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The Chemistry of the Future: CO_2 Alcohol in the Creation of Innovative Fragrances

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1. Introduction

The fight against climate change involves diversified actions that drive the reduction of greenhouse gas (GHG) emissions, eliminate waste and pollution, and promote the regeneration of natural resources. Currently, the transition from energy sources to renewable alternatives can mitigate around 55% of global GHG emissions. However, the remaining 45% is directly associated with the way products, materials and food are produced and consumed in today's linear and extractive economy, with an emphasis on industrial processes, deforestation, landfills and incineration – practices driven by consumption [1]. Given this scenario, the development of technologies that capture, rather than emit, pollutants such as carbon dioxide (CO_2) is becoming urgent, complementing already consolidated strategies such as upcycling.

In addition to generating energy, biomass from plants and organic waste - urban agricultural or industrial - stands out as a strategic raw material for decarbonization solutions. In contrast to fossil refineries, biorefineries transform biomass into renewable fuels and chemical compounds, including ingredients for cosmetics and bioplastics [2]. In Brazil, sugarcane accounts for around 96% of the total production of first-generation ethanol (1G), with around 350 plants in operation [3] and a production of 610.1 million tons in the 2022/2023 harvest, resulting in 27.37 billion liters of ethanol [4].

Despite its plant origin, sugarcane ethanol faces questions about the sustainability of its production, mainly due to agricultural expansion in natural areas and competition for land use between food and biofuels. Even so, sugarcane is considered one of the most productive energy crops in the world, with high energy efficiency per cultivated area and ample availability of land outside the Amazon [5]. This plant is made up of juice (the basis for sugar and ethanol), bagasse and straw, the last two of which have a high lignocellulosic content, meaning that they are viable sources for the production of second-generation ethanol (2G) [6,7]. Already used in the cosmetics industry, 2G represents a significant advance in environmental sustainability. While 1G comes from sugarcane sucrose, 2G is obtained through processes that convert cellulose, demonstrating the full use of agricultural biomass.

In recent years, researchers have been pushing the boundaries of innovation by exploring third generation ethanol (3G) - an alcohol obtained not from biomass, but from the catalytic conversion of atmospheric CO_2. A search on Scopus for the terms “ethanol” or “third generation ethanol” shows 52 publications between 1958 and 2022, 27 of which occurred in the last five years [8], which indicates growing scientific interest in the subject. This approach does not compete with the agricultural sector, significantly reduces water use compared to traditional routes, relieves pressure on land use and can even be integrated with renewable energy sources.

In perfumery, ethanol is an essential ingredient - it acts as a vehicle, gives a refreshing sensation, speeds up drying time and solubilizes formula’s ingredients, guaranteeing stability and safety for cosmetic use. It is the most common solvent in fine fragrances, usually combined with water, due to its dual polarity and olfactory compatibility.

In this context, the integration of ethanol obtained from CO_2 (3G) into the perfumery production chain is promising as a concrete strategy for reducing the sector's carbon footprint. Life Cycle Assessment (LCA), a methodology based on the ISO 14040:2009 and ISO 14071:2014 standards [5,6], was used to measure the environmental impact of partially replacing traditional ethanol with 3G in a cosmetic product. This tool makes it possible to scientifically assess environmental impacts throughout a product's life cycle, from the extraction of raw materials to disposal, and has become essential for decisions on sustainable innovation and environmental labeling.

This work investigates the potential of ethanol derived from CO_2 as an innovative and sustainable solvent for fragrance formulations. The partnership between a cosmetics company and a 3G alcohol producer, through a patented process for capturing and converting CO_2, resulted in the practical application of this alcohol in a real product - mixed with 2G and 1G - promoting circularity and innovation. The analysis includes olfactory compatibility, sensory performance and the final quality of the product, demonstrating that the use of ethanol captured from CO_2 can combine high performance with less environmental impact, effectively contributing to a greener future for perfumery.

