“Innovative Ecodesign Methodology for Efficient and sustainable rinse-off Cosmetic Formulations: combining LCA with Physicochemical Property Analysis”

1.Introduction

The cosmetic industry is increasingly challenged to develop products that deliver exceptional performance while minimizing environmental impact. This dual objective requires innovative methodological approaches that can quantitatively assess both aspects simultaneously. The growing focus on environmental sustainability in the cosmetic industry has driven the development of innovative approaches that integrate environmental impact assessments with functional performance measures through analytical methods. In this context, our study introduces a pioneering screening phase within the eco-design of rinse-off hair care cosmetic formulations, combining Life Cycle Assessment (LCA) [1,2] with electrokinetic measurements. A fundamental part of this approach involved using various types of hair tresses—virgin, curly, bleached, and bleached subjected to UV stress (sun test)—to realistically represent the conditions of use for the formulations. The selection of the most suitable tresses was conducted through contact angle measurements, which allowed evaluation of the wettability characteristics of hair surfaces. The results revealed significant differences among the various types of tresses, with high contact angles for virgin and curly tresses, and very low or zero values for bleached tresses.

Following the selection process, the formulations were further characterized through measurements of conductivity and zeta potential to evaluate electrostatic interactions between formulations and hair fiber under realistic conditions [3]. Analyses conducted on several cosmetic samples allowed data collection on the variation in conductivity of pre- and post-washing solutions and in the electrochemical behavior of treated surfaces.

This integrated and multifactorial approach enables simultaneous evaluation of cosmetic efficacy and environmental sustainability, aiming to identify formulations that optimize washing and rinsing performance while minimizing water consumption during the use phase. The results obtained validate the effectiveness of the proposed methodology and lay the foundation for future extension to in-vivo studies, further strengthening the scientific reliability of the protocol. The strategy presented here represents an important advancement toward ethical and sustainable practices in the field of cosmetic formulation, in line with the industry's responsible innovative objectives. Our research objectives were to: (1) develop a reproducible methodology combining LCA with physicochemical characterization; (2) apply this methodology to create an improved rinse-off conditioner formulation; and (3) quantitatively demonstrate improvements in both environmental impact and product performance parameters.

2. Materials and Methods

The method adopted consisted of three sequential phases (Figure 1).

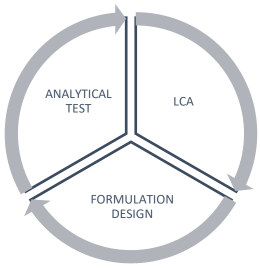


Figure 1. The figure represents the workflow process.

Initially, a preliminary Life Cycle Assessment (LCA) was conducted, using SimaPro software [4], to evaluate the environmental impacts associated with the entire life cycle of a product and to identify critical areas for improvement. Based on the results of the initial LCA, a formulation design phase was carried out, aimed at optimizing the selection of raw materials and processes in accordance with sustainability criteria and product performance. The developed formulations were then subjected to analytical testing to assess their physical, chemical, and functional performance.

For this study, human hair tresses (weighing between 600–700 mg) were used and classified into four categories: virgin hair, curly hair, bleached hair, bleached hair subjected to light exposure (Sun Test). The hair tresses, supplied by Imhair S.r.l. (Italy), were standardized in size (20 × 4.5 cm).

To select the most suitable type of hair, a wettability test of the different hair types was assessed by measuring the dynamic contact angle using a goniometer (KRÜSS DSA). Measurements were taken at three acquisition times (100 ms, 5100 ms, and 10100 ms).

For the assessment of the rinsability of the product, the surface charge was characterized through zeta potential analysis, a portion of treated hair tress (600–700 mg) was mounted in the Cylindrical Cell of the SurPASS 3 electrokinetic analyzer (Anton Paar, Austria).

Measurements were conducted using0.003 mol/L KCl solution for the evaluation of the native hair-water interfacial charge,and the interaction between hair and cosmetic formulations.

