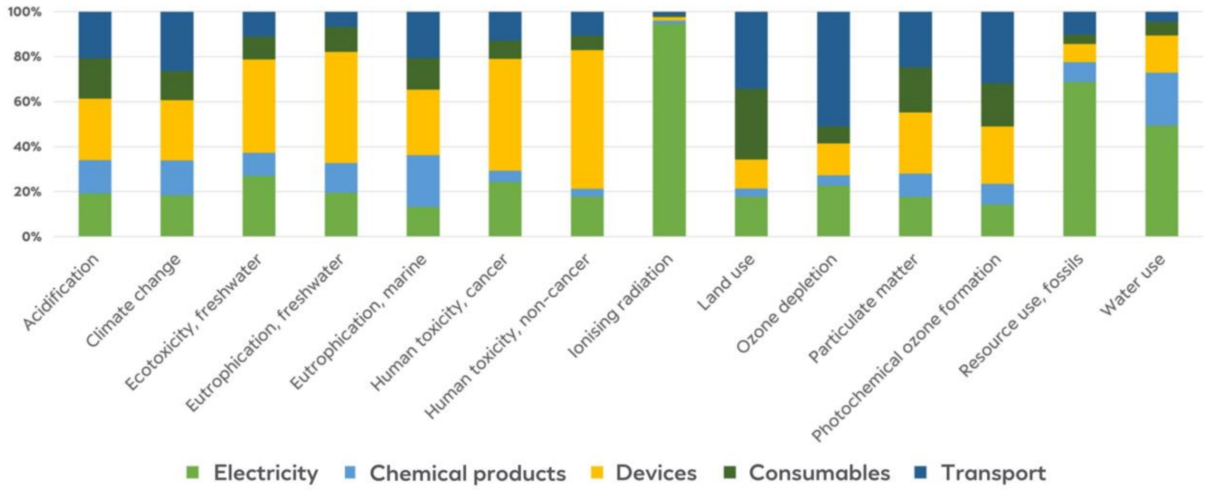

Figure 3: Contribution analysis for each indicator

Equipment depreciation (devices) was the dominant contributors across nearly all impact categories, with exceptions observed for electricity regarding ionizing radiation, fossil resource depletion, and water depletion. These preponderances are primarily attributed to the two-day data processing step involving a desktop computer (monitor, tower, keyboard, and mouse). Ionizing radiation (IR) impact stemmed largely from electricity use due to the prevalence of nuclear power in France. Nuclear fuel extraction and power plant operation release radionuclides (e.g., radon-222), contributing to this impact.

A strong correlation was observed between the number of injections within a sequence and the contribution to all indicators. Analyzing a natural extract involves injecting blanks, standards, and samples with repetitions (approximately 20 in practice, reflecting the average sequence length). In such scenarios, increasing the number of injections reduces the relative contribution of equipment depreciation, shifting the burden to other impact categories, notably chemicals, consumables, and electricity (Figure 4).

