https://doi.org/10.31891/2307-5732-2025-353-27
УДК 632:654.672

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SIMULATION OF THE RECIPE COMPOSITION OF SAUCES FOR HEALTH PURPOSES BASED ON THE FUNCTIONAL COMPOSITIONS OF DIETARY SUPPLEMENTS

The article provides the scientific basis and development of a methodology for creating functional sauce recipes based on functional compositions. This process is founded on the principle of food combinatorics, which ensures a well-reasoned selection of quantitative ratios between the main raw materials and food additives. This allows for the formation of the necessary organoleptic and physicochemical indicators, as well as achieving the required levels of nutritional and biological value. Modeling functional products involves creating a unified system whose parameters cannot be considered in isolation. Scientific approaches to modeling functional compositional mixtures and products utilizing them are aimed at optimizing the selection and ratio of ingredients, which ensures the achievement of a composition maximally compatible with nutritional value requirements and medico-biological standards. Considering the aforementioned aspects, the modeling results provide effective optimization of the product composition and its manufacturing process parameters. After the completion of multi-level experimental modeling, the functional components and product manufacturing technologies undergo testing in laboratory and industrial conditions, and are then adjusted. At the final stage, a comprehensive analysis of the key quality indicators of finished products is conducted, economic indicators are calculated, the technology is improved directly in production, regulatory documentation is prepared and approved, and industrial implementation is established. The application of this methodology for developing model functional compositions and food products contributes to increasing the efficiency of raw material utilization and expanding the assortment of products with a defined composition and health-promoting properties.

Keywords: sauces, model compositions, macro- microelements, vitamins, functional compositions, biotechnology, protein, fats, carbohydrates, energy value.

АНТОНЕНКО АРТЕМ
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МОДЕЛЮВАННЯ РЕЦЕПТУРНОГО СКЛАДУ СОУСІВ ОЗДОРОВЧОГО ПРИЗНАЧЕННЯ НА ОСНОВІ ФУНКЦІОНАЛЬНИХ КОМПОЗИЦІЙ ДІЄТИЧНИХ ДОБАВОК

У статті обґрунтувано та розробку методики створення рецептур функціональних соусів на основі функціональних композицій. В основі цього процесу лежить принцип харчової комбінаторики, що забезпечує обґрунтований вибір кількісних співвідношень між основною сировиною та харчовими добавками. Це дає змогу сформувати необхідні органолептичні та фізико-хімічні показники, а також досягти необхідних рівнів харчової та біологічної цінності. Моделювання функціональних продуктів полягає у створенні єдиної системи, параметри якої неможливо надати окремо. Наукові підходи до моделювання функціональних композиційних сумішей та продуктів з їх використанням орієнтовані на оптимізацію підбору та співвідношення інгредієнтів, що забезпечує досягнення композиції, максимально сумісної з вимогами харчової цінності та медико-біологічними стандартами. Беручи до уваги вищезазначені аспекти, результати моделювання, забезпечують ефективну оптимізацію складу продукту та параметрів його виробничого процесу. Після завершення багаторівневого експериментального моделювання функціональні компоненти та технології виготовлення продукції проходять випробування в лабораторних і промислових умовах, а потім коригуються. На завершальному етапі проводиться комплексний аналіз ключових показників якості готової продукції, розраховуються економічні показники, удосконалюється технологія безпосередньо на виробництві, готується та затверджується нормативна документація, а також налагоджується промислове впровадження. Застосування методики розробки модельних функціональних композицій і харчових продуктів сприяє підвищенню ефективності використання сировини та розширенню асортименту продукції з визначеним складом і оздоровчими властивостями.

Ключові слова: технологія, соуси, модельні композиції, макро- мікроелементи, вітаміни, функціональні композиції, біотехнологія, білки, жири, вуглеводи, енергетична цінність.

