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DETERMINATION OF MULTI-CRITERION OPTIMIZATION FEATURES IN CREATING SYSTEMS FOR RECOMPLEXING ANHYDROUS COSMETICS

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This study explores formulation systems for anhydrous cosmetics, specifically, solid shampoos. They have predicted quality indicators and a high level of resource efficiency.

The main issue in designing such systems is the high complexity of optimization, due to technological contradictions between the product's functional effect, physicochemical stability, environmental safety indicators, and composition. This work identifies features of the multi-criteria optimization method based on the Harrington desirability function for such systems. It involves normalizing experimental indicators and aggregating them into an integrated quality indicator D. Based on this indicator, the formulation composition of sample S2 is the most balanced across all criteria.

The results are attributed to synergistic interactions among composition components and the establishment of a nonlinear dependence between the composition and properties. It has been shown that the desirability function successfully describes such interactions. It is shown that the deviation of at least one criterion beyond the limits of acceptability leads to a sharp decrease in the integrated assessment. The use of multi-criteria optimization based on the Harrington desirability function minimizes subjectivity and enables the comparison of alternative compositions of formulation technological systems.

Multi-criteria optimization using the Harrington desirability function could be applied at the stage of laboratory design of environmentally friendly formulation systems, provided that technological regimes are adhered to and an identical raw material base is used

Keywords: multi-criteria optimization, formulation technological systems, Harrington desirability function, eco-oriented design

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1. Introduction

One of the most common examples of formulation technological systems in the chemical industry is cosmetic products. Their main quality feature is not so much the presence of individual properties but the consistency among them. This applies primarily to the balance between functional, physicochemical, and environmental characteristics, which is difficult to achieve in actual industrial settings.

The current stage of development of the cosmetic industry is accompanied by an expansion of product range, which is accompanied by the accumulation of environmental risks because of the use of natural resources. High levels of water and energy consumption, the formation of significant amounts of waste are the root cause of increased regulatory pressure on manufacturers. Therefore, recently, new environmentally friendly products, namely, anhydrous ones, have increasingly appeared on the cosmetic market.

In the context of technological advancements, there is a need to optimize individual parts of production in accordance with the principles of resource conservation. The basis of this process is the minimization of material flows at all stages of the product life cycle. by optimizing while preserving the quality of the finished product.

Synergistic effects are the main factor affecting the quality of multi-component products. They determine the integral, structural, and operational characteristics that form a nonlinear relationship between the composition of the product and its properties.

Taking into account these characteristics and establishing the features of their interaction is a prerequisite for designing an effective technological system of the formulation type. In these systems, the determining way to achieve the optimal balance between such properties as functionality, stability, resource efficiency, and environmental friendliness is the selection and multi-criteria coordination of the product composition.

Conventional design methods do not allow for the full consideration of the emergence of synergistic effects between components as they are based on the alternate variation of factors and are mostly focused on optimizing individual properties without taking into account the compromise between composition, quality, and resource efficiency. The empirical process of designing cosmetic products leads to overspending of resources and limitations in predicting the properties of the final product. This is especially evident when designing anhydrous cosmetic products for which requirements for stability, functionality, and environmental friendliness are increased, which makes it difficult to achieve optimal properties. Under such conditions, multi-criteria optimization and mathematical modeling are urgent tools of today when designing anhydrous cosmetic products. Their application makes it possible to reveal quantitative regularities of influence of formulation factors on a set of quality indicators and to define the optimal composition.

The results of such research make it possible to reduce duration and cost of design, to increase stability of quality, and to reduce energy and material costs. Scientifically guided design of cosmetic products could make it possible to design competitive anhydrous products which meet a set of requirements.

2. Literature review and problem statement

One of the sources of information that shapes the quality of products is the base of regulatory documents. In Ukraine, for cosmetic products, the basic document is the technical regulation on cosmetic products, harmonized with EU Regulation No. 1223/2009[1], which orients the Ukrainian market to European requirements.

Analysis of the provisions in regulation [1]reveals emphasis on strengthening the requirements for safety, labeling, and notification. At the same time, the document focuses mainly on human chemical safety, without taking into account systemic environmental optimization and the principles of “green” chemistry, which leaves this issue unresolved. Currently, there are systemic gaps in the regulatory and methodological aspects of sustainable development in the field of cosmetic production.

Life cycle assessment (LCA) is one of the key tools for ensuring the environmental sustainability of cosmetic products. Paper [2] shows the application of LCA of shampoo based on plant components. The authors analyze the impact of packaging and refill systems on the ecological footprint of production. In [3], the authors summarize modern approaches to sustainable development in the cosmetics industry, including the assessment of environmental impact at all stages of the product life cycle. However, the issues of implementing LCA for a whole range of formulation systems remain unresolved due to the complexity of data collection, variability of product formulations, and changes in consumer behavior. In addition, the authors draw attention to the lack of unified approaches to the assessment of multicomponent systems.

In [4], the integration of circular economy principles in the process of designing cosmetic products using the ANP-QFD approach is considered. The authors indicate that taking into account the principles of closed material cycles makes it possible to increase the sustainability of the finished cosmetic product. However, the issue of practical implementation of such circular models in industrial settings remains unresolved. The implementation of circular economy principles is limited by the technical capabilities of the equipment, the weak development of the infrastructure for the reuse of materials, and the lack of economic benefits from entering a new market.

In [5], the requirements for cosmetic products within the framework of the current technical regulations are analyzed. Attention is paid to the issues of safety standards, compliance procedures, and requirements for the labeling of the finished product. At the same time, the issues of environmental optimization and support for innovative solutions in the field of sustainable development are not considered sufficiently. This is due to the orientation of the regulation on the prevention of possible risks, while the development of environmentally friendly approaches is not a priority.

