AN APPROACH TO THE CHOICE OF ALTERNATIVES OF THE OPTIMIZED FORMULATIONS

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Abstract: The scientific direction of the food product designing with a specified set of indicators of nutritional value is currently topical in the world. The mathematical bases for solving formulation problems are well studied. The problems concerning the multi-objective optimization of formulations for multicomponent products are frequently met. At the same time, only one, the most important, criterion is to be optimized, and the rest criteria act as the additional constraints, since the intersection of sets of the optimal solutions for all single-objective problems usually turns out to be an empty set. As a result, several formulation alternatives are obtained, which are optimized according to any single or several (but not all) criteria. The purpose of the work is to theoretically substantiate a universal approach to choosing out of the set of alternatives of the optimized formulations of food products. The authors suggest reasserting the problem of choice as the problem of assessing the degree of the product’s composition conformance with the recommended physiological standards. When assessing the balanced state of the formulation alternatives, the conclusions are made by comparing the relative degree of conformance of the generalized Harrington's desirability function value with the reference standard, and not of the absolute value of the generalized desirability function. To select from a variety of the optimized formulation alternatives of the multicomponent food products, it is proposed to use the following 6 criteria: a balanced state index of the product’s macronutrient composition; a balanced state index of the vitamin composition; a balanced state index of the mineral composition; a balanced state index of the amino acid composition; a balanced state index of the fatty acid composition; and a balanced state index of the energy value. Wherein, it is proposed to calculate the generalized Harrington's desirability function as a geometric mean of the partial balanced state indices. A universal approach is suggested for making a choice out of the variety of the optimized formulation alternatives. At the same time, the subjectivity is eliminated in choosing the nomenclature and numerical values of the physical indicators of quality of the compared variants of multicomponent products.

Keywords: Formulation, food product, multicomponent product, mathematical design of a product composition, optimization of formulation

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INTRODUCTION

Since the human diet consists of a variety of products, this generally compensates for the shortage of any substances in a daily diet, though it is still desirable to provide people with food products balanced in chemical composition. Therefore, the design of food products with a given set of nutritional value indicators is currently topical.

The fundamental principles for designing products and diets with the specifiable nutritional value are inherent in the works written by the academics I.A. Rogov and N.N. Lipatov (junior). They stated the basic principles of composition design of the balanced products with the required set of indicators and of the diets containing such products [4–6, 13]. Later, this methodology was developed in the works by A.B. Lisitsin, E.I. Titov, S.B. Iudina, Iu.N. Nelepov, Yu.A. Ivashkin, A.M. Brazhnikov, G.I. Kas’ianov, A.E. Krasnov, A.T. Diplock, A. Wollen, Ruguo Hu, and other scientists [1, 3, 8, 19, 21]. The method of neural networks is proposed by the A.G. Khramtsov School [16].

Currently, this trend retains its relevance and not only in the scientific, but also in the applied aspects. For many years, the domestic (Fig. 1) and foreign scientists [17–21, 22–26] have been working on solving this problem including through the methods of mathematical modeling [1, 2, 7, 9–10, 20]. The basic methodological principles and approaches have been developed for designing quality and balanced state of the food products according to the main macro- and micronutrients [14, 15].
A key objective in designing the multicomponent food products is to establish a preferred set and ratio of components. The difficulty in solving a formulation problem consists in frequent usage of a large number of ingredients in designing, while the optimization can involve more than two criteria.

At the present stage of the science and technology development, it is impossible to solve this problem without involving the formal approaches, wherein the numerical information is used and the desired properties of composition are provided. Moreover, the solution of this problem is very complicated without applying appropriate software, since the manual solution of the system of linear equations and inequalities with a large number of variables is of significant difficulty, at which the computational errors cannot be excluded [9, 10].

The mathematical framework for solving such problems is well known. Among the various models of the technological processes, the so-called linear models hold a specific place, i.e. the models, wherein the mathematical relationships (equalities or inequalities) are linear with respect to all the variables included into the model. The essence of such problems consists in choosing according to the specified criterion an optimal alternative out of the variety of possible alternatives of the process studied. The development of general methods for their solution was started in 1939 by the Russian mathematician and academician L.V. Kantorovich. Later, in the works by the American scientist G. Dantzig, this method was called a simplex method. The simplex method is a universal method for solving linear programming problems. The simplex method is based on the algorithm of simplex transformations of a system, which is supplemented by the rule ensuring a transition to the best basic solution, and not just to the any solution. That is, at first, an admissible alternative is obtained, which satisfies all the constraints, but it is not necessary to be the optimal alternative (an initial basic solution). The optimality is achieved through a consistent improvement of the initial alternative of a certain number of steps (iterations).