Стаття надійшла до редакції / Received 21.03.2025
Прийнята до друку / Accepted 16.04.2025

Formulation of the problem

The scientific concept of creating technologies of special food products is based on the main provisions of the theory of rational nutrition, theoretical and practical principles of technologies of health products, with optimized nutritional and energy value, sensory and structural characteristics, based on a purposeful combination, through mathematical modeling, of functionally active ingredients of plant origin. [1,2]

The basis of the modeling is the principle of food combinatorics, which consists in the justified quantitative selection of the main raw materials and food additives, which together ensure the formation of the necessary organoleptic and physicochemical properties, a given level of nutritional (food, biological) and energy value. [3]

Modeling of food products is the process of creating a product as a single integrated system consisting of elements that do not individually provide the specified properties. Conceptual approaches to the modeling of functional compositions and products based on them consist in optimizing the selection and ratios of ingredients, by which it is possible to obtain a composition that, in terms of quantitative content and qualitative composition, best meets nutritional value indicators and medical and biological requirements. [4] The application of a mathematical apparatus based on the formalization of qualitative and quantitative indicators of composition, nutritional value of individual ingredients and their combinations in the composition of model functional compositions allows, through simulation modeling, to determine the total content of an individual component. [5,6]

Analysis of recent sources

The scientific justification and development of a methodology for modeling the recipe composition of functional food products is an urgent task. Solving it will allow us to expand the range of dishes with enhanced nutritional and biological value, and to create products with specified functional properties [7-9].

Significant contributions to addressing the fundamental issues of modeling the recipe composition of functional products, as a means of preventing and eliminating micronutrient deficiencies, have been made by the research of the following domestic and foreign scientists: M.I. Peresichny, G.O. Simakhinoi, O.O. Grinchenko, A.B. Horalchuk, A.M. Dorokhovych, I.Yu. Zhigalenko, A.V. Ziolkovska, P.O. Karpenka, M.B. Kolesnykova, V.N. Korzuna, M.F. Kravchenko, H.M. Lysyuk, L.P. Malyuk, L.M. Mostovoi, N.Ya. Orlova, P.P. Pivovarova, N.V. Prytulska, G.B. Rudavska, M.R. Ennis, J.C.F. Murray, G.O. Phillips, W.C. Weling, P.A. Williams et al. [10-15]

This work aims to justify and develop a methodology for creating health-promoting food products by modeling their recipes using functional compositions.

The primary focus of this study is the methodology itself: how to effectively model the recipe composition of health foods based on their functional components.

Our research delves into specific elements, including: model compositions, functional compositions, and key nutritional components like proteins, fats, carbohydrates, macro- and microelements, vitamins, and overall energy value.

Presenting main material

The modeling process is provided by an information base containing experimentally obtained data on the macro- and micronutrient composition of the ingredients and consists of the following stages:

Stage 1. Development of raw data for modeling products based on functional compositions.

- Determination of the goal: to create technologies for products with food additives of plant origin for health nutrition (develop a competitive product, reduce the cost price, realize the available raw materials);
- familiarization with existing domestic and foreign analogues and prototypes (scientific and patent sources, Internet publications), assessment of technical capabilities, selection of basic technology;
- determination of restrictive criteria for the composition of model functional compositions and products based on them (according to individual types of raw materials and ingredients, protein, fat, carbohydrate content, etc.);
- selection of ingredients based on characteristics (chemical composition, functional properties, cost), which, when varying their content in the model composition, can most significantly influence the nutritional value, structural and mechanical properties of the food system, organoleptic indicators of the finished product, and its price;
- formation of a database on the general chemical composition of the components of the model composition (including the content of essential amino acids in the mass fraction of total protein; lipid composition - the content of saturated (sum), monounsaturated (sum) and polyunsaturated fatty acids in the composition of fats of possible recipe ingredients; carbohydrate composition - mass fraction of mono-, di- and polysaccharides; mineral and vitamin composition, energy value);
- formulation and specification of medical and biological requirements for the quantitative and qualitative composition of the modeled product.

Stage 2. Formalization of requirements for the composition and properties of the initial ingredients and product quality based on model functional compositions.