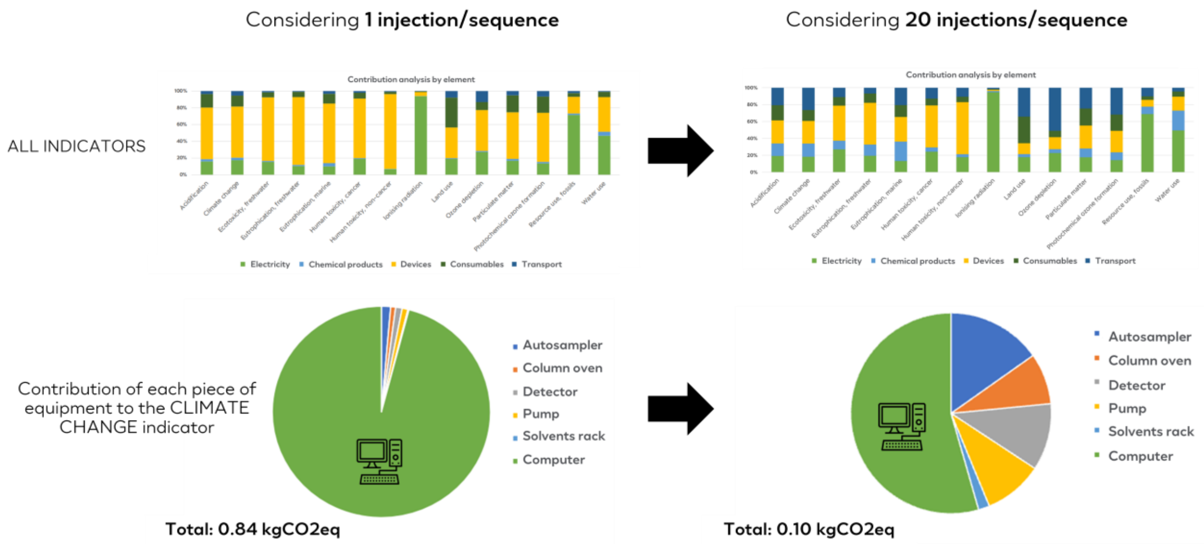

Figure 4: Impact of number of injections per sequence in contribution results

In Figure 4, focusing on the equipment contribution to climate change, while computer depreciation remains substantial, the contribution from instrument parts becomes significantly more pronounced. Consequently, managing IT resources as well as analytical instruments presents two major levers for reducing energy consumption and mitigating environmental impacts. The reduction of data processing time with automated process and the use of refurbished computer and equipment are optimization options. Additionally, this example underscores the crucial role of precise study definition in ensuring accurate result interpretation and the development of effective action plans.

3.2. Normalization

To identify environmental hotspots and prioritize their importance, the results were normalized according to ISO 14040:2006. This involved dividing each impact value by a reference quantity, specifically the equivalent annual emissions of an average European (Table 1, Figure 5).

Table 1. Values considered for normalization

Impact category	Unit	Annual emissions of an Average European
Climate change	kg CO2 eq	7553.08
Ozone depletion	kg CFC 11 eq	0.05
Acidification	mol H+ eq	55.57
Eutrophication (freshwater)	kg P eq	1.61
Eutrophication (marine)	kg N eq	19.55
Photochemical ozone formation	kg NMVOC eq	40.86
Resource depletion - fossils	MJ, net calorific value	65004.26
Water use	M3 world ea. deprived	11468.71
Fine particles matter	Disease incidence	0.00
Ionizing radiation	kBq U235 eq	4220.16
Ecotoxicity	CTUe	56716.59
Human toxicity (carcinogen)	CTUh	0.00
Human toxicity (non-carcinogen)	CTUh	0.00

