Technical Sciences
Academy of Romania
www.jesi.astr.ro

Journal of Engineering Sciences and Innovation
Volume 7, Issue 1 / 2022, pp. 45-58
http://doi.org/10.56958/jesi.2022.7.1.45

C. Chemical Engineering, Materials Science and Engineering

Received ***30 August 2021*** *Accepted* ***7 March 2022***
Received in revised form ***19 November 2021***

Systems theory and the study of cosmetic products

ADELA ELENA MANEA[*], MARIA DELIA PERJU, ANDRA TĂMAȘ

Politehnica University Timisoara, Romania

Abstract. The principles of systems theory apply today to all existentialist fields of man, whether it is economics, agriculture, industry, philosophy, medicine, research or even politics. As such, mathematical modeling as a tool for using systems theory is used as a technique for studying phenomena and processes specific to those fields. In the case of applying systems theory in researching problems related to cosmetic emulsions, mathematical modeling is a technique for quantitative and qualitative study of phenomena and physical-chemical processes that characterize cosmetics from obtaining them to using them as a finished product by man.

Mathematical modeling is the basis for studying all processes and phenomena in terms of the principles of systems theory.

In this context, we aimed to study the possibilities of using mathematical modeling in the characterization of cosmetic products, having the conviction that the results obtained will improve the performance possibilities of the quality of these products.

Keywords: mathematical modeling, systems theory, cosmetic emulsion, quality indicators, cosmetology.

1. Introduction

People need to pay more attention to the care of the skin organ (skin) from birth to old age. A healthy and well-groomed complexion offers everyone a state of comfort both physically and mentally (it gives self-confidence).

Cosmetology is the science that deals with the study of maintaining the health and beauty of the human body, especially the epidermis, by making cosmetic and dermato-cosmetic products [1].

In all the technologies of some finished products, regardless of the field of use, there has been a pronounced tendency in recent years to quantitatively address the

---

[*] Correspondence address: adelamanea@gmail.com

problems of design and operation of physical-chemical processes. This trend was ensured by the progressive use of computers to solve the mathematical equations of complex systems [2-6].

2. Cosmetics products

According to the European Community Directives, the Cosmetic Product is defined as: "Any substance or preparation which is intended to come into contact with various external parts of the human body (epidermis, hair, nails, lips, external genitalia) or teeth or membranes. mucous membranes of the oral cavity, with the sole or main purpose of cleaning, perfuming, modifying the appearance, correcting the body odor or protecting and maintaining them in good condition" [1].

In recent years, the frequency of dermatological problems has increased worldwide, for various reasons, both in children (affecting between 10-12% of the world's children) and in adults (1-3% of them). These health problems cannot always be cured, but the use of emulsions / creams in the applied treatments can alleviate certain unpleasant effects and prevent their recurrence, thus improving people's health. For these reasons, the field related to the manufacture of cosmetics and dermato-cosmetics, as well as research on improving their quality indicators, has developed a lot worldwide. Research has been carried out on new raw materials, respectively, revolutionary active ingredients (natural and synthetic) with clinical efficacy studies, which aim to restore and maintain the natural beauty and health of the skin. In this way, those active substances appeared, called cosmeceuticals, which are considered cosmetic ingredients and which improve the appearance of the skin thanks to a pharmacological effect that can be identified at the intracellular level. The name "cosmeceutical" appeared by combining the terms "cosmetic" and "pharmaceutical" [7-9].

The basic objective of the preparation specialist is to create a product that is as stable as possible from a physical-chemical and microbiological point of view.

3. The qualities of a high-performance cosmetic cream

The highest desideratum of cosmetics is the tendency to give the skin its normal parameters, namely: gloss, tone, elasticity, hydration, suppleness. The conditions of a high-performance cosmetic cream are: to be specific to a certain type of skin; be harmless to the skin (do not contain toxic or allergenic substances); to be easily absorbed; to ensure a sufficient (physiological) lubrication of the face; to ensure a good hydration of the skin; to keep well; the emulsion has a very high degree of homogenization; to form a protective and emollient layer in any season; to bring extra nutrients and / or minerals to the skin [1,7].