The algorithm for solving the problem involves the calculation and assessment of the balance of the overall chemical composition of model functional compositions and optimization of protein, fat and carbohydrate components, energy value of the developed product. Computer modeling consists of structural optimization of the composition, content and ratio of individual nutrient components of multicomponent food products and allows, based on the components selected from the database and the characteristics of their nutrient composition, to determine the composition that is as close as possible to the specified reference requirements. The methodology of food modeling based on model compositions involves determining the desired content:

- protein in the product and modeling of its amino acid composition, with the aim of approaching the standard (the "ideal" protein, which takes into account the daily human need for essential amino acids, is defined as the standard);
- fat (reference ratio between saturated, mono- and polyunsaturated fatty acids);
- carbohydrates (ratio of simple and complex carbohydrates, including dietary fiber content);
- macro- and microelements (quality composition, ratio of individual elements);
- vitamins (quality composition and ratio);
- energy value and its comparison with the desired Q (standard).

Mathematical modeling of functional compositions and products based on them is reduced to the construction of their model according to the given parameters of adequacy and quality, selection of initial components and recipe optimization according to the criteria of nutritional and biological value.

To achieve this, we develop a parametric product model. This model incorporates the chemical composition (like protein, fat, moisture, and carbohydrates) and the mass fractions of the primary ingredients. It also accounts for the structural ratios of biological value indicators, such such as the amino and fatty acid profiles. Crucially, the model is designed to specifically consider the unique characteristics of health food products. The minimum deviation from the given structure of the corresponding group of indicators of nutritional and biological value is set as the target function of multicomponent product optimization.

1. Optimization criterion based on indicators of chemical composition, which determines the nutritional value of the simulated functional composition:

$$P(z) = \sum_{i=1}^{n} \left(z_i^0 - \sum_{j=1}^{m} b_{ij} x_j \right)^2 \to \min \quad (1)$$

x_j – represents the mass fraction of the *j*-th component within a given compositio;
b_{ij} – specific content of the *i*-th chemical element (such as protein or fat) found in the *j*-th component;
z_j^0 – reference content of the *i*-th element serves as a benchmark.

2. Criterion of minimal deviation from the given structure of indicators of biological value:

$$P(A) = \sum_{k=1}^{n} \left(\left(A_k^0 - \frac{\sum_{j=1}^{m} a_{ki} b_{ij} x_j}{\sum_{j=1}^{m} b_{ij} x_j} \right)^2 \right) \to \min \quad (2)$$

a_{kj} – the specific content of the k-th ingredient in the ith element of the chemical composition

3. The mass fraction of the lth amino acid (should not exceed the specified threshold $A_l^{\max}$ in g/100g of protein):

$$\sum_{j=1}^{m} a_{lj} b_j^a x_j \leq A_l^{\max} \quad (3)$$

a_{lj} – mass fraction of the lth amino acid in the jth component, g/100 g of protein.

Regarding plant proteins, they typically exhibit lower levels of essential amino acids like lysine, leucine, threonine, methionine, and tryptophan, while being rich in glutamic acid. The biological value of proteins is quantified through their amino acid score: (amino acid score = (g of AA in 100g of the studied protein / g of AA in 100 g of "ideal" protein) 100%.

An amino acid score less than 100% indicates that the amino acid is limiting. The smallest values correspond to the main limiting acid. To improve the amino acid composition of proteins, the level of the main limiting amino acid is increased in accordance with the amino acid formula of needs and the content levels of the second limiting amino acid. The number of the first and second limiting amino acids is correlated with the number of the third amino acid.

4. The mass fraction of lysine in relation to the total mass fraction of methionine and cystine (in the pursuit of unity):

$$\sum_{j=1}^{m} \left[a_{ліз} - (a_{мет} + a_{цис}) \right] \cdot b_j^a \cdot x_j \leq eps \quad (4)$$

де, $a_{ліз}$, $a_{мет}$, $a_{цис}$ – the proportion of lysine, methionine, and cystine per 100 grams of protein;
b_j^a – the protein's mass fraction in the *j*-th component;
eps – small value.