Land use	dimension less	819498.18

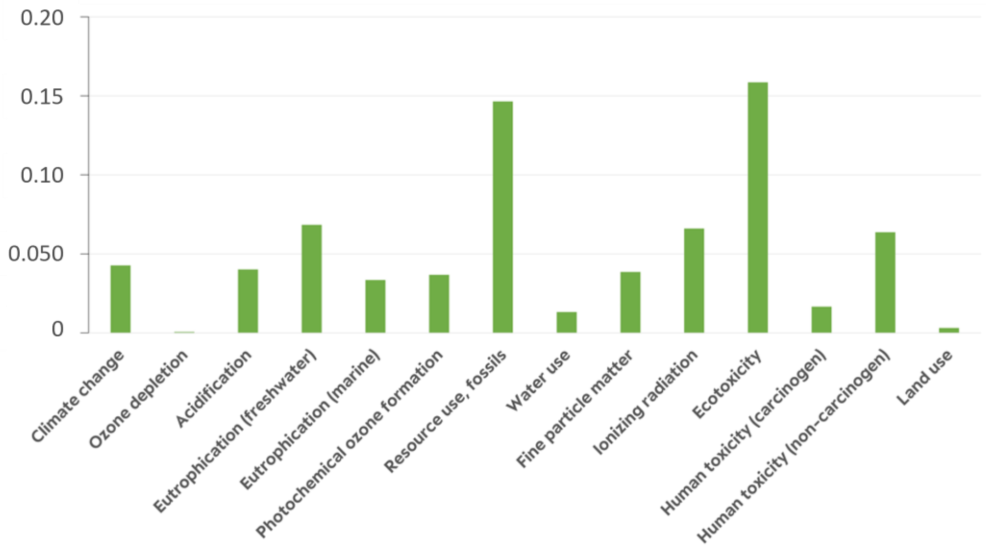

Figure 5: Normalization results considering 800 injections (40 sequences) per year

Normalization highlighted ecotoxicity as the primary impact, primarily attributed to extensive computer use and the metals contained within its components. Metals persist in the environment, enriching soils and potentially hindering plant growth. Even at low concentrations, they can pose health risks to animals inhabiting contaminated land. Human non-carcinogenic toxicity ranked second, also stemming from computer metals. Personnel involved in metal extraction and processing may experience direct exposure to potentially toxic forms, leading to bioaccumulation and health issues [**6**]. Furthermore, metal accumulation in soils can lead to plant uptake and subsequent entry into the food chain. Metal processing also generates wastewater and waste, potentially contaminating local water sources. These impact categories predominantly involve imported emissions, as the metals are largely extracted in countries like China and Russia.

3.3. Quantified units

Expressing LCA results in standardized units, such as $kgCO_2eq$ for climate change impact, allows for direct comparison of this analytical method with alternative approaches. The environmental impact of this analytical method, expressed as its carbon footprint, is estimated at 0.40 $kgCO_2eq$ per injection. Consequently, analyzing a single natural extract, which requires 20 injections and 2 days of data processing, results in a total carbon footprint of approximately 8 $kgCO_2eq$ [**7**].

4. Discussion

As demonstrated, the computer's usage, encompassing both its depreciation and the electricity mix powering it, predominantly drives the analysis's environmental impact. Employing a refurbished computer offers a compelling strategy for eco-design. ADEME reports indicate that refurbished computers can reduce Greenhouse gas (GHG) emissions by 43-97% [**8**]. A scenario modeling the use of a refurbished computer and equipment and a reduced data processing time of one day shows a potential 22% decrease in gas emissions compared to laboratory's current practices.

Given global presence of cosmetic companies, including in China, where analyses may be transferred, it is pertinent to assess potential impacts under different electricity mixes. Referencing the "market for electricity, low voltage" data in the ecoinvent database, 1 kWh in France generates 0.09 kgCO_2eq, while in China, it generates 1 kgCO_2eq—an elevenfold increase. Therefore, the GHG impact of the analyzed method would increase significantly in China compared to France.

Based on 40 analyses per year, the total impact reaches 320 kgCO_2eq, which is comparable to a round-trip flight between Paris and Toulouse, according to ADEME organization [**9**].

5. Conclusions

The environmental impact of this method is 0.40kgCO2eq (climate change indicator) per injection. For an analysis of one natural extract, including an average 20 samples per sequence and 2 days of data processing, the impact is 8kgCO2eq.

The LCA revealed that computer and equipment in global are the hotspots of this method. The equipment depreciation, particularly of the computer, and its energy consumption during the 2 days data processing stage are the primary sources of environmental impact.

This LCA successfully identified key optimization levers for minimizing the environmental footprint and reducing operational costs through enhanced resource efficiency.
The reduction of data processing time with automated process and the use of refurbished computer and equipment are optimization levers. Sharing equipment is another option.
A scenario modeling the use of a refurbished computer and equipment and a reduced data processing time of one day shows a potential 22% decrease in gas emissions compared to the laboratory's current practices.

References

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