2. Materials and Methods

We present the cosmetic application of alcohol obtained from the biosynthesis technology that converts atmospheric CO_2 into ethanol. We investigated the viability of this use in perfumery applications, using sensory and physicochemical tests in order to assess the quality of cosmetic formulations. We also carried out an environmental performance analysis of different alcohol manufacturing processes.

2.1. Olfactory evaluation of alcohol obtained from carbon capture and its impact on the product

Ethyl alcohol from sugar cane has a characteristic odor that should be monitored by the perfume industry, since it can impact on the olfactory perception of the product. In certain cases, it can even interfere with the fragrance performance. Its properties, specific and difficult to replace with other solvents, require caution when it comes to alterations and/or additions in order to avoid changes in the consumer's perception. Therefore, in order to introduce 3G alcohol into a specific item in its portfolio, the cosmetics industry opted for a new item for the market, which avoided the risk of altering the perception of a product already known to the consumer.

The olfactory evaluation of the alcohol 3G in question by olfactory experts from the cosmetics industry brought up a major challenge: its smell, even after purification, also has a characteristic odor, not similar to ethyl alcohol, more pungent and to some extent unpleasant, when compared to the 1G and 2G alcohols used by the company. To mitigate this obstacle in product development, the flow in Figure 1 was established for the development of the fragrance.

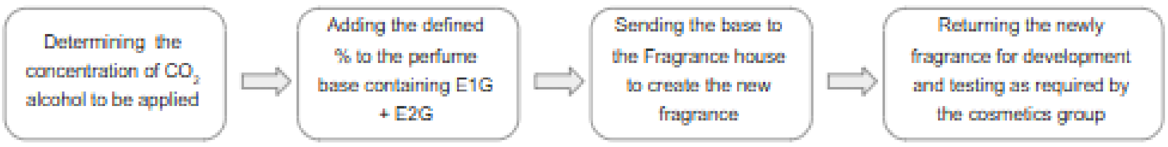

Figure 1. Flow of creating a new fragrance to cover the odor of the alcohol base containing 1G, 2G and 3G.

In the return of the new fragrance developed, its potential to cover up the specific odor of the new alcohol was assessed, to ensure the pleasantness of the new item. A Home Use Test was also carried out to assess consumer interest in the product, a quantitative research carried out with 176 consumers, 88 cases in São Paulo and 88 in Recife.

2.2. Evaluation of 3G alcohol characteristics and product stability

In addition to the olfactory aspect, the physical and chemical characteristics of the alcohol used in the composition of cosmetic items must be well monitored to ensure the quality of the product as a whole. Characteristics such as density, impurities and alcohol content are important to ensure the clarity and solubility under different conditions.

Another crucial point to be observed in any inclusion of raw materials is product safety. Thus, the evaluation of each raw material used in the composition of the product as well as its mixture in the final product is necessary to avoid skin sensitization in users considering the recommended conditions of use.

In this context, the inclusion of 3G in the cosmetic group in question required rigorous testing. The stability of the final formulation was assessed in 2 scenarios, with and without the 3G studied here.

2.3. Application of LCA tool

In order to use the LCA tool to quantify the potential greenhouse gas emissions from different scenarios of proposed formulations of the analyzed product, all the guidelines presented in the ISO 14040 and 14071 standards were used.

In this context, a comparative attributional analysis was carried out using the 100-year Global Warming Potential method, with the aim of assessing the environmental performance in terms of greenhouse gas emissions of different formulation scenarios for the product in question, covering different types of alcohols.

The analysis followed the scope established in the product system shown in Figure 2. Thus, the scope adopted in this analysis allowed a cradle-to-grave assessment of the formulations analyzed, considering the stages of extraction and transformation of the raw materials used, their transport to the production plant and finally, the production stage of the formulations considered.