4. Creams (emulsions) - general notions

The emulsion, in its simplest form, represents a biphasic system composed of two immiscible liquids, one of which is dispersed in the other in the form of microscopic or submicroscopic droplets [1,8,10].

From a physical point of view, cosmetic creams are prepared in the form of emulsions.

The usual types of emulsions are:

1) oil-in-water emulsions (U / A)
2) oil-in-oil emulsions (A / U)

There are also multiple emulsions:

1) multiple U / A / U emulsions
2) multiple A / U / A emulsions

Emulsification is performed with the help of surfactants (emulsifiers) that make it possible to disperse the internal phase in the form of droplets in the external phase and that stabilize the emulsion, preventing the separation of the two phases [1,8,10].

The type of emulsion (A / U or U / A) is imposed by: the amount of emulsifier, the ratio between the aqueous and the oily phase, the presence of surfactants and the preparation temperature [8].

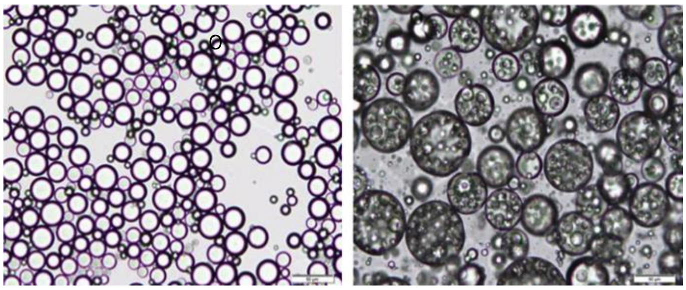

Fig. 1. Optical microscopic images of emulsions: oil-in-water (U / A) emulsion on the left and oil-in-water-in-water (A / U / A) emulsion on the right.

5. Stability of cosmetic emulsions [1,11-14]

Cosmetic emulsions may show instability during storage, from chemical changes of components, the presence of microorganisms in products or physical changes (mechanical or visual). The first two causes of instability are generally unacceptable.

It is the responsibility of the preparation specialist to correct the damage of the emulsions from the chemical, biological or physical ones. The basic goal is to create a product as stable as possible.

As a rule, slow losses of emulsion ingredients due to chemical (or oxidative) changes should not be tolerated. Similarly, the presence of an excessive number of microorganisms, even harmless ones, is a warning that pathogens can invade the product and it should not be distributed.

6. Mathematical modeling theory

Process modeling in order to improve knowledge methods is constantly evolving, being driven by the explosion in computer science, which has led to the emergence of new languages, which provide real facilities in simulating process behavior based on mathematical models. The application of mathematical modeling and simulation is gaining ground, being of real use in areas such as parameter measurement techniques, automation and optimization of physical and chemical processes [15,16].

Thus, it can be used successfully both in the scientific research of various laboratories or research centers, as well as in the design, construction and actual realization phases in obtaining the finished products.

Mathematical modeling is useful in all phases of development of a theory, scientific or technical research, it brings a number of definite advantages [2,5,6]:

1. deepening the knowledge and understanding of the phenomenon or process (complex cause-effect sequences, interdependencies between variables must be taken into account);
2. optimal design of research or production facilities (sizing of equipment and evaluation of parameters based on data obtained on pilot plants, study of the effects of changes in size, optimal structure of technological flow);
3. optimization of the operation of the installations in operation;
4. optimal control.

The mathematical model of a system is a set of mathematical relations, equations and inequalities, which characterizes and describes the interdependencies between the constructive and functional parameters of the system. The presence of inequalities in the model is due to physical-chemical, technological or constructive restrictions. The models aim at the behavior of the systems in stationary regime or in dynamic regime [2,17-19].

The elaboration of a correct and efficient model of an original system represents a synthesis of what is known about that system. Paradoxically, in order to model a phenomenon correctly, it is necessary to know it as comprehensively as possible, which is in opposition to the need to research it. The model must also be appropriate to the intended purpose [20-22].

Modeling, in a narrow sense, represents the activity of proper elaboration of the model of a source system, the activities carried out in this sense being materialized also through: search and analysis techniques and procedures; simulation techniques; complementary techniques and procedures [2,23].