The ratio of protein content to fat content:

$$\sum_{j=1}^{m} b_j^a x_j \,/\, \sum_{j=1}^{m} b_j^ж x_j = K \quad (5)$$

де, b^a_j, $b^ж_j$ – mass fraction, respectively, of protein and fat in the j-th recipe component of the composition;
x_j – the fraction by mass for the *j*-th component;

5. The mass fraction ratio of saturated, monounsaturated, and polyunsaturated fatty acids should adhere to the specified K1:K2:K3 proportion:

$$K_2\sum_{k=1}^{7}\sum_{j=1}^{m}q_{kj}b_j^{ж}x_j = K_1\sum_{k=8}^{10}\sum_{j=1}^{m}q_{kj}b_j^{ж}x_j; \quad (6)$$

$$\sum_{k=1}^{7}\sum_{j=1}^{m}q_{kj}b_j^{ж}x_j + \sum_{k=8}^{10}\sum_{j=1}^{m}q_{kj}b_j^{ж}x_j = K_3\sum_{k=11}^{13}\sum_{j=1}^{m}q_{kj}b_jx_j, \quad (7)$$

де, k=1-7 – corresponds to saturated fatty acids;
k=8-10 – monounsaturated fatty acids;
k=11-13 – polyunsaturated fatty acids;
$b_j^{ж}$ – mass fraction of fat of the jth component of the composition;
q_{kj} – mass fraction of the k-th fatty acid in the j-th component, g/100g of fat;
On average, the amount of PUFA should provide about 4% of the energy value of the diet.

6. Criterion of minimum deviation from the given structure of vitamin composition, mineral substances:

$$P_i(V) = \sum_{k=1}^{n}\left(V_k^0 - \frac{\sum_{j=1}^{m}b_{kj}x_j}{\sum_{j=1}^{m}x_j}\right)^2 \to \min \qquad i = 1, 2, 3 \quad (8)$$

As a limitation, the ratios derived from the structural-parametric models of rational nutrition are used.

7. Restrictions on the elemental chemical composition of the product:

$$L_r^{\min} \le \sum_{j=1}^{m}t_{rj}x_j \le L_r^{\max} \qquad r = \overline{1,\chi}, \quad (9)$$

де, t_{rj} – the content of the r-th element in the j-th component of the composition;
$L_r^{\min}, L_r^{\max}$ – admissible restrictions on the content of the r-th element.

8. Restrictions on prescription components:

$$\sum_{j=1}^{m}x_j = 1; \qquad x_j^{\min} \le x_j \le x_j^{\max}; \qquad j = \overline{1,m}, \quad (10)$$

де, $x_j^{\min}, x_j^{\max}$ – permissible limits on the content of the i-th component in the product formulation.

9. Restrictions on value indicators:

$$\sum_{j=1}^{m}d_ix_j \le D_p^{\max} \quad (11)$$

де, d_i – unit cost of the jth component;
$D_p^{\max}$ – the maximum value of the product.

Optimizing multi-component products, considering various formulations and combinations of linear and nonlinear criteria and constraints, is achieved through simulation modeling. This involves systematically evaluating all possible initial ingredient combinations, then verifying constraints and their correlation with the optimization criterion.

To identify the optimal composition for a product containing *m* components, the process begins by selecting the mass fraction of the first component (x_1). Subsequently, we systematically evaluate the ratio coefficients (K_j). This involves iterating through values from an initial n_0 up to 0.9, in increments of h. Through this simulation, all possible combinatorial variations of the *m*-component product recipe are explored. For each variation, the mass fraction of the *j*-th component (x_j) is precisely calculated using a specific formula:

$$X_j = \frac{(1-K_{j-1})}{K_{j-1}} \cdot X_{j-1} \cdot K_j, \quad j = \overline{2,m-1} \quad (12)$$