The zeta potential (ζ) was calculated based on the Helmholtz–Smoluchowski equation (Eq. 1):

$$\zeta = \frac{\mathrm{d}U_{str}}{\mathrm{d}\Delta p} \times \frac{\eta}{\varepsilon_{rel} \times \varepsilon_0} \times \kappa_B$$

dUstr/dΔp is the streaming potential coupling coefficient calculated as the slope of the linear dependence of the streaming potential Ustr on the pressure gradient Δp applied between both ends of the permeable hair plug, η and εrel are the dynamic viscosity and the dielectric coefficient of water, ε0 is the permittivity of free space, and κB is the electric conductivity of the aqueous solution [5]. Each sample was collected in triplicate.

The conductivity (mS/m) of the rinse solutions were performed using conductivity meters (XS Instruments, Italy) to confirm the results collected with the electrokinetic analysis. Each sample was analyzed in triplicate.

Several cosmetic formulations were evaluated. In this study, we present the evaluation of two rinse-off hair conditioners formulated for long, easily detangled hair: a commercial benchmark and a newly developed, eco-designed alternative formulated without silicones and with a reduced number of raw materials. While full formulation details are proprietary, key performance aspects are discussed and compared.

Analytical test results were ultimately used to enhance the accuracy of the LCA.

Table 1. The Table illustrates a summary of the analytical test performed.

Hair Type	Formulation Tested	Analysis Performed
Virgin, Curly Bleached Bleached+UV stress	None	Contact Angle Measurement (Wettability)
Bleached	New Conditioner Benchmark Conditioner	Conductivity Zeta Potential

3. Results

3.1 LCA assessment

The LCA conducted on the conditioner benchmark (Table 2) allowed us to identify the main area of improvement. To maintain a clear focus on results-oriented objectives, we selected the following impact categories: climate change, eutrophication, land use, resource use and water use. In this article, we discussed only the four main areas of contribution that could be influenced by the product formulation (raw material, production process, use phase, end of life product).

Table 2. The table shows the contribution analysis of the conditioner benchmark considering the impact categories selected.

Impact categories	Raw materials	Production process	Use phase	End of life Product
Climate change	4.8%	0.1%	87.7%	2.8%
Climate change - Biogenic	4.9%	0.1%	5.7%	69.5%
Climate change - Fossil	3.3%	0.1%	89.6%	2.5%
Climate change - Land use and LU change	97.0%	0.2%	1.7%	0.2%
Eutrophication, marine	12.8%	0.1%	18.9%	64.1%
Eutrophication, freshwater	3.5%	0.1%	18.5%	75.5%
Eutrophication, terrestrial	17.8%	0.2%	62.7%	8.4%
Land use	55.2%	0.7%	21.6%	5.2%
Resource use, fossils	3.2%	0.1%	89.5%	2.1%
Resource use, minerals and metals	16.8%	0.8%	67.9%	7.2%
Water use	1.3%	0.0%	36.7%	61.9%

Considering the main contribution and taking into account our operational boundaries, we worked on the selection of the raw materials and on the rinsability of the formulation in order to act on the water consumption in the use phase and in the end of life product.

We redesigned the formulation to improve the impact on the different categories as much as possible, as shown by the table below (Table 3).

Table 3. The table displays a summary of the contribution analysis of the conditioner benchmark considering the impact categories selected.

Impact categories	Raw materials	Production process	Use phase	End of life Product
Climate change	3.4%	0.1%	89.1%	2.9%
Climate change - Biogenic	8.4%	0.1%	5.5%	66.9%
Climate change - Fossil	2.0%	0.1%	90.8%	2.5%
Climate change - Land use and LU change	96.8%	0.3%	1.8%	0.2%
Eutrophication, marine	10.5%	0.1%	19.4%	65.8%
Eutrophication, freshwater	7.7%	0.1%	17.7%	72.2%
Eutrophication, terrestrial	14.3%	0.2%	65.5%	8.8%
Land use	50.9%	0.8%	23.8%	5.7%
Resource use, fossils	2.1%	0.1%	90.6%	2.2%
Resource use, minerals and metals	11.7%	0.9%	72.2%	7.7%
Water use	0.3%	0.0%	37.1%	62.5%

Comparing the benchmark and the new conditioner (Table 4), the percentage delta confirmed that the new product is better than the benchmark for most of the impact categories in particular thanks to a careful selection of raw materials endowed with specific conditioning and emollient properties.