Historically, cosmetic requirements have been formulated for liquid forms (shampoos, gels) in which water is the main component and solvent. Paper [6]reports the results from analysis of cosmetic products according to environmental standards. It is shown that liquid systems can be easily standardized by pH, viscosity, and microbiological purity, which provides and emphasizes the importance of a comprehensive assessment. Issues related to the environmental impact throughout the life cycle remain unresolved. The reason for this is the aqueous nature of liquid products, which necessitates the use of preservatives, complicates logistics and leads to the formation of a significant amount of wastewater. An additional factor is the heavy dependence on plastic packaging. As a result, formal compliance with the regulations does not guarantee the actual environmental effectiveness of the product.

Modern environmental management requires reviewing not only the composition but also the aggregate state of cosmetic products. In [7], a solution to the above problems is proposed by switching to anhydrous products. It is shown that the exclusion of water makes it possible to abandon preservatives, reduce the use of plastic packaging, and significantly optimize logistics costs, combining functional efficiency with current environmental strategies. However, problems remain associated with scaling and dissemination of this concept. The reasons for this are the technological aspects of implementation, ensuring the stability of the resulting cosmetic formulas, changing consumer habits, and insufficient level of trust in the new product.

The conceptual basis for the evolution of anhydrous cosmetics is based on three strategies, including WaterlessBeauty – as a transition from a marketing trend to an environmental necessity. As noted in [7], the rejection of the aqueous environment reduces the carbon footprint and the need for preservatives that are capable of bioaccumulation. The use of this approach is reflected in [8, 9], in which the concept of WaterlessBeauty is considered as part of an integrated quality that encompasses functional, technological, and dermatological indicators. However, problems such as lack of hydration and a limited range of products, compared to conventional cosmetics, may restrain market growth.

Similar issues were also analyzed in work[10]. The basis of the study is the implementation of the ZeroWaste approach, which involves an engineering method for preventing waste generation. This is achieved by using an alternative type of packaging or abandoning it. It is noted that the solid form allows the use of paper packaging, the recycling rate of which is 81%(compared to 10–15% for plastic). However, there is a decrease in the level of consumer confidence in such cosmetic products. This is explained by the fact that the product is offered on some online platforms without proper confirmation of the origin of the raw materials. This complicates the objective perception of the quality of cosmetic products, and therefore the relevance of ensuring the stability of their characteristics both at the development stage and during the circulation process increases.

The generalization of approaches to reducing environmental impact is reflected in the GreenChemistry concept, the methodological basis of which is a system of 12 principles of green chemistry [11]. In works [12, 13] it is noted that the implementation of this principle includes the use of renewable raw materials and energy-efficient technologies (for example, hot mixing at 50–60°C instead of complex synthesis). In [14, 15] the key basis of GreenChemistry is the use of biodegradable ingredients (in particular, instead of surfactants) with the introduction of GreenScore formulation assessment tools.

Comparing the above concepts, it should be noted that each of them contains its own special approach to characterizing the quality of formulation technological systems in the form of waterless shampoos. For example, ZeroWaste focuses on packaging and reuse, WaterlessBeauty on the concentration and form of the product, and GreenChemistry on reducing toxicity and ensuring biodegradability. Each of these approaches has its advantages, as they all contribute to ensuring certain environmental components regarding the quality of the final product. At the same time, the use of only one of these concepts does not make it possible to fully predict the quality of the product, which is determined by both the chemical safety of the starting raw materials and the composition of the packaging, that is, in general, the assessment of the product's life cycle.

At the same time, the transition to anhydrous systems cannot be based only on declarative "environmental friendliness". As noted in [16, 17], the product must be stable, safe, and effective. Conventional methods for assessing the quality of shampoos are often fragmentary: as noted in [18], they analyze indicators in isolation, ignoring the complex interaction and possible conflicts between properties.

However, when designing formulations of anhydrous cosmetics, one often encounters the problem of high sensitivity of the system to variations in the constituent ingredients. Minor changes in the ratio of formulation components can lead to disruption of structural and mechanical properties, changes in dissolution kinetics, instability of the pH level, increased foaming, and excessive dissolution. For example, increased foaming can reduce dermatological softness, and excessive hardness of the bar can worsen its dissolution. The optimal product should be in the compromise zone, where all characteristics (functional, environmental, consumer) are acceptable. Therefore, the efficiency of such technological systems requires the search for features of their optimization.

The key in this direction is the use of multi-criteria decision-making methods. The use of the Analytical Hierarchy Process (AHP), the technique of preference by similarity to the ideal solution (TPSIP), and the desirability function (Harrington) are crucial for modern engineering and technological systems. In [19], this is explained by their ability to effectively process complex scenarios with conflicting goals.

AHP as a structuring and weighing tool makes it possible to decompose a complex problem into a hierarchical structure consisting of a goal, criteria, and alternatives. The method is based on a process of pairwise comparisons where experts use the Saati scale (from 1 to 9) to determine the relative importance of parameters. The consistency of judgments is also checked using the consistency index, the consistency ratio. If the consistency ratio does not exceed 10%, the results are considered reliable.

TPSIP is used for objective ranking of alternatives. The method is based on the concept of choosing a solution that is at the shortest distance to the positive-ideal solution and is remote from the negative-ideal. Paper [20] emphasizes the advantages of this approach. It is characterized by high computational efficiency, independence from the number of criteria and understandable logic, which makes it possible to find compromises in which the weakness of one indicator is compensated by the strength of another.

There are hybrid approaches, in particular AHP-TPSIP, which combine the advantages of both methods: AHP is used to calculate the weight of criteria, and TPSIP is used for ranking.

In complex systems, parameter values are aggregated using Harrington desirability functions, which makes it possible to combine different physical units of measurement into a single solution acceptability index. This method is most often used at the laboratory design stage, which makes it possible to transform heterogeneous qualitative and quantitative indicators into a single integrated quality indicator. A characteristic feature of the method is the consideration of "zero points" – critical discrepancies at which the product cannot be considered high-quality regardless of other advantages.