The steps by which modeling is performed, in the classical way, in a narrow sense are, in general, the following [2,23]:

I. Building the model based on;
II. Model analysis by simulation;
III. Comparing the results of the analysis with the behavior data of the source system under equivalent conditions;
IV. Correction of the model, in the sense of bringing the behavior closer to that of the source system.

Figure 2 shows the logical scheme for the methodology of modeling a process [24].

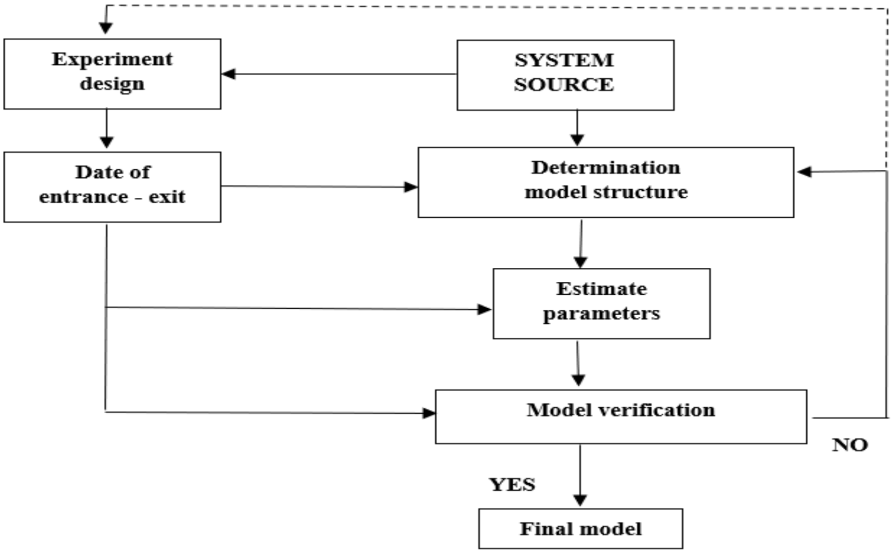

Fig. 2. Logical scheme for the methodology of modeling a process.

Figure 3 shows the block diagram of a system that is a cosmetic emulsion. It consists of several microsystems represented by the aqueous phase with all raw materials, the fatty phase with all raw materials, active ingredients (vitamins, minerals, enzymes, liposomes, peptides, proteins, biofirms, plant extracts), perfume compositions.

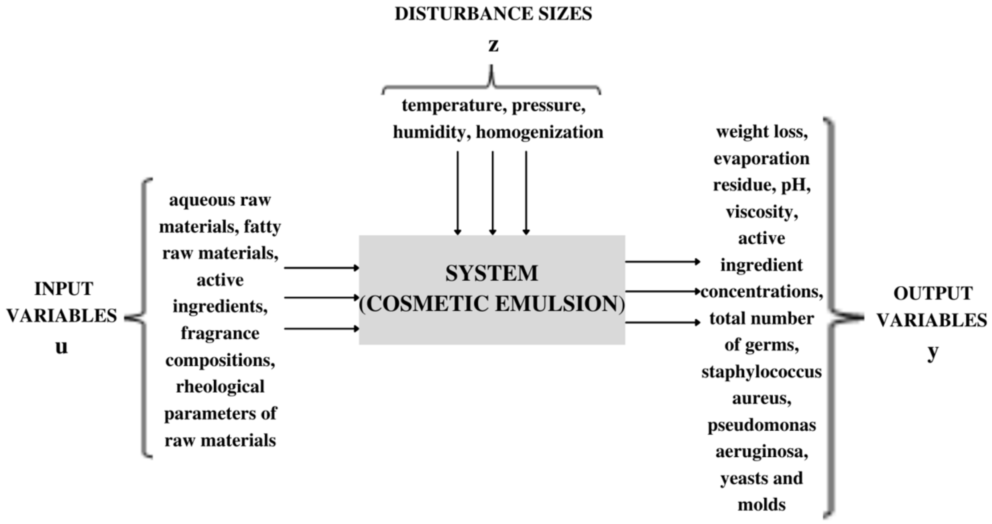

Fig. 3. Block diagram of a system consisting of an emulsion.