Table 4. The table highlights the LCA assessment of the new product in comparison to the benchmark.

Impact categories	Unit	Benchmark	New	Δ %
Climate change	kg CO2 eq	6.92E+00	6.82E+00	-1.5%
Climate change - Biogenic	kg CO2 eq	3.56E-02	3.70E-02	3.8%
Climate change - Fossil	kg CO2 eq	6.78E+00	6.68E+00	-1.4%
Climate change - Land use and LU change	kg CO2 eq	1.09E-01	9.98E-02	-8.2%
Eutrophication, marine	kg N eq	1.08E-02	1.05E-02	-2.6%
Eutrophication, freshwater	kg P eq	2.34E-03	2.44E-03	4.5%
Eutrophication, terrestrial	mol N eq	3.44E-02	3.29E-02	-4.3%
Land use	Pt	1.68E+01	1.53E+01	-9.3%
Resource use, fossils	MJ	9.53E+01	9.41E+01	-1.3%
Resource use, minerals and metals	kg Sb eq	1.18E-05	1.11E-05	-6.0%
Water use	m3 depriv.	-17.11	-17.82	-4.1%

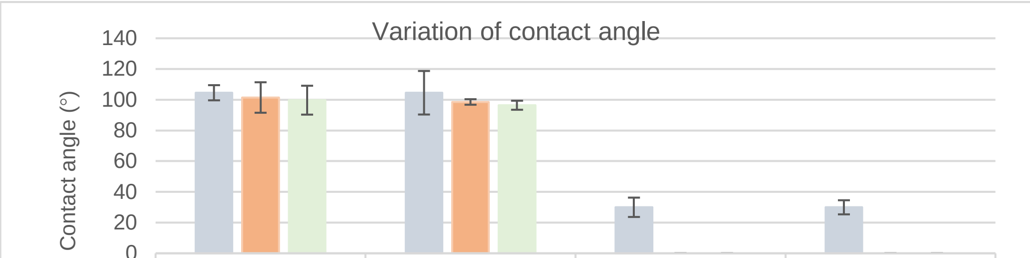
During the analytical test we attempted to optimize the percentage delta of the categories that were not improved by working on rinsability, keeping in mind that Life Cycle Assessment (LCA) studies have shown that one of the most significant environmental impacts in the cosmetic product lifecycle occurs during the use phase, primarily due to the substantial water consumption required for rinsing [6].

3.2 Wettability test

The wettability analysis, conducted on different hair types, allowed us to identify the most suitable tresses for use in this study. The results (Figure 2) clearly show significant differences in hydrophobic properties among the hair samples: virgin and curly hair maintained high contact angles (around 100°) across all measurement times, indicating strong hydrophobic characteristics. These samples exhibited only slight decreases in contact angle over time, demonstrating their resistance to water absorption. In sharp contrast, bleached and Sun test-treated bleached hair showed dramatically lower initial contact angles (approximately 30° at 100 ms), which rapidly dropped to 0° at subsequent time points (5100 ms and 10100 ms). This behavior indicates complete wetting and absorption of water droplets.

The substantially lower contact angles observed in both bleached hair samples confirm significant cuticle damage and loss of natural hydrophobicity due to the bleaching process; UV stress application did not induce any appreciable alteration.

This damage makes bleached hair more prone to water uptake and, therefore, more appropriate as a model substrate for evaluating interactions with cosmetic formulations in subsequent stuy phases.



	Virgin hair	Curly hair	Bleached hair	Bleached hair + UV stress
100 ms	104,533	104,533	29,950	29,950
5100 ms	101,433	98,533	0	0
10100 ms	99,7	96,4	0	0

Figure 2. The figure illustrates dynamic contact angle measurements for four types of hair (virgin, curly, bleached, and bleached + UV stress) at three specific time points (100 ms, 5100 ms, and 10100 ms).

Overall, the results confirm that chemical treatments such as bleaching fundamentally alter the surface properties of hair fibers, rendering them more hydrophilic. For this reason, we selected bleached hair to conduct the other analytical techniques.