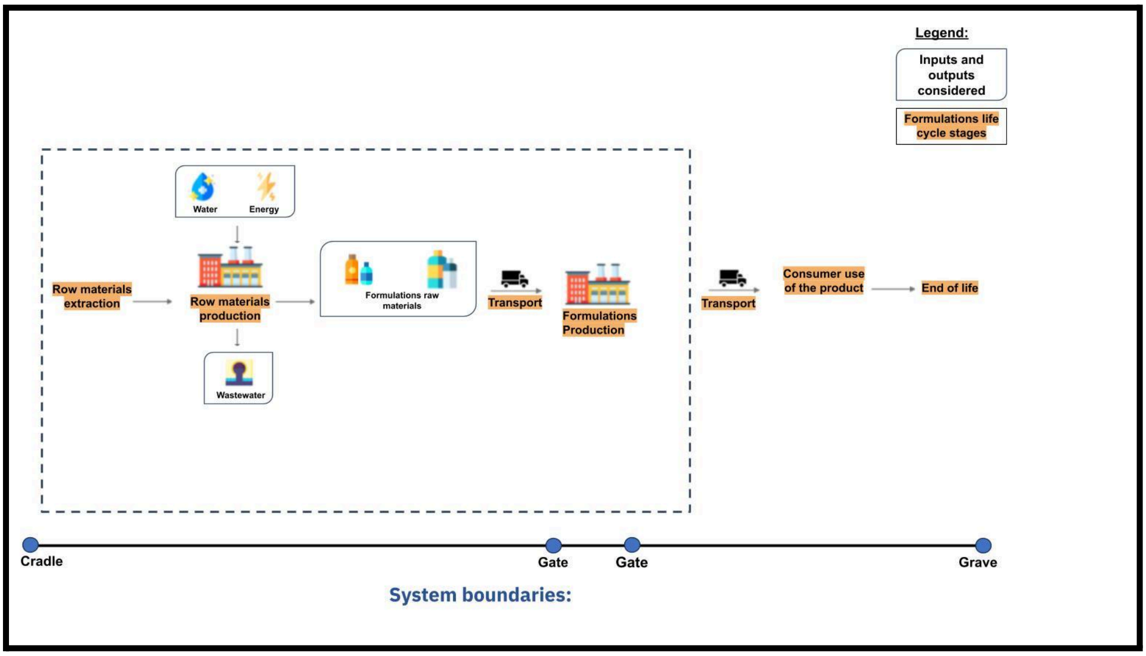

Figure 2. Cradle-to-grave evaluation of the formulations analyzed.

Thus, within the scope described, the analysis focused on the functional unit of the volume of alcohol required to produce a cosmetic. Considering the established definitions, three formulation scenarios were evaluated and presented in Table 1. Ethanol from sugar cane was designated as G1; ethanol from sugar cane residues as G2; and ethanol produced from the capture of atmospheric CO_2 as G3. With these guidelines as a reference, it was possible to assess the difference in atmospheric emissions from the 3 scenarios established, thus evaluating the environmental performance of the presence of the 3 types of alcohol in the formulation of the cosmetics considered.

Table 1. Composition scenarios for the alcohols in the formulations analyzed

Scenarios	Composition
1	Alcohol G1
2	Alcohol G1 + G2
3	Alcohol G1 + G2 + G3

3. Results

3.1 Olfactory evaluation of alcohol obtained from carbon capture and its impact on the product

In the return of the fragrance developed in question, its potential to cover up the specific odor of the new alcohol was assessed, to ensure the pleasantness of the new item. As Figure 3 shows, it was possible to have a product with the desired and pleasant smell for the target audience, even with the unwanted smell of CO_2 alcohol.

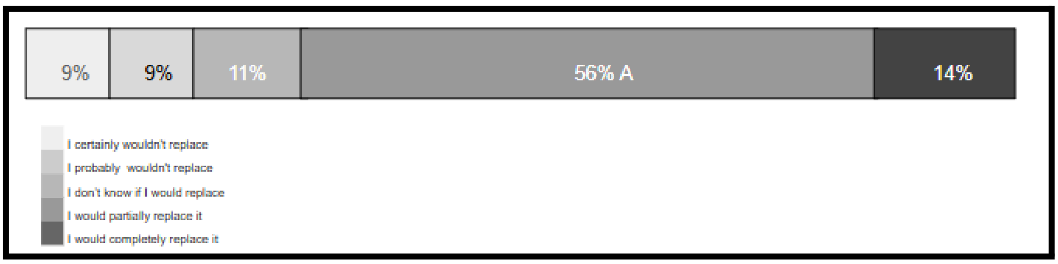

Figure 3. Replacement the new fragrance created compared to the usual fragrance

3.2 Evaluation of 3G alcohol characteristics and product stability

Only an olfactory difference was observed between the alcohol obtained by capturing CO2 when compared to the alcohols already used by the company.