Mathematical modeling of physical-chemical processes involves the following steps [25,26]:

A. Collection, analysis and interpretation of experimental data.
B. Formulation of empirical laws that describe the process.
C. Elaboration of the mathematical model.
D. Testing the mathematical model and validating it.
E. Using the mathematical model.

7. Mathematical elements of experimental modeling (statistics)

The elaboration of experimental models is based on the statistical correlation of the concrete data obtained during the experiment. The validity of these models is limited by the field in which the variables were modified. The error function, E, depends on the output quantities of the process and the model (y and y_m respectively) [2, 27]:

$$E = E\,(y, y_m) \qquad (1)$$

The steps in the modeling methodology are as follows [2, 27]:

- establishing the structure of the model;
- organizing and conducting experiments on the real installation;
- interpretation and processing of results;
- deduction of the final form of the model equations and calculation of the coefficients from the equations (model parameters);

- model verification.

The approach to the issue of statistical modeling in stationary regime is done using the following steps: inventory of variables, choice of model form, obtaining and testing data, determining model coefficients, testing and assessing model quality [2].

8. Indicators of model adequacy

8.1. Fischer's F test

In the language of mathematical statistics, the F test or the F criterion shows that based on a small number of observations the dispersions must be compared [2,23,29,30].

The Fischer, F_C criterion is calculated by the expression

$$F_c = \frac{s^2_{e,max}}{s^2_{e,min}}. \tag{2}$$

This is the ratio of the largest (maximum) dispersion, $S^2_{e,max}$ and the smallest (minimum) dispersion, $S^2_{e,min}$.

Where

$$S^2_e = \frac{\sum_i^{n_e}(y_i - \bar{y})}{n_e - 1} \tag{3}$$

S_e^2 - the dispersions of the values of the variables beside to their arithmetic means;

$\bar{y}$ - medium value;

y_i - calculated value;

n_e – number of experiences.

Depending on the degrees of freedom of the two tests, in the case of a confidence level P = 95%, from the tables in the literature is the value of the Fischer criterion (F_T).

Compare the calculated Fischer criterion, F_C with the tabulated Fischer criterion, F_T.

If:

- ✓ $F_C<F_T$ – the dispersions are homogeneous, they do not differ significantly;
- ✓ $F_C>F_T$ – the dispersions are inhomogeneous, the maximum dispersion is considered to correspond to an erroneous test and it is restored. Test the dispersion immediately below the maximum, continuing in this way until it is obtained $F_C<F_T$.

8.2. Adequacy dispersion, σ^2 [2, 23,28-30]:

- for a single independent variable and ”n” determinations:

$$\sigma^2 = \frac{\sum_{i=1}^{n}(\hat{y}_i - y_{icalc})^2}{n-1} \tag{4}$$

- for ”m” independent variables and for ”n” determinations:

$$\sigma^2 = \frac{\sum_{i=1}^{n}(\hat{y}_i - y_{icalc})^2}{n-m-1} \tag{5}$$

8.3. Standard deviation (square mean deviation), $\boldsymbol{\sigma}$ [2, 23,29,30]:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_{icalc})^2}{n-\mathrm{m}-1}} \tag{6}$$

8.4. Model accuracy indicator, R² [2, 23,29,30]:

$$R^2 = \frac{\sum_{i=1}^{n}(y_{icalc} - \bar{y})^2}{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2} \tag{7}$$

8.5. Multiple correlation coefficient, R [2, 23,29,30]:

$$R = \sqrt{1 - \frac{\sum_{i=1}^{n}(\hat{y}_i - y_{icalc})^2}{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}} \tag{8}$$

where:

n – number of data sets (determinations),
m – number of independent variables,
y – dependent variable,
y_{icalc} – the resulting value for y based on the regression equation,
$\hat{y}_i$ - experimental value,
$\bar{y}$ - experimental value.

The multiple correlation coefficient is a measure of the overall capacity of the model to represent the experimental data, even if in portions the model is less adequate.

This coefficient must be greater than 90%, and it is advisable to use it only in conjunction with other tests of suitability for the model and the quality of the estimate.