3.3 Zeta potential

The analysis of surface potential kinetics (Figure 3) revealed that the increased slope of the curve associated with the new formulation reflects an accelerated desorption rate, indicative of enhanced rinsing efficiency from the substrate interface.

As shown in Figure 3, the benchmark and the new conditioner modified the hair structure contributing to the development of a positive potential on the surface. These results indicated that the new product deposits onto the hair similarly to the benchmark, thereby contributing to the conditioning of the hair surface.

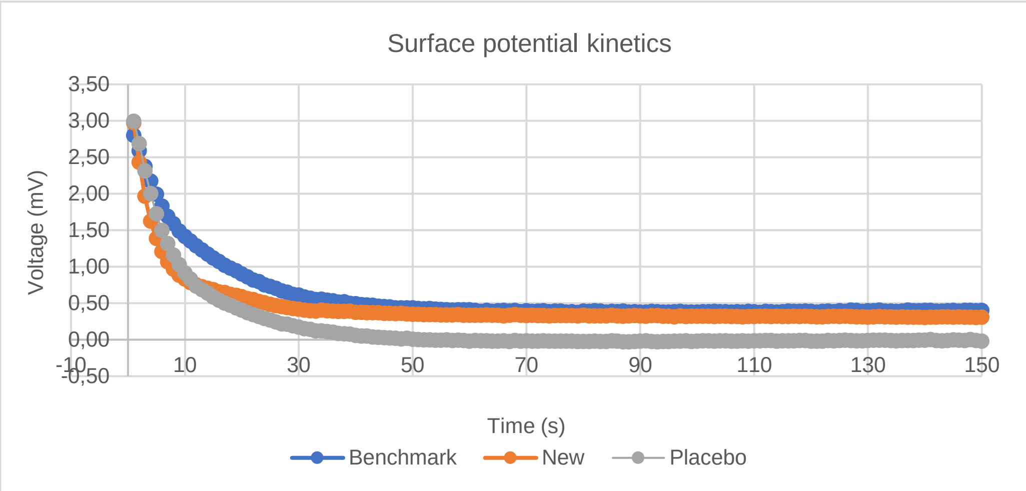


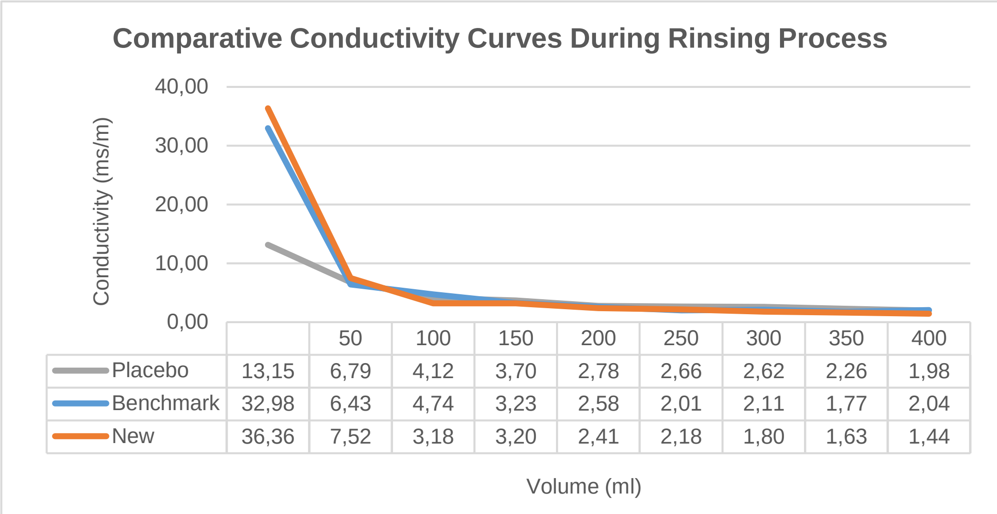
Figure 3. The figure illustrates the comparison of the surface potential kinetics of the placebo, benchmark and new conditioner considering the first 150s.