Our analysis of the above studies reveals that despite the greening of the cosmetic industry, the problem of establishing quantitative patterns of the relationship and comprehensive coordination between the composition of formulation systems and heterogeneous criteria that form the quality of anhydrous cosmetic products still remains unresolved. There are no unified approaches to integrating heterogeneous criteria into a single evaluation system suitable for predictive design. Evaluation approaches are often fragmented, do not establish patterns between composition and quality, and do not make it possible to predict properties even during design. There are a number of reasons for this, which include the diversity, multicomponent nature, variability of formulations, and constant updating of the range of cosmetic products, including the emergence of new formulation anhydrous systems. Insufficient regulatory limitations, the predominance of empirical approaches, and focusing only on individual key quality indicators in the design of anhydrous cosmetic products also do not make it possible to solve the issue of comprehensive optimization of their compositions.

3.The aim and objectives of the study

The purpose of our research is to achieve predicted quality indicators of formulation systems of anhydrous cosmetics by determining the features of their multi-criteria optimization using the desirability function (Harrington). This will make it possible to optimize the formulations of such systems, taking into account the heterogeneity of their quality indicators and minimizing internal conflicts of the system.

To achieve the goal, the following tasks were set:

– to analyze the influence of the composition of anhydrous cosmetics on their functional, technological, and dermatological quality indicators;

– to normalize the resulting indicators and integrate them through partial desirability functions into an integrated quality indicator of the system;

– to rank the derived integrated quality indicators to determine the optimal composition for an anhydrous cosmetic.

4. The study materials and methods

The object of our study is the formulation systems for anhydrous cosmetics, namely, solid shampoos with predicted quality indicators and a high level of resource efficiency.

The principal hypothesis assumes that:

– formulation systems of anhydrous cosmetics are characterized by multiparametric quantitative patterns of the relationship between the formulation composition and quality and resource efficiency indicators;

– the use of multicriteria optimization using the Harrington desirability function will make it possible to determine these patterns and establish the boundaries of rational formulation parameters, establishing a compromise between heterogeneous quality indicators of anhydrous cosmetics.

The following assumptions were adopted in the study:

– there are continuous and approximate dependences between the formulation composition and quality indicators of formulation systems;

– formulation factors can be varied within specified limits to determine target indicators;

– quality and resource efficiency criteria can be translated to a dimensionless scale and aggregated into a generalized desirability function.

At the same time, the number of criteria is limited to key indicators, and the environmental friendliness of the product is formed by the optimal values of functional, technological, and dermatological indicators under specific technological conditions. Interactions of higher orders of components are not taken into account. The process of manufacturing anhydrous cosmetics is considered stable.

Given the multicomponent nature of the formulation of a solid cosmetic product and the need to analyze the synergistic effect of ingredients on the quality characteristics of the finished product, a fractional factorial design of type 3^{3-1} was used to study the influence of ingredients. The sample formulations (Table 1) were based on a combination of the content of the main anionic and amphoteric surfactants, structuring agents, and auxiliary components (lipid phase, active additives).

The technological process of obtaining solid shampoos took place by heating in a glass laboratory reactor with stirring by a bladed overhead mixer and included the following stages [21]:

1. Preparation of raw materials, weighing of solid surfactants and grinding of lipid components took place using electronic analytical balances with mechanical grinding in a laboratory mill.
2. Melting of the lipid phase: heating of cetyl alcohol and shea oil to 50–55°C and mixing them at 250 rpm until a homogeneous melt was obtained.
3. Emulsification: heating at a constant temperature within 50°C with the gradual introduction of liquid surfactants and water into the melt, as well as the addition of solid surfactants until a homogeneous plastic paste was formed.
4. Cooling: lowering the mass temperature to 30–35°C and introducing thermolabile additives (essential oils, panthenol, glycerin, preservatives).
5. Forming: placing the mass in silicone molds followed by manual pressing of the samples to remove air cavities.
6. Maturation: keeping the samples in a laboratory cabinet for 24–48 hours at a temperature of 20–22°C to crystallize lipids and remove excess moisture.

Table 1

Solid shampoo formulations

Component	Sample, g								
	S1	S2	S3	S4	S5	S6	S7	S8	S9
Sodium Cocoyl Isothionate	60	60	60	40	40	40	20	20	20
Sodium Coco-Sulfate	–	–	–	20	20	20	40	40	40
Cocamidopropyl Betaine	5	10	15	5	10	15	5	10	15
Cetyl Alcohol	2	3	4	3	4	2	4	3	2
Shea Butter	2	3	4	3	4	2	4	3	2
Decyl Glucoside	5								
Sodium Lauroyl Oat Amino Acids	3								
Glycerin	4								
Panthenol	2								
Hydrolyzed Wheat Protein	2								
Lavender Essential Oil	0,2								
Water	To100								

Key quality indicators of anhydrous cosmetics [22] were selected as optimization criteria, which are given in Table 2.

Foaming ability and foam stability are key to consumer perception of shampoo quality. The most common and acceptable for research is the modified Ross-Miles method or its laboratory analogs [23].

Dissolution time is a kinetic indicator that characterizes the resistance of the bar to soaking and its economy of use. When determining it, the time of complete dissolution or disintegration under the action of mechanical stirring of a 1 g sample of solid shampoo in 100 ml of deionized water at a temperature of 25°C is recorded.

The content of solids by dry residue was determined by the gravimetric method. The method involved preliminary drying and weighing of a porcelain (evaporation) cup, obtaining an aqueous solution of shampoo after a standard cycle of use and selection of a 50 ml sample. The sample cup was dried in a drying oven at 105°C until complete removal of moisture, followed by cooling in a desiccator and weighing on an analytical balance. The mass of the dry residue was determined by the difference between the masses of the cup with the dry residue and the empty cup [24].