If the model is not suitable, the following decisions can be made [2,30]:

- which does not involve changing the shape of the model (completing the experimental data, changing the range of variation of the factors, etc.);
- which involves changing the shape of the model and resuming experimental determinations.

The quality of a model is expressed, first of all, by the fidelity with which the model reproduces the known behavior of the modeled system. The behavior of the model is relevant by operation, so in the operations related to modeling, related to simulation. Fidelity depends on the following: the correctness with which the assessment of what is essential, relevant to the purpose pursued; the procedures for establishing the model; the quality and quantity of available knowledge that could be used [3].

The above can be constituted in fidelity criteria, with the help of which the models of a source system can be qualitatively differentiated. The quality of a model is also determined by other aspects: simplicity, intelligibility, cost, etc [30].

As examples for the use of systems theory (mathematical modeling) we further present the studies performed in two concrete cases. [31,32]:

a. Determining the stability over time and the shelf life for 4 cosmetic emulsions. Measurements were performed on physico-chemical and microbiological parameters for 4 years. These were analyzed physico-chemically and microbiologically in order to obtain the initial values of their specific quality indicators, and then they were analyzed annually in order to verify the stability over time of these indicators. Based on the experimental data obtained, the equations of the statistical mathematical models were determined and the adequacy (concordance) indicators were calculated. Figures 4, 5, 6 and 7 show the variations over time of the evaporation residue.

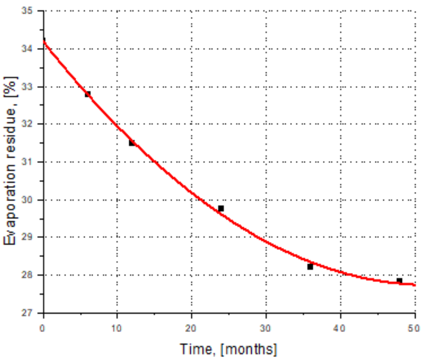

Fig. 4. Time evolution of the evaporation residue for the moisturizer 1.

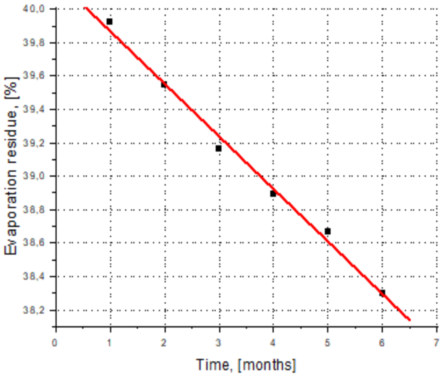

Fig. 5. Time evolution of the evaporation residue for the moisturizer 2.

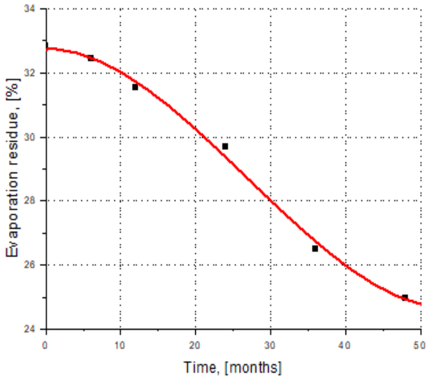

Fig. 6. Time evolution of the evaporation residue for the body milk 1.

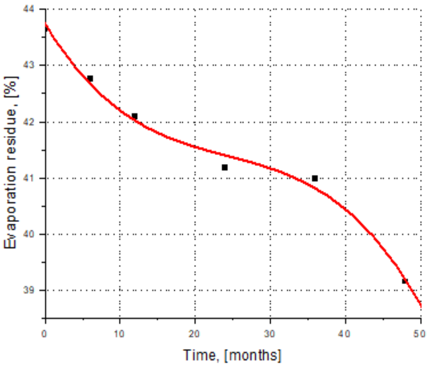

Fig. 7. Time evolution of the evaporation residue for the body milk 2.