3.4 Conductivity assessment

After applying 1gr of the product on the hair, the samples were rinsed after agitation in 50ml of distilled water for 10sec. This rinsing step was repeated and for each aliquot was performed conductivity (mS/m) analysis. The variation in this parameter was evaluated and the test was stopped until the plateau was reached (Table 5, Figure 3).

Table 5. The table shows a summary of the average conductivity data collected in triplicate with the relative standard deviation.

	Placebo		Benchmark		New	
Volume (ml)	**Conductivity average (ms/m)**	**Std. Dev.**	**Conductivity average (ms/m)**	**Std. Dev.**	**Conductivity average (ms/m)**	**Std. Dev.**
	13,15	0,09	32,98	0,27	36,36	0,66
50	6,79	0,10	6,43	0,06	7,52	0,07
100	4,12	0,03	4,74	0,06	3,18	0,05
150	3,70	0,04	3,23	0,05	3,20	0,04
200	2,78	0,04	2,58	0,04	2,41	0,05
250	2,66	0,05	2,06	0,04	2,18	0,02
300	2,62	0,04	2,11	0,03	1,80	0,03
350	2,26	0,05	1,77	0,03	1,63	0,03
400	1,98	0,04	2,04	0,03	1,44	0,02



		50	100	150	200	250	300	350	400
Placebo	13,15	6,79	4,12	3,70	2,78	2,66	2,62	2,26	1,98
Benchmark	32,98	6,43	4,74	3,23	2,58	2,01	2,11	1,77	2,04
New	36,36	7,52	3,18	3,20	2,41	2,18	1,80	1,63	1,44

Figure 3. The figure presents the conductivity curves as a function of rinsing volume for placebo, benchmark, and new product formulations.

Comparing the conductivity values quantified during the following rising steps, we considered different indicators to assess the best product in terms of rinsability.
Area Under the Curve (AUC): the area under the conductivity curve, lower AUC values indicate a reduced amount of residual product throughout the rinsing process. We measured the integral of the conductivity curve across rinsing steps (Equation 2).

$$\mathrm{AUC} = \sum_{i=1}^{n-1} \frac{(y_i + y_{i+1})}{2} \cdot (x_{i+1} - x_i)$$

Initial curve slope: the slope of the initial portion of the curve was determined considering the first three values. A steeper slope corresponds to a faster removal of the product during the early rinsing steps.
Volume required to reach conductivity < 2.0 mS/m: the volume of water needed to reduce conductivity below 2.0 mS/m was determined. This threshold represents minimal residual presence and reflects the baseline level associated with bleached hair treated with water alone (placebo), corresponding to its equilibrium state. Furthermore, it's close value to the ideal one that represents the water without residue (1.0 ms/m), and it has a significative reduction compared to the initial value (94% reduction).
Final conductivity: conductivity was measured after the final rinse. Lower final conductivity values are indicative of a more complete removal of the product.

Table 6. The table provides a comparison of the conductivity values between the benchmark and the new conditioner, based on specific indicators.

Indicator	Benchmark	New	Result
AUC	40.39	40.81	Benchmark is slighlty better
Initial curve slope	-14.12	-16.59	New has a steeper slope
Volume (ml) required for conductivity < 2.0	350	300	New requires less water
Final conductivity (ms/m)	2.04	1.44	new has a lower score

The data (Table 6) showed that the new conditioner is removed more rapidly during rinsing based on three indicators out of four.
The initial curve slope is faster in the new conditioner; it requires less water to reach the conductivity target < 2.0 ms/m and it achieves a lower final conductivity. Only for the area under the curve, the benchmark performs slightly better, but with a minimal difference of around 1.0%.
To conclude the workflow, the LCA assessment of the new conditioner versus the benchmark was repeated, incorporating the data on water consumption reduction obtained from in vitro tests. The results are presented in the following table (Table 7).

Table 7. The table highlights the LCA comparison between new conditioner and benchmark.