Organoleptic examination was based on expert evaluation on a 5-point scale (appearance, color, odor, texture, homogeneity, where 5 is excellent (solid block, smooth surface, pleasant odor), and 1 is unsatisfactory (stickiness, heterogeneity, pungent odor) [18].

Table 2

Categories of quality indicators for solid shampoos

Category	Key indicators	Scientific, technological, and environmental significance	Consequences of insufficient indicator values
Functional	Foaming ability, foam stability, dissolution time	Determine consumer value, product competitiveness, and resource efficiency (LCA)	Increased consumption of raw materials, energy, and water
Technological	Solids content, organoleptic characteristics	Ensure ease of use, sample lifetime, economic feasibility of production and water footprint	Reduced resource efficiency, short life cycle
Dermatological	pH indicator	Guarantee safety of use, preservation of skin barrier function and biocompatibility	Increased overall chemical load, increased environmental impact

The pH of the sample solution was determined according to DSTU EN1262:2007[25] by the potentiometric method, using a digital pH meter in a 5% aqueous solution of solid shampoo in triplicate. To improve solubility, the samples were heated to a temperature of about 50°C with subsequent cooling to room temperature. Before measurements, the device was calibrated using standard buffer solutions. Preparation of the glass electrode included rinsing and immersion in the test solution until the values stabilized. Measurements were performed for all samples, with subsequent calculation of the average value with an accuracy of 0.1 units.

Optimization of the composition and properties of solid shampoos was carried out by applying the Harrington desirability function [26], which makes it possible to integrate several heterogeneous quality indicators into a single generalized criterion according to the algorithm in Fig. 1.

The methodology is based on the transformation of each experimental indicator y_i into a dimensionless partial desirability function d_j, the value of which varies in the interval from 0 (unacceptable quality) to 1 (optimal quality).

The evaluation process consisted of the following stages:

1. Defining the system of factors and quality indicators.

The formulation technological system is described by a number of variables

$$X = \left(x_1, x_2, \ldots x_n\right), \quad (1)$$

where x_i – ingredient concentrations.

The quality indicator is formed as a series

$$Y = \left(y_1, y_2, \ldots y_n\right), \quad (2)$$

where y_i – experimentally determined quality indicators of solid shampoo (Table 2).

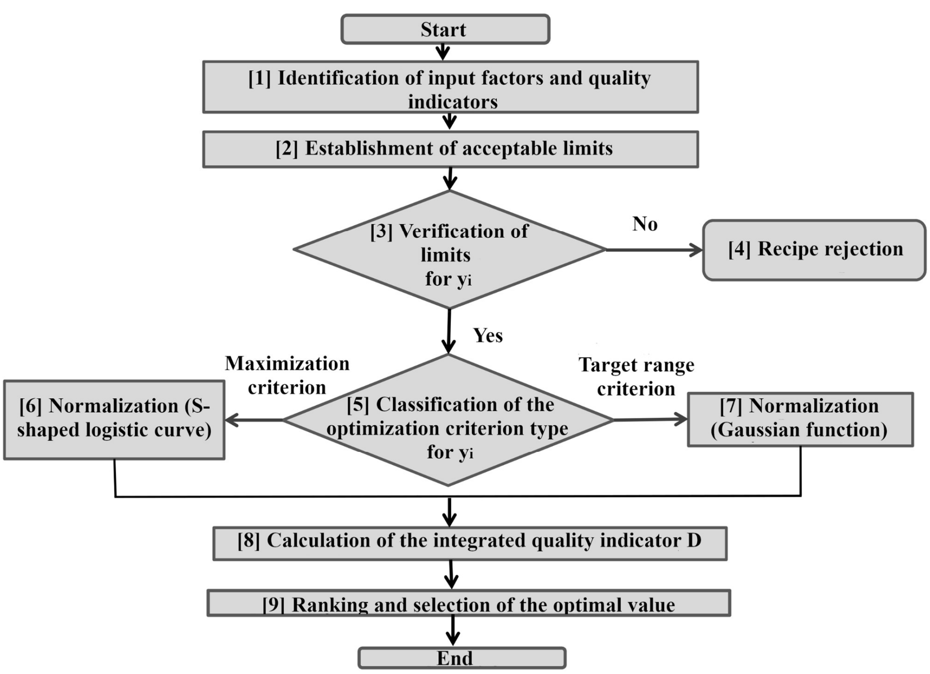

Fig. 1. Multi-criteria optimization algorithm using Harrington desirability function

2. Establishment of acceptable limits

Acceptance limits are determined for each indicator

$$y_{\min} \le y_j \le y_{\max}. \quad (3)$$

If the indicator value goes beyond these limits

$$d_j = 0, \quad (4)$$

which means unacceptable system quality.

3. Classification of optimization criteria.

Each quality indicator is assigned to one of the types of criteria: maximization criteria (foaming ability, foam stability, organoleptic characteristics)

$$y_j \to \max, \quad (5)$$

target range criteria (dissolution time, solids content, pH)

$$y_j \to y_{opt}, \quad (6)$$

where y_{opt} is the optimal value of the quality indicator.

4. Normalization of indicators and determination of desirability functions.

The normalization of indicators was carried out using an S-shaped logistic curve (for maximization criteria) and a Gaussian function (for target ranges) within d_j[0;1].

For maximization criteria

$$d_j = e^{\left(-e^{\left(-\left(a_i + b_i \cdot y_j\right)\right)}\right)}, \quad (7)$$

where a_i, b_i– coefficients for converting the values of actual indicators into normalized ones, setting the corresponding desirability values for the two values y_j, preferably in the interval $0.2 < d_j < 0.8$.

For target range criteria

$$d_j = e^{\left(-\left|\frac{y_j - y_{opt}}{\sigma}\right|^2\right)}, \quad (8)$$

where σ is the permissible deviation.