Table 1. The equations of the statistical mathematical models obtained for the 4 studied samples

Emulsions	Equations of statistical mathematical models
Moisturizer 1	Evaporation residue = $34{,}18947 - 0{,}2485 \cdot T + 0{,}0024 \cdot T^2$
Moisturizer 2	Evaporation residue = $40{,}18267 - 0{,}31457 \cdot T$
Body milk 1	Evaporation residue = $32{,}7615 + 6{,}70792 \cdot 10^{-4} \cdot T - 0{,}00843 \cdot T^2 + 1{,}04447 \cdot 10^{-4} \cdot T^3$
Body milk 2	Evaporation residue = $43{,}7335 - 0{,}21894 \cdot T + 0{,}00756 \cdot T^2 - 1{,}03475 \cdot 10^{-4} \cdot T^3$

Table 2. Adequacy indicators of the determined statistical models

Adequacy indicators	Moisturizer 1	Moisturizer 2	Body milk 1	Body milk 2
Standard deviation, σ	0.1196	0.05867	0.30441	0.22147
Model accuracy indicator, R^2	0.99868	0.99605	0.99605	0.99209

b. For the 4 emulsions above, other physico-chemical and microbiological analyzes were performed monthly, for 4 years, thus obtaining much more experimental data, with the help of which statistical mathematical models were developed using the program. STATSOFTSTATISTICA 13.3.0. With the help of the program, the graphic representations of the desired dependencies in 3D format were obtained. Figures 8, 9, 10, 11 show the variations of the evaporation residue (RE) of the 4 emulsions as a function of time (T) and total number of germs (NTG).

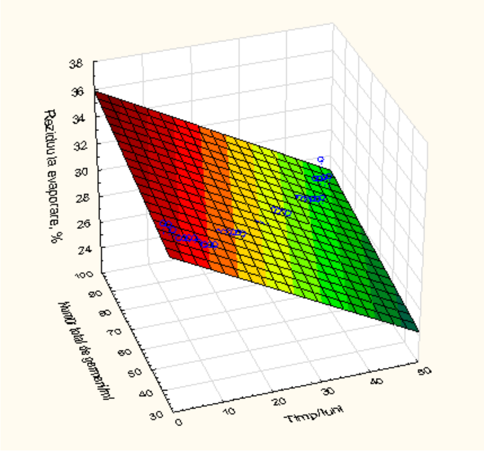

Fig. 8. Evaporation residue as a function of time and total number of germs - emulsion 1.

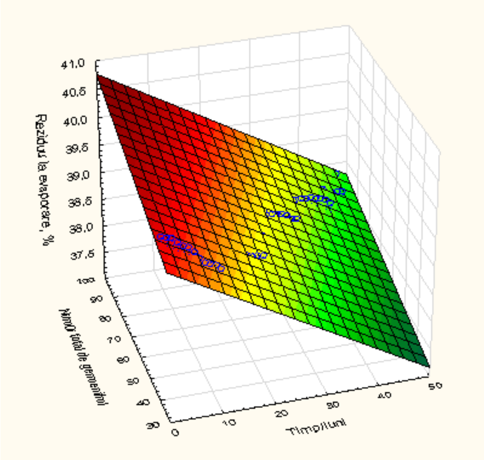

Fig. 9. Evaporation residue as a function of time and total number of germs - emulsion 2.

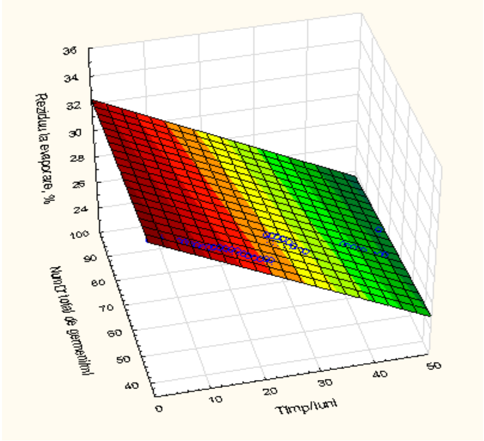

Fig. 10. Evaporation residue as a function of time and total number of germs - emulsion 3.