Impact categories	Unit	Benchmark	New	Δ %
Climate change	kg CO2 eq	6.92E+00	6.04E+00	-12.8%
Climate change - Biogenic	kg CO2 eq	3.56E-02	3.36E-02	-5.6%
Climate change - Fossil	kg CO2 eq	6.78E+00	5.90E+00	-12.9%
Climate change - Land use and LU change	kg CO2 eq	1.09E-01	9.96E-02	-8.5%
Eutrophication, marine	kg N eq	1.08E-02	9.42E-03	-13.0%
Eutrophication, freshwater	kg P eq	2.34E-03	2.17E-03	-7.3%
Eutrophication, terrestrial	mol N eq	3.44E-02	2.99E-02	-13.2%
Land use	Pt	1.68E+01	1.47E+01	-12.7%
Resource use, fossils	MJ	9.53E+01	8.32E+01	-12.7%
Resource use, minerals and metals	kg Sb eq	1.18E-05	1.00E-05	-15.4%
Water use	m3 depriv.	-17.11	-15.56	9.1%

Thanks to the analytical analysis the LCA fine tuned improved even more.
The only impact categories that change in worst was the water use, this seemed counterintuitive: use less water result in a higher impact. This is due to the modelling approach used for the LCA analysis and is linked to the product end of life phase of the conditioner life cycle. Wastewater treatment faciclities have certain fixed environmental impacts, such as the construction of treatment plants and installation of equipment. These impacts don't change

based on the amount of water treated. In the LCA assessment when you treat a smaller volume of wastewater, these fixed impacts are spread over fewer units, making environmental benefit per unit appear smaller. In essence, treating less water still provides environmental benefits, but the fixed costs associated with the infrastructure are less efficiently distributed.

Combing LCA with the analytical evaluation was the best choice to overcome the impacts of this fixed infrastructure.

4. **Discussion**

The integration of LCA and laboratory-based analytical testing enabled a systemic approach to the development of the new cosmetic product, with a targeted focus on both environmental sustainability and functional performance. The initial LCA assessment highlighted that the main environmental hotspots were concentrated in the use phase, particularly related to water consumption and fossil CO_2 emissions. In response, the reformulation strategy focused on selecting raw materials with specific conditioning properties and enhancing rinsability.

Zeta potential analysis revealed that the new formulation exhibited a kinetic profile similar to the benchmark, suggesting effective conditioning action, but with a faster rate of surface charge development, demonstrating lower residue persistence. These observations were further supported by conductivity measurements, which corroborated improved rinsing efficiency: the new formulation showed a steeper initial slope, required less water to reach the target conductivity threshold (< 2.0 mS/m), and achieved a lower final conductivity value compared to the benchmark.

The improvements observed in most environmental impact categories confirm the effectiveness of the combined LCA and in-vitro testing approach.

An apparently paradoxical result was observed in the “water use” impact category, where the new product showed a slightly higher impact. This counterintuitive outcome is attributed to limitations in the LCA modelling approach: when the volume of treated water is reduced, the fixed environmental burdens of treatment infrastructure are distributed over fewer units, leading to a seemingly higher per-unit impact. This underlines the need to complement LCA data with experimental evidence to avoid misinterpretation.

The findings validate the proposed workflow as a valuable tool in sustainable product development.

This work represents only the starting point for further investigations, paving the way for in vivo studies and the extension of the methodology to a wider range of rinse-off cosmetic formulations.

5. **Conclusion**

This study demonstrated that integrating Life Cycle Assessment (LCA) with in vitro analytical testing provides a strategic approach to the sustainable development of cosmetic formulations. The application of this methodology allowed for the identification and mitigation of key environmental hotspots associated with the life cycle of a hair conditioner, leading to a reformulated product that reduced environmental impacts across most assessed categories, particularly climate change, land use, and water consumption.

From a functional perspective, rinsability and zeta potential measurements confirmed the effectiveness of the new formulation in both cosmetic performance and post-application residue reduction. Although water use impact appeared to increase, this was attributed to inherent limitations in the LCA model, highlighting the importance of a critical and integrated interpretation of environmental data.

In conclusion, this work presents a replicable methodology for the eco-design of cosmetic products, capable of balancing sustainability, performance, and formulation innovation, and offering a meaningful contribution toward circular economy goals and environmental responsibility in the cosmetics industry.

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