The process continues by checking if the calculated mass fraction for component *j* (x_j) meets the predefined boundary conditions. If it does, we establish the admissible relationship $n_j=K_j$ and proceed to the next component (j=j+1) to determine its ratio coefficient (K_j). However, if x_j falls below its minimum threshold ($x_j<min_j$), its proportion relative to subsequent components is increased by a step size (h). Conversely, if xj exceeds its maximum limit ($x_j>maxj$), the system reverts to the initial ratio for component *j* ($n_j=n0$). The previous cycle then resumes for component j−1, with its starting value incremented by h ($n_j=n_j+h$). Once acceptable ratios for all recipe components are selected, ensuring their mass fractions sum to unity, both parametric and balance constraints are validated. This step involves accumulating all valid options, which are then evaluated for their functional adequacy to identify the best alternative solution. The overall product quality is assessed based on a set of values or deviations of determining factors and their significance. This evaluation is typically achieved through additive, multiplicative, or mixed functionals. It's important to note that all measurement parameters are standardized and converted to a dimensionless scale of relative values for consistent analysis:

$$Z_i = \frac{X_i - X_i^0}{\Delta X_i} \quad (13)$$

X_i, X^0_i – the actual and desired value of the parameters;

ΔX_i – the maximum permissible deviation from the desired.

Taking into account the weighting factors b_i of the ith parameter at $\sum_{i=1}^{n} bi = 1$ the expression of the functional has the following form:

$$\Phi(z) = 1 - \sqrt{\sum_{i=1}^{n} b_i z_i^2} \quad (14)$$

or taking into account the group of critical indicators Zk, the deviation of which beyond the limits clearly excludes the possibility of using the product,

$$\Phi(z) = \prod_{k=1}^{m_k}(1 - z_k^2) \cdot \left[\ 1 - \sqrt{\sum_{i=1} b_i z_i^2}\ \right] \quad (15)$$

When leaving the tolerance field of any parameter of the critical group Zk, the functional turns into 0. When finding the critical indicators within the norm, the value of the criterion changes from 1, when the measurement values of Chi completely match the reference values (better quality) to 0, when the limit of the quality level is reached (limit value). With negative values of the functionality, the product does not meet the specified quality level. To determine the weighting coefficients and the graduated scale of the generalized functional, it is advisable to use the method of expert evaluations or a full factorial experiment. The value of the quality function of the modeled product is graded from 1 to 0 on the desirability scale, respectively from the highest to the satisfactory level of quality according to the equations of the separating surfaces, which are obtained as a result of the full factorial experiment: 1.0-0.7 - excellent; 0.7-0.3 – good; 0.3-0.1 – satisfactory; 0.1-0.0 - bad, negative functional values correspond to unsatisfactory product quality.

The proposed multi-criteria model can be used in various settings for any specific criterion, for example, for the analysis of amino acid, fatty acid, carbohydrate, macro- and microelement, vitamin composition of multicomponent prescription systems. Thus, operating with the initial data characterizing the composition and properties of the ingredients, setting the boundary conditions and necessary levels of individual indicators and using the computer modeling system, it is possible to determine the optimal model functional compositions that meet the given criteria. Computer design systems of model functional compositions and food products based on them function in the Windows 2000, XP, NT environment. The interfaces are written in Delphi, and the main procedures are written in Object Pascal.

Stage 3. Design of model compositions with given structural characteristics. The stage of computer design allows to obtain functional compositions through modeling that maximally satisfy the formalized needs, the level of nutrient content and the total biological value. However, the composition of the "optimal" compositions determined at the first stage does not guarantee their transformation in the process of technological processing under production conditions into a system with the necessary organoleptic indicators, structural and mechanical properties. This is due to the fact that the individual components of the formulations have certain individual and often mutually exclusive functional-technological properties (FTV). For the effective implementation of the second stage of design, it is necessary to have information not only about the chemical composition and biological value of individual components of the recipes, but also information about the actual values of FTV of the main raw materials and auxiliary ingredients in multicomponent food systems with analytical and imperial dependencies, which characterize the main patterns of behavior of heterogeneous dispersed systems with varying physical and chemical factors.