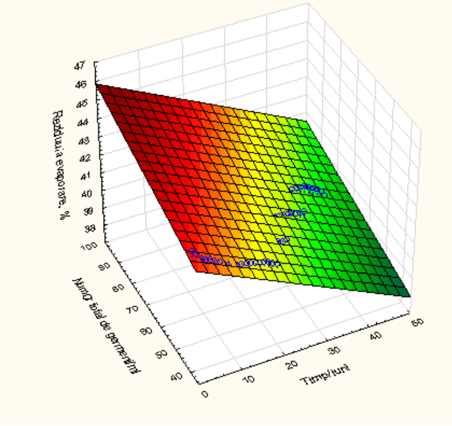

Fig. 11. Evaporation residue as a function of time and total number of germs - emulsion 4.

Table 3. Equations of statistical mathematical models

Emulsii	Equations of statistical mathematical models
Emulsion 1	$RE = 32{,}2978 - 0{,}1814 \cdot T + 0{,}036 \cdot NTG$
Emulsion 2	$RE = 39{,}2088 - 0{,}0502 \cdot T + 0{,}0156 \cdot NTG$
Emulsion 3	$RE = 34{,}4746 - 0{,}1746 \cdot T + 0{,}0217 \cdot NTG$
Emulsion 4	$RE = 41{,}9099 - 0{,}1075 \cdot T + 0{,}0396 \cdot NTG$

Table 4. Adequacy indicators of the statistical models obtained

Adequacy indicators	Emulsion 1	Emulsion 2	Emulsion 3	Emulsion 4
Adequacy dispersion, σ^2	0,1296	0,0104	0,1092	0,0569
Standard deviation, σ	0,3601	0,1021	0,3306	0,2386
Model accuracy indicator, R^2	0,9670	0,9479	0,9849	0,9503
Multiple correlation coefficient, R	0,9834	0,9736	0,9924	0,9749

From the two studies presented, a series of important aspects were highlighted on the existing dependencies, aspects that can lead both to the improvement of the manufacturing processes and to the stability and effectiveness of cosmetic creams, such as moisturizers, anti-wrinkle, sensitive skin, anti-acne, etc.

The determined mathematical models will also offer the possibility to predict improved manufacturing methodologies that will ensure the obtaining of high-performance quality indicators both in the storage and storage of cosmetics and in their use.

9. Conclusions

The use of mathematical modeling techniques in order to improve the physical-chemical and microbiological quality indicators is beneficial for the more in-depth study of the physical-chemical processes that take place during the manufacture, storage and use of cosmetic creams.

The systemic approach to the problems related to maintaining the stability of cosmetic creams using mathematical modeling and numerical simulation brings important improvements in the study of cosmetic creams.

Specifically, applying the principles of systems theory to several types of cosmetic creams or emulsions, statistical mathematical models have been obtained that allow a quantitative and qualitative characterization of the possibilities to improve the properties and quality indicators of these products, as well as rheological properties.

References

[1] Merică E., *Tehnologia produselor cosmetice*, vol.1, Ed. Corson, Iaşi, 2000.

[2] Todinca T., Geantă M., *Modelarea şi simularea proceselor chimice. Aplicaţii în Matlab*, Ed. Politehnica, Timişoara, 1999.

[3] Savii G., Luchin M., *Modelare şi simulare*, Ed. Eurostampa, Timişoara, 2000.

[4] Imre-Lucaci A., Agachi P.Ș., Optimizarea proceselor din industria chimică, Ed. Tehnică, București, 2002.

[5] Perju D., Todinca T., *Automatizarea proceselor chimice*, vol. 2, Centrul de multiplicare al UTT, Timişoara,1995.

[6] Perju D., Geantă M., Şuta M., Rusnac C., *Automatizarea proceselor chimice*, vol. 1, Ed. Mirton, Timişoara, 1998.

[7] Dragomirescu A.O., *Dermatocosmetologie farmaceutică*, Ed. Brumar, Timişoara, 2020.

[8] Sakamoto K., Lochhead R.Y., Maibach H.I., Yamashita Y., Cosmetic Science and Technology: Theoretical Principles and Applications, Elsevier, 2017.

[9] Dragomirescu A.O., *Cosmeticele: substanțe active în formularea cosmetică*, Ed. Victor Babeș, Timișoara, 2019.