Table 2. Comparative evaluation of the 1G, 2G and 3G alcohols used:

Characteristics	Specification Alcohol 1st and 2nd generation	Specification Alcohol 3nd generation
Aspect	Clear liquid, free of suspended materials	Clear and Transparent, and no visible suspended solids and sediment
Color	Incolor	Incolor
Odor	According to standard	According to standard
Density	max. 0,8071	max. 0,8071
Alcohol content	min. 96,1ºGL	min. 96ºGL
Free Acidity	max. 10 ppm	max. 10 ppm
Methanol content	max. 10 ppm	max. 12,5 ppm

The impact of the difference on the product was assessed by means of a comparative stability study, which evaluated the impact of the formulation containing a mixture of 1G, 2G and 3G alcohols versus the formulation containing only 1G and 2G. The studies, which looked at initial evaluation, 7, 15, 30 and 63 days in the conditions of 25ºC, 40ºC, 5ºC and LED light, did not identify any significant differences between the samples in terms of appearance, color or smell.

According to SCCS (Scientific Committee on Consumer Safety) the safety of cosmetic products is based on the safety of the ingredients. The rationale behind the safety of the cosmetic product being based on the safety of its ingredients comes from the fact that many thousands of different cosmetic products on the market are all derived from a limited number of substances. The product fulfills the definition of the cosmetics according to the current regulation.

3.3. Life Cycle Assessment results

Figure 4 shows the evolution of the reduction in atmospheric emissions associated with the inclusion of 2G and 3G alcohols in the cosmetic product analyzed.

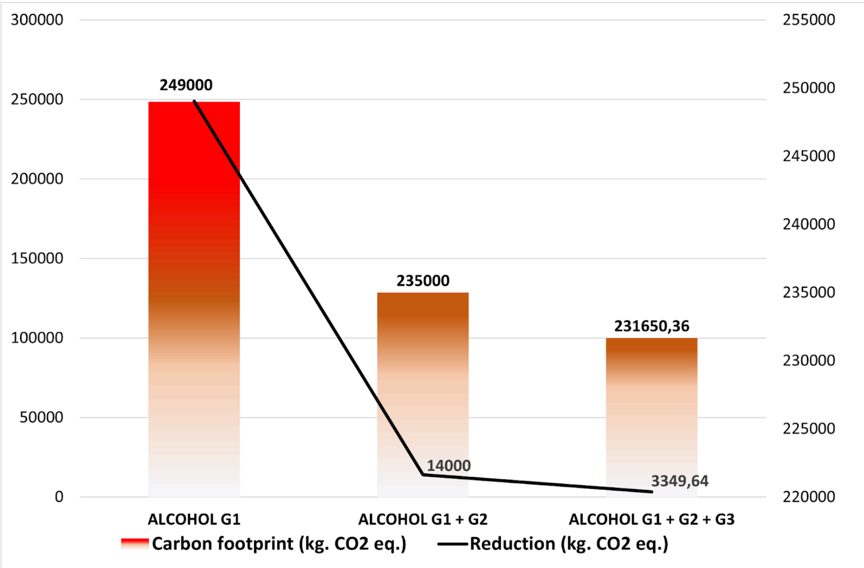

Figure 4 - Evolution of the reduction in atmospheric emissions associated with the inclusion of 2G and 3G alcohols in the formulation of the product analyzed.