5. Calculation of the integrated quality indicator.

The integrated quality indicator of the system D was determined by geometric aggregation of partial functions. This ensures the sensitivity of the integrated indicator to critically low values of individual parameters

$$D = \sqrt[n]{d_1 \cdot d_2 \cdot d_3 \cdot \ldots \cdot d_n}, \quad (9)$$

where n is the number of quality indicators by which optimization was performed.

6. Ranking and selection of the optimal value.

The obtained integrated indicators were ranked and used to select the optimal formulation, which provides a balanced combination of functional, technological, and dermatological properties according to the Harrington scale (Table 3) under the condition $D \to$max.

The proposed algorithm guarantees transparency, reproducibility, and applicability of the method for multi-criteria evaluation and sustainable design of cosmetic products.

Table 3

Harrington scale

Range of values D	Psychophysical quality assessment	Technological acceptability of the formulation
0.80–1.00	Very good	The formulation meets the standards of «green» cosmetics and premium quality
0.63–0.80	Good	High quality, safe and effective product
0.37–0.63	Satisfactory	Limit of acceptability, requires refinement in individual parameters
0.20–0.37	Poor	Does not meet the requirements of sustainable development or functionality
0.00–0.20	Very bad	The product is unacceptable for release to the market

5. Results of research on multi-criteria optimization of solid shampoo composition

5. 1. Comparative analysis of quality indicators of solid shampoo samples

Fig. 2, *a–f* shows experimental values of key functional, technological, and dermatological indicators for nine solid shampoo formulations.

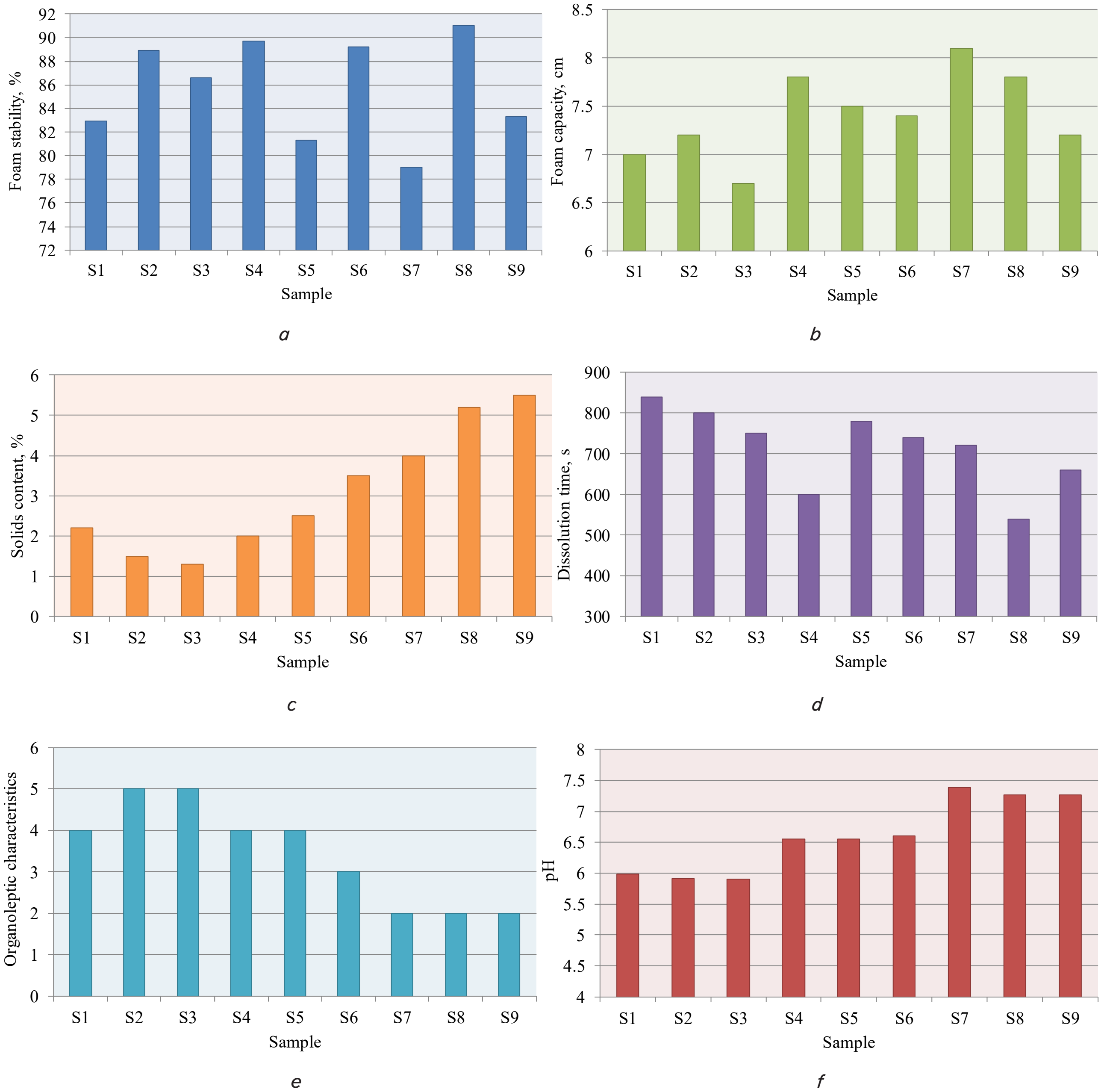

Fig. 2. Efficiency indicators of solid shampoo formulations: *a* — foam stability; *b* — foaming ability; *c* — dissolution time; *d* — solids content; *e* — organoleptic characteristics; *f* — pH value

The constructed plots (Fig. 2) clearly show the nature of the influence of each parameter on quality.

Analysis of experimental data revealed that no sample achieves maximum efficiency simultaneously in all indicators, which confirms the presence of compromises between functional efficiency and resource saving. In particular, formulations with high foaming ability (S7–S8) are characterized by simultaneously excessive solids content in the working solution (4.0–5.5%), low organoleptic ratings, and pH deviation into the alkaline region.