Consideration of the theoretical foundations of the processes of structure formation, in particular, in test systems and the possibility of their adaptation to the design methodology, testify to the high level of complexity of the task, which is due to:

• the diversity and multicomponent nature of the main raw material, its morphological heterogeneity, lability as a result of the development of biochemical and microbiological processes;

• high variability of its properties with different methods of technological processing and under the influence of physical and chemical factors (pH of the environment, temperature, etc.).

It is almost impossible to predict the final properties of combined food systems based only on the general chemical composition and physicochemical properties of individual ingredients of the formulation. Even assuming that the acquisition of individual structural forms (consistency, appearance, structure, etc.) by the model composition is due to the peculiarities of colloidal-chemical processes, it cannot be confidently predicted that after technological processing the ingredients of the composition will turn into a stable dispersed system with the necessary properties. When modeling functional compositions, it is necessary to take into account that the ingredients must have certain functional and technological properties that ensure the production of stable food dispersion systems with the necessary structural-mechanical and organoleptic properties.

The main FTVs include swelling, solubility, ability to stabilize dispersed systems (drag-forming, water-absorbing, emulsifying ability), rheological properties. Thus, the degree of expressiveness of certain FTV of specific composition ingredients determines the degree of their participation in the performance of certain structural functions in food systems. In turn, the level of manifestation of specific FTV of various types of raw materials and ingredients depends both on their composition (proteins, polysaccharides, their mixtures), and on physico-chemical and microbiological factors. The relative values of the main functional and technological properties of model functional compositions are interpreted in a five-point scale. The study and systematization of the FTV of individual ingredients of compositions and products, the nature of their changes under the influence of physico-chemical and technological methods of processing, the development of theoretical foundations of the basic processes of structuring in food systems, make it possible to form an information base and approach the process of modeling food products, taking into account the specifics of possible interaction recipe components.Computer multi-level modeling allows you to significantly speed up the process of developing technologies, create the basis of a systematic approach to the selection of model functional compositions, taking into account the possible influence of individual ingredients on the formation of organoleptic indicators, structural and mechanical properties, output, etc.

After the completion of the computer modeling stage, the "optimal" compositions are subjected to further comparative analysis from the point of view of the possibility of obtaining, on the basis of the selected set of ingredients, a stable structured dispersed system of a certain type with the required level of structural and mechanical properties (for model functional compositions) and organoleptic indicators (for finished products). Taking into account the initial data for design (type of product, basic technology, technical means), they analyze the food system and the processes of its production, evaluate the FTV of each of the ingredients of the composition, the nature of their changes, depending on physical and chemical factors, determine the degree of their functional and technological compatibility, choose basic structure-forming parameters that allow effective regulation of FTV and the structuring process that determines the physical stability and rheological properties of the food system.

At the next stage, through multi-level experimental modeling, the level of stability of systems made on the basis of "optimal" compositions is checked and, if necessary, targeted regulation of the FTV of individual ingredients and model systems, as well as the organoleptic indicators of products, is carried out by selecting and applying certain mechanical and physicochemical factors

Conclusions

Therefore, the features of the biotechnological potential of the used ingredients of the model compositions, the probability and intensity of the development of microbiological processes are simultaneously taken into account during modeling. Taking into account the above-mentioned factors, the modeling results, as a rule, provide effective optimization of the product composition and parameters of individual operations of the technological process. Upon completion of the stage of multi-level experimental modeling, the functional compositions and technologies of the products are tested in laboratory and production conditions, after which their final adjustment is made. At the final stage, comprehensive studies of the main indicators of the quality of finished products, calculation of economic indicators, development of the technology in production conditions, preparation, coordination and approval of regulatory documents and organization of industrial implementation are carried out. The application of the design methodology of model functional compositions and food products allows to increase the degree of use of raw materials and expand the assortment of products with a given composition and properties for health purposes.

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