Production based exclusively on G1 alcohol has an emission of 249,000 kg of CO_2 eq. The incorporation of G2 alcohol represents a significant step forward in terms of sustainability, with a reduction of 14,000 kg of CO_2 eq., totaling 235,000 kg - showing environmental gains from the use of waste. The introduction of G3 alcohol, in turn, is a significant additional step in the direction of technological innovation, promoting an even greater reduction in emissions, totaling 3,349.64 kg of CO_2 eq. and resulting in emissions of 231,650.36 kg of CO_2 eq. for the specific volume of alcohol destined for the product analyzed. These results demonstrate the cumulative potential of 2G and 3G technologies in mitigating emissions, reinforcing their strategic role in the transition to a formulation scenario with a lower climate impact and as qualified as the G1 alcohol-only scenario.

4. Discussion

The results obtained highlight both the challenges and opportunities related to the introduction of third generation ethanol, derived from the capture of atmospheric CO_2, into cosmetic formulations. The main sensory limitation observed was associated with the residual olfactory profile of the new alcohol, whose pungency and distinctive characteristics, even after purification, set it apart from the 1G and 2G alcohols traditionally used. This finding is in line with the literature which indicates that the origin and production processes of ethanol can significantly influence its organoleptic profile [7,8], especially in sensitive applications such as fragrances.

Despite this sensory challenge, the approach adopted - based on the formulation of a new product and the collaborative development of the fragrance with the fragrance house - proved to be effective in mitigating the perceptual impact of the unwanted odor. The success of the fragrance in the HUT test confirms that end consumer acceptance can be assured even in the face of technical changes to the base ingredients, provided that the formulation and development strategies are carefully conducted.

From a physicochemical point of view, the equivalence between 3G and conventional alcohols in critical parameters ensures the technical viability of its application, without compromising product stability. Although the methanol content showed a slight increase (12.5 ppm vs. 10 ppm), the values remain within the safety limits established for cosmetic applications, and no visual or organoleptic instabilities were observed in the comparative stability tests.

The Life Cycle Analysis study reinforces the strategic importance of adopting alcohols from renewable sources in the cosmetics production chain. The significant reduction in greenhouse gas emissions with the partial replacement of 1G with 2G and 3G reflects a tangible environmental gain. The accumulated reduction of 17,349.64 kg of CO_2 eq. in the volume analyzed represents not only a direct mitigation of climate impacts, but also a concrete sign of alignment with global sustainability and circular economy goals. The potential of 3G, in particular, is associated with the possibility of carbon neutrality or even negativity, a concept widely explored in recent literature on renewable carbon technologies [9,10].

It is also worth noting that the introduction of 3G ingredients in new products is an intelligent sensory and commercial risk management strategy, as it avoids direct comparisons with previous fragrances that are already fixed in consumers' olfactory memory [11]. This practice respects the strong association between scent and brand recognition, a fundamental aspect in the perfumery sector.

Captured CO_2 converted into cosmetic raw materials demonstrates a promising technical and environmental 3G viability, contingent on sensory evaluation and collaborative development. This technological advancement represents a new era for sustainable innovation and market distinction. Consumers increasingly value environmental transparency, carbon neutrality, and regenerative ingredients [12,13], making CO_2-derived ethanol a potential value-add that aligns with their ethical and environmental expectations alongside sensory performance.

5. Conclusion

In terms of environmental performance, the integration of 2G and 3G alcohols in the formulation of the cosmetic product analyzed represents a significant technological advance towards decarbonizing the sector. The partial replacement of 1G alcohol with 2G already demonstrates a significant reduction in the carbon footprint, reflecting the use of waste and greater process efficiency. The introduction of 3G alcohol further enhances these gains, indicating the promising role of innovations based on alternative raw materials. The results show that adopting these more advanced technologies is an effective strategy for mitigating greenhouse gas emissions and promoting a more sustainable economy.

The production of ethanol from the capture of atmospheric CO_2 represents a notable technological advance, with high potential to boost the decarbonization of the cosmetics production chain. The integration of second- and third-generation alcohols into the product evaluated proves to be a viable and environmentally effective technical strategy, promoting a significant reduction in greenhouse gas emissions, as evidenced by the life cycle analysis shown. The partial replacement of sugar cane ethanol with an alternative originating from agro-industrial waste reflects a more efficient use of resources and a concrete alignment with circular economy principles.