In contrast, samples S1–S3 demonstrate moderate but balanced values of most indicators. This confirms that the improvement of one parameter is often accompanied by the deterioration of others, and therefore, a single-criteria assessment is methodologically incorrect.

5. 2. Results of normalization of the obtained quality indicators and their integration into the integrated quality indicator of the system

The indicators were normalized using an S-shaped logistic curve (for maximization criteria) and a Gaussian function (for target ranges) (Table 4) [26].

A bell-shaped function (Gaussian curve) is used for the target range criteria (pH, dissolution time, solids content). This models a situation where deviations in either direction (both too little and too much) are detrimental.

The transformation of the normalized values into partial desirability functions is given in Table 5.

Foaming ability is normalized according to the principle of "maximum" since an increase in this indicator improves consumer perception and reduces reapplication of the product. However, even high absolute values (S7–S8) do not guarantee high values of the desirability function if they are accompanied by other negative effects. This is reflected in moderate d_{fc}values (0.77–0.80), rather than maximum.

Table 5

Harrington desirability functions for quality indicators

Sample	d_{fc}	d_{fst}	d_{dt}	d_{sc}	d_{org}	d_{pH}
S1	0.68	0.76	0.85	1.00	0.67	0.99
S2	0.71	0.82	0.90	1.00	0.86	0.99
S3	0.64	0.80	0.94	0.85	0.86	0.99
S4	0.77	0.83	1.00	1.00	0.67	0.89
S5	0.74	0.74	0.91	1.00	0.67	0.89
S6	0.73	0.82	0.95	0.37	0.36	0.88
S7	0.80	0.71	0.96	0.02	0.08	0.59
S8	0.77	0.84	0.99	0.00	0.08	0.64
S9	0.71	0.76	0.99	0.00	0.08	0.64

Foam stability directly affects the quality of washing and comfort of use. Values below 60% are considered unacceptable, as they lead to overconsumption of shampoo. Samples S2, S4, and S8 demonstrate high d_{fs}(above 0.82), while S7 has a reduced value of 0.71, indicating less efficient use.

Dissolution time is a conventional indicator of the target range. The optimal interval of 300–600 s ensures controlled dissolution and minimizes mass loss per cycle. Sample S4 reaches d_{dt}=1.0, which indicates an optimal balance between convenience and economy. Too short or too long a dissolution time reduces the value of the desirability function.

Table 4

Normalization of indicators taking into account their functional content

Indicator, y_i	Constraint type	Target range (d_j=0)	Acceptability limit (d_j≈0,37)	Harrington function
Foaming ability, cm	maximum	>8.0 cm	5.0 cm	$d_{fc} = e^{\left(-e^{-(-2.33+0.47\cdot y)}\right)}$
Foam stability, %	maximum	85–100%	60%	$d_{fst} = e^{\left(-e^{-(-3.36+0.056\cdot y)}\right)}$
Dissolution time, s	target range	300–600 s	<180 s or >1200 s	If $300 \le y_{dt} \le 600: d_{dt}$=1.0. If $y_{dt} < 300:\ d_{dt} = e^{\left(-\left\|\frac{y-300}{120}\right\|^2\right)}$. If $y_{dt} > 600:\ d_{dt} = e^{\left(-\left\|\frac{y-600}{600}\right\|^2\right)}$
Solids content, %	target range	1.5–3%(in solution)	<1.5% or >3.0%	If $1.5 \le y_{sc} \le 3.0: d_{sc}$=1.0. If $y_{sc} < 1.5:\ d_{sc} = e^{\left(-\left\|\frac{y-1.5}{0.5}\right\|^2\right)}$. If $y_{sc} > 3.0:\ d_{sc} = e^{\left(-\left\|\frac{y-3}{0.5}\right\|^2\right)}$
Organoleptic characteristics	maximum	4.5–5.0 points	3.0 points	$d_{org} = e^{\left(-e^{-(-2.8+0.93\cdot y)}\right)}$
pH value	target range	5.3–5.8	<4.5 or >8.0	If $5.3 \le y_{dt} \le 5.8: d_{pH}$=1.0. If $y_{pH} < 5.3:\ d_{pH} = e^{\left(-\left\|\frac{y-5.3}{0.8}\right\|^2\right)}$. If $y_{pH} > 5.8:\ d_{pH} = e^{\left(-\left\|\frac{y-5.8}{2.2}\right\|^2\right)}$

The solids content in the working solution is a critical indicator of the dosage per wash.

The optimal range of 1.5–3.0% provides sufficient cleaning effect without overspending. Samples S7–S9 have d_{sc}≈0, which indicates excessive discharge of substances into wastewater.

The organoleptic assessment is an integrated indicator of consumer acceptability. At values less than three points, the values of the partial desirability functions (S7–S9) drop sharply.

The optimal pH (5.3–5.8) ensures dermatological safety. Deviations to the alkaline side (S7–S9) sharply reduce d_{pH}.

5. 3. Results of determining the optimal composition of solid shampoo based on Harrington's integrated quality index

Geometric aggregation of partial desirability functions allowed us to obtain an integrated quality index *D* (Fig. 3), which is sensitive to any critically low parameter.

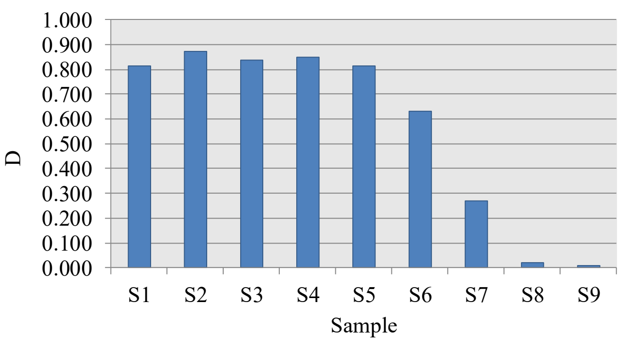

Fig. 3.Integrated indicator of the quality of solid shampoo formulations

The Harrington integrated quality index serves as a quantitative tool for making optimal decisions in the development of cosmetic formulations and allows for effective resolution of contradictions between technological and functional characteristics of anhydrous cosmetic products. Its values are interpreted in accordance with the established psychophysical thresholds of the Harrington scale, which makes it possible to classify the resulting formulations (Table 5).