[10] IFSCC Monograph Number 4, *Introduction to cosmetic emulsions and emulsification*, Micelle Press, Weymouth, Dorset, England, 1997.

[11] Popovici I., Lupuleasa D., *Tehnologie farmaceutică*, vol. 2, Ed. Polirom, Iași, 2017.

[12] IFSCC Monograph Number 5, *An introduction to cosmetic microbiology*, Micelle Press, Weymouth, Dorset, England, 1999.

[13] *Farmacopeea Română*, ed. X, Ed. Medicală, București, 1993.

[14] IFSCC Monograph Number 2, The fundamentals of stability testing, Micelle Press, Weymouth, Dorset, England, 2006.

[15] Moldovan R., *Îmbunătățirea performanțelor funcționale ale microdebitmetrelor electrotermice utilizând metode de modelare matematică și simulare numerică*, Teză de doctorat, Universitatea Politehnica Timișoara, 2008.

[16] Chapra S. C., Canale R.P., *Numerical methods for Engineers*, 6th ed., McGraw-Hill, New York, 2010.

[17] Meerschaert M.M., *Mathematical Modeling*, 4th ed., Academic Press, 2013.

[18] Dym C.L., *Principles of Mathematical Modeling*, 2nd ed., Academic Press, Burlington, 2004.

[19] Luchin M., *Clasificarea și descrierea modelelor*, a XXVIII-a sesiune de comunicări științifice cu participare internațională a Academiei Tehnice Militare, București, 1999.

[20] Busenberg S., Forte B., Kuiken H.K., *Mathematical Modelling of Industrial Processes*, Springer Verlag, Berlin, Heidelberg, 1990.

[21] Perju D., Șuta M., Todinca T., Rusnac C., *Echipamente de automatizare pneumatice de joasă presiune. Aplicații*, Ed. Politehnica, Timișoara, 2001.

[22] Perju D., Șuta M., Rusnac C., *Echipamente de automatizare pneumatice de joasă presiune*, Ed. Politehnica, Timișoara, 2003.

[23] Cameron I., Gani R., *Product and Process Modelling*, 1st ed., Elsevier, 2011.

[24] Tertişco M., Stoica P., *Identificarea şi estimarea parametrilor sistemelor*, Ed. Academiei RSR, Bucureşti, 1980.

[25] Perju D., Dalea V., Şuta M., Rusnac C., *Main Aspects Concerning Teaching of Environmental and Chemical Process Modeling at the Faculty of Industrial Chemistry and Environmental Engineering from the Politehnica University of Timişoara*, Chem. Bull. Politehnica Univ., 45 (59), 1, 2000, p. 147-150.

[26] Tănăsescu N., *Modelarea matematică şi simularea numerică a proceselor tehnologice din industria alimentară*, Ed. Matrix Rom, Bucureşti, 2000.

[27] Mishra S., Datta-Gupta A., *Applied Statistical Modelling and data Analytics*, 1st ed., Elsevier, 2017.

[28] Montogomery D.C., Runger G.C., *Applied statistics and probability for engineers*, 6th ed., John Wiley & Sons Inc., 2014.

[29] Ross S., *Introduction to Probability and Statistics for Engineers and Scientists*, 6th ed., Academic Press, 2020.

[30] Calisevici M.N., *Studii asupra posibilităților de îmbunătățire și optimizare a indicatorilor de calitate pentru apele potabile și de fântână cu ajutorul tehnicilor moderne de măsurare și a modelării matematice*, Teză de doctorat, Universitatea Politehnica Timișoara, 2011.

[31] Manea E.A., Perju D., Brusturean G.A., Calisevici M., Marinescu S., *Contributions to the Stabilization Processes of the Cosmetic Creams*, Proceedings of the microCAD 2008 International Scientific Conference, Miskolc, Hungary, 2008, p.65-70.

[32] Manea E.A., Pârlea H., Perju D., Brusturean G.A., Calisevici M.N., *Study of cosmetic creams stability as a function of temperature*, Chem. Bull. Politehnica Univ., **53**, 67, 2008, p.50-55.