The results indicate that, even in the face of sensory challenges such as the residual odor of third-generation ethanol, the use of formulation strategies and co-creative development makes it possible to mitigate impacts on the olfactory experience and ensure the physicochemical stability of the final product. Taking advantage of 3G not only expands the technological frontiers available to the industry, but also contributes directly to sustainability goals on a global scale, reinforcing the cosmetics sector's potential as a vector for climate innovation.

Although the focus of this study is on the technical and environmental viability of the new inputs, it is important to note that sustainable initiatives such as this also resonate with the consumer market. The growing appreciation of environmentally responsible cosmetics can act as a catalyst for the adoption of these technologies, offering an additional competitive advantage to the brands that lead this movement.

6. References

[1] ELLEN MACARTHUR FOUNDATION. In: The circular economy: a missing piece in city climate action plans?. Reino Unido, 17 set. 2023.
[2] ELLEN MACARTHUR FOUNDATION. **Towards the Circular Economy:** Opportunities for the Consumer Goods Sector. Ellen MacArthur Found, vol. 2, 2013.
[3] EIA - U.S. ENERGY INFORMATION ADMINISTRATION. **Country Analysis Brief:** Brazil. Washington, DC, 4 dec. 2023. Disponível em: https://www.eia.gov/international/analysis/country/BRA. Acesso em: 24 abril 2025
[4] CONAB - COMPANHIA NACIONAL DE ABASTECIMENTO. Acompanhamento da safra brasileira de cana-de-açúcar, Brasília, DF, v. 10, n. 4 abril 2023.
[5] Associação Brasileira de Normas Técnicas. ABNT NBR ISO 14040: Gestão ambiental-avaliação do ciclo de vida-princípio e estrutura. ABNT, 2009.)
[6] INTERNATIONAL ORGANIZATION FOR STANDARDIZATION. **ISO 14071: Environmental management — Life cycle assessment — Critical review processes and reviewer**

competencies. Geneva: ISO, 2014.
[7] Muñoz, Ivan & Flury, Karin & Jungbluth, Niels & Rigarlsford, Giles & Milà i Canals, Llorenç & King, Henry. (2014). Life cycle assessment of bio-based ethanol produced from different agricultural feedstocks. The International Journal of Life Cycle Assessment. 19. 10.1007/s11367-013-0613-1.
[8] Goldner, Maria & Zamora, María & Dileo, Paola & GIANNINOTO, HERNANDO & Bandoni, Arnaldo. (2009). Effect of ethanol level in the perception of aroma attributes and the detection of volatile compounds in red wine. Journal of Sensory Studies. 24. 243 - 257. 10.1111/j.1745-459X.2009.00208.x.
[9] Assia Mansouri, Rachida Rihani, Aicha Nadia Laoufi, Melek Özkan. Production of bioethanol from a mixture of agricultural feedstocks: Biofuels characterization, Fuel, Volume 185, 2016; 612-621, ISSN 0016-2361, https://doi.org/10.1016/j.fuel.2016.08.008.
[10] Khojasteh-Salkuyeh, Yaser & Ashrafi, Omid & Mostafavi, Ehsan & Navarri, Philippe. (2021). CO2 utilization for methanol production; Part I: Process design and life cycle GHG assessment of different pathways. Journal of CO2 Utilization. 50. 101608. 10.1016/j.jcou.2021.101608.
[11] Herz RS. The role of odor-evoked memory in psychological and physiological health. Brain Sci. 2016;6(3):22.
[12] Niinimäki K, Peters G, Dahlbo H, et al. The environmental price of fast fashion. Nat Rev Earth Environ. 2020;1:189–200.
[13] Lee J, Kwon KH. Sustainable changes in beauty market trends focused on the perspective of safety in the post-coronavirus disease-19 period. J Cosmet Dermatol. 2022 Jul;21(7):2700-2707. doi: 10.1111/jocd.14493. Epub 2022 Apr 9. PMID: 35397181; PMCID: PMC9115195.