The ranking of the results showed that:

– S2–S4: "very good" zone (*D*>0.84);

– S1, S3, S5 have high scores (*D*≈0.81–0.84), but are inferior to the leader in foam stability or organoleptics;

– S7–S9: unacceptable (*D*<0.37) because they have critical shortcomings: high solids content, alkaline pH, low organoleptics.

Based on the established features, a multi-criteria technological profile of the optimal solid shampoo formulation is shown inFig. 4.

The multi-criteria compromise profile of sample S2 confirms the content of the research hypothesis regarding the possibility of establishing regularities between the formulation and quality indicators using the Harrington desirability function, which underlies the multi-criteria optimization method. As a result, such a formulation of solid shampoo forms a holistic technological system with a sufficiently high value of psychophysical quality assessment by the integrated indicator, despite the heterogeneity of the quality indicators that form it.

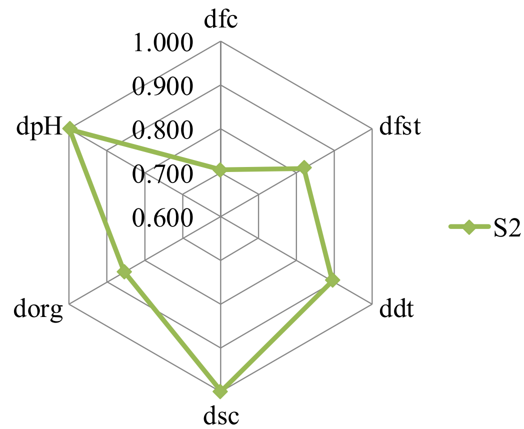

Fig. 4.Multi-criteria technological profile of the optimal formulation of solid shampoo

6. Discussion of results based on determining the features of multi-criteria optimization

The experimental data (Fig. 2) demonstrate significant variability in the properties of samples S1–S9. This is explained by the complex pattern of nonlinear interaction between anionic surfactants and other structure-forming agents of the formulation technological system (Table 1). In particular, sample S2 demonstrated optimal foaming according to a balanced indicator of foam stability and foaming ability, which is explained by the synergy of the selected combination of components and provides high micellar activity while maintaining a solid structure.

Due to the balanced dissolution time (falling into the "target range"), sample S2 is consumed economically. It does not soak, preserving the structure, which makes it possible to use100% of the product without residues. The high stability of the S2 foam means effective cleaning with a smaller amount of product, which reduces the concentration of surfactants that enter the wastewater. pH5.92 (S2) is safe for the biocenosis of water bodies if it enters the sewage system, unlike the more alkaline samples S7–S9.

The mathematical transformation of the indicators y_j into dimensionless responses d_j (Table 4) using the formulas of exponential and Gaussian dependences allowed us to balance the contradictions between the criteria and determine the patterns for each key quality indicator. For example, for pH and dissolution time, a "two-sided restriction" (Gauss curve) was used, which is explained by the need to maintain the system within the physiological norm and prevent excessive soaking of the product.

Geometric aggregation into a generalized desirability function ensured the sensitivity of the integrated quality indicator *D* to critically low partial values. This allowed us to methodically correctly approach the assessment of the quality of formulation technological systems, where a low value of one parameter can make the product unacceptable. The calculation of the integrated indicator *D* (Fig. 3) revealed that only sample S2 (*D* = 0.87) falls into the "very good" zone on the Harrington scale. The multi-criteria profile (Fig. 4) visualizes the harmony of this system: unlike other samples, S2 does not have "sharp dips" in any of the criteria, which indicates the high technological maturity of this formulation and correctly established features during multi-criteria optimization according to the desirability function.

The established features of multi-criteria optimization by the desirability function make it possible to implement the integration of key quality indicators into a single integrated indicator, taking into account their dependence on the formulation composition of the anhydrous cosmetic product. At the same time, critical thresholds of unacceptability are taken into account, the choice of the optimal formulation is formalized with the achievement of a technological compromise. The range of criteria by which cosmetic products are optimized is also expanded, avoiding limitations in terms of organoleptics or foaming.

Compared with the fragmentary assessment given in [7–9] (without taking into account functional indicators), multi-criteria optimization by the desirability function provides simultaneous environmental and technological optimization.

Analyzing various methods of multi-criteria decision-making, such as AHP or TPSIP, in which the weight of the criteria is determined expertly, the Harrington function minimizes subjectivity, taking into account nonlinear dependences between properties and composition. This is achieved by formalizing responses in a desirability scale and smoothing out extreme deviations, highlighting the most stable zone, and also allows for the integration of target range criteria.

In the context of the WaterlessBeauty, ZeroWaste and GreenChemistry strategies, the established features also have their results. Thus, when compared with conventional liquid shampoos, in which the water content reaches 80–90%, the developed S2 formulation system provides a similar functional effect at a mass 7–8 times smaller. In known alternative solutions (for example, natural shampoos without synthetic surfactants), the foam stability indicator is often underestimated, and the obtained dependences between the composition of anhydrous formulation systems and quality criteria (Fig. 2) show stability at the level of 93%, which is achieved precisely through the optimal dosage of the surfactant mixture. Determining the pattern, the influence of the composition of the product on the dissolution time (sample S2) solves the issue of excessive product consumption, which directly corresponds to the "ZeroWaste" concept [10].

Our studies and their results allowed us to determine quantitative patterns for coordinating the formulation composition of anhydrous cosmetic formulations with a complex of heterogeneous quality indicators. This takes into account nonlinear interactions, as well as the possibility of determining the area of technological compromise that satisfies the maximum level of quality. Such consistency makes it possible to ensure structural stability, control dissolution time, and effective foaming, without violating the environmental friendliness of the system.

Our results provide the possibility of transition from fragmentary assessment of properties to a comprehensive establishment of regularities between the composition of anhydrous cosmetics and their quality. The identified features of multi-criteria optimization make it possible to predict the influence of the formula composition of systems on the stability of the integrated quality indicator and its partial functions at the stage of laboratory development, increasing the resource efficiency of products.

When applying the results in practice, one should take into account the limitations in the technological regimes of the processes of obtaining solid shampoos, their raw material composition and equivalence when determining the weight of the effectiveness indicators of the formulations.

The main drawback of the research is the absence of criteria for long-term stability and microbiological stability in the list. Also, the assessment of organoleptic indicators, although based on a point assessment, still contains a share of subjectivity of the expert group.

Further advancement of research is advisable in order to expand the factor space, technical and economic optimization, and integration of LCA. Automation of calculations according to the above algorithm could be used for rapid design of formulation technological systems. At the same time, this will make it possible to increase the predictive capacity of formulations, minimize uncertainty, and integrate environmental and economic criteria into a single management system for formulation systems of anhydrous cosmetics.

7. Conclusions

1. A range of six key quality indicators (foaming ability, foam stability, dissolution time, solids content, organoleptics, and pH)has been substantiated, which describe the state of the formulation system of solid shampoo and make it possible to avoid fragmented evaluation. Based on the established patterns between them, a high sensitivity of the system to changes in surfactant concentrations was revealed, which is explained by the complex processes of micelle formation in concentrated mixtures without an aqueous solvent. During the experimental study, it was found that no sample demonstrates maximum values for all functional, technological, and dermatological indicators simultaneously. Samples S7–S8 are characterized by increased foaming ability (up to 8 cm) but have an excessive solids content (4.0–5.5%), a pH deviation in the alkaline region, and a low organoleptic assessment. Instead, formulations S1–S4 demonstrate a more uniform distribution of indicators without critical deviations. It has been proven that the results could become the basis for further mathematical processing, replacing the subjective selection of ingredients with quantitative characteristics.

2. The regularities of transformation of heterogeneous quality indicators of solid shampoos into dimensionless partial desirability functions $d_j$have been established. A feature of such a solution is the use of two-sided restrictions (Gaussian curve) for pH and dissolution time indicators, which makes it possible to keep the system within technological tolerances. This provides an advantage over known methods of simple linear normalization since it makes it possible to introduce restrictions for indicators exceeding the norm, which is critical for the engineering design of stable forms. An integrated quality indicator for each formulation has been determined. The highest value of the integrated quality indicator ($D = 0.87$)was established for the S2 formulation and corresponds to the "very good" level. The high score is explained by the pronounced synergism between anionic surfactants. Compared with other samples (for example, S9 with $D = 0.0001$), the chosen solution guarantees the stability of the technological system at extremely low moisture content. It has been quantitatively established that the deviation of at least one indicator beyond the limits of acceptability leads to a significant decrease in the overall quality of the product, regardless of the high values of other indicators. Unlike linear aggregation, geometric aggregation prevents the compensation of unacceptable parameters by high values of

others. The resulting effect is explained by the multi-criteria nature of the Harrington function, where partial desirability close to zero determines an extremely low integrated result.

3. The ranking of the integrated index D showed that formulations S2–S4 belong to the category of "very good" ($D > 0.84$), S1, S3, S5 – to a high level of quality ($D \approx 0.81–0.84$), while S7–S9 are unacceptable ($D < 0.37$). The optimal composition is characterized by balanced values of partial functions without critical minima, which is confirmed by the multi-criteria profile. The result is explained by the consistency of functional, technological, and dermatological parameters within the target ranges, which minimizes internal conflicts of the system. The advantage of the result is the quantitative determination of the optimal formulation based on a single integrated criterion, which allows us to formalize the selection process and minimize expert subjectivity. The multi-criteria profile of the optimal sample was visualized. The assessment of its resource efficiency confirmed the advantage of the solid form over liquid analogs. It was found that due to the optimized amount of active ingredients and balanced dissolution rate, 50 g of the developed S2 shampoo is functionally equivalent to 350–400 ml of liquid product. This allows for a 7–8-fold reduction in material flows in the logistics chain and minimizes anthropogenic load, which alleviates the problematic part of the high resource intensity of conventional cosmetic products identified in the study.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study and the results reported in this paper.

Funding

The study was conducted without financial support.

Data availability

All data are available in the main text of the manuscript.

Use of artificial intelligence

The authors declare the use of generative AI in the research and manuscript preparation process. According to the GAIDeT(2025) taxonomy, the following tasks below were delegated to generative AI tools under full human supervision.

The generative AI tool applied: ChatGPT-5 was used as an auxiliary tool for the preliminary development of the research methodology in order to generate methodological approaches and did not determine the final scientific results. The proposed methodology was further analyzed in accordance with the approaches of modern methods of mathematical modeling of multi-component and multi-criteria systems. The resulting approaches were also compared with known studies in this field, given in peer-reviewed papers on optimization methods and indicated in the list of sources used.

The verification of the results provided by the AI tool was carried out on the basis of experimental studies in several repetitions (to confirm reproducibility). Mathematical processing of the results allowed us to confirm the adequacy and reliability of the chosen methodology. It was found that the use of generative AI at this stage contributed to the application of a conceptual approach to the study of these objects.

Authors' contributions

Tetiana Ivanishena: Methodology, Validation, Formal analysis, Data Curation, Writing – original raft, Project administration; **Zoriana Chereshnia**: Conceptualization, Software, Investigation, Visualization; **Anna Mahdiichuk**: Resources, Writing – review&editing, Supervision.

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