The application of the simplex method in the dairy industry was considered by Yu.P. Markin and Yu.A. Ivashkin. To implement the simplex method, either the specially written programs (KSIMP, ESIMP, ISIMP) or the universal mathematical software packages (MathCAD, Maple) are applied. The Solver Microsoft Excel add-in uses the Generalized Reduced Gradient, a nonlinear optimization algorithm developed by Leon Lasdon and Allan Waren. The simplex method algorithms for solving linear and integer problems with constraints are developed by John G. Watson and Daniel Fylstra [7]. In the United States, this approach with reference to designing the food product formulations is perfectly described in the book by Ruguo Hu [21].

It should be noted that in practice, we often meet problems that require finding the best solution in the presence of different irreducible criteria of optimality – the problems of multi-objective optimization. For example, when designing a multicomponent dairy product, it is necessary to take into account such
frequently controversial facts as the quantity and ratio of the essential amino acids, the balance of fatty acids, the low energy value, the minimum cost, the technologically or organoleptically limited content of vegetable components, and many others. In other words, there are several objectives that cannot be reflected by a single criterion. Some partial criteria may be controversial, others may act in single direction, and others can be indifferent to each other.

Usually, in order to cope with such a situation, we have to make the following compromises: the optimization of single criterion recognized as the most important one, whereas all the rest criteria act as the additional constraints (in particular, the authors have implemented this approach in the "Minimum-Maximum" computer program); the ordering of a given set of criteria and a consistent optimization of each of them.

Theoretically, in an ideal case, it is possible to search for such a solution that belongs to the intersection of the sets of optimal solutions for all single-objective problems. However, it is known that such an intersection usually appears to be an empty set [7]. Therefore, a set of effective solutions should be considered at the time when the optimization means the enhancement of some indicators provided that the others do not deteriorate.

As a result, we obtain a set of alternatives optimized according to any single criterion of formulations. The purpose of this work is to theoretically substantiate a universal approach to choosing out of the set of alternatives of the optimized formulations of food products.

OBJECTS AND METHODS OF STUDIES

The problem of mathematical design of the food product formulations can be interpreted as the problem concerning the optimal use of the limited resources. The essence of the formulation optimization for a food product consists in finding such a solution \( X = (x_1, x_2, ..., x_n) \), wherein \( x_i \) are the formulation components, which would be the best to take account of the optimality criteria. An optimality criterion can be represented for example by a minimum cost, a maximum macronutrient content, etc. In addition, a number of conditions are superimposed on the solution, i.e. the choice \( \bar{X} \) is carried out from a certain area of possible solutions \( R \). Within the framework of this article, the term "to optimize a formulation of a food product" means to solve a problem of the following type: \( \max(\min) f (\bar{X}), \bar{X} \in R \), where \( f(\bar{X}) \) is an objective function (the mathematical notation of an optimality criterion).

In solving an optimization problem, an uncertain system, i.e. a set of non-negative solutions of a system of linear equations, is of practical interest. From a technologically point of view, this means finding a set of formulation alternatives, which correspond to the predetermined constraining conditions. It should be emphasized that the objective of the present article involves not just a discussion of the methods for solving optimization problems, but the scientific substantiation of the methodology for choosing a product formulation out of the set of possible optimized formulation alternatives.

One of the known methods for choosing an optimal formulation out of the set of formulation alternatives consists in using the generalized Harrington's desirability function. The construction of a generalized Harrington's desirability function is based on the idea of converting the natural values of partial responses into a dimensionless scale of desirability or preferable.

The partial response value converted into a dimensionless scale of desirability is denoted by \( d_i \) \((i = 1, 2, ..., n)\) and called a partial desirability. The formulation of a designed product should be evaluated in the units of partial desirability function \( (d_i) \). All the partial desirability functions \( d_i \) are to be combined into the generalized desirability function. The generalized index of desirability \( (D) \) is calculated as a geometric mean according to the following formula:

\[
D = \sqrt[n]{\prod_{i=1}^{n} d_i} = \sqrt[n]{d_1 \cdot d_2 \cdot d_3 \cdot d_n}.
\]

The scale of desirably has a range from zero to one. The \( d_i = 0 \) value corresponds to the absolutely unacceptable level of this property, and the \( d_i = 1 \) value corresponds to the best value of the property. The \( d_i = 0.37 \) value usually corresponds to the lower boundary of the permissible values.

The desirability function reflects the dependence of assessments or indicators of the desirability \( d \) on the dimensionless indicators \( y \), into which the dimensional (physical) quality indicators are converted. If the top or bottom unilateral constraints are imposed on a parameter, then the desirability function is to be calculated according to the following formula:

\[
d_i = \exp(-\exp(-y_i)).
\]

If the optimization parameters possess the bilateral constraints, i.e. they are of the \( y_{\text{min}} \leq y \leq y_{\text{max}} \) form, then the desirability function is to be calculated according to the following formula:

\[
d_i = \exp\left[-\left|y_i\right|^n\right],
\]

where \( n \) is a positive figure.

By choosing different values of \( n \), it is possible to specify different curvature of the desirability curve. This provision allows taking into account the particular importance of the individual parameters of optimization: therefore \( n \) will make a big value, and thus, a small change of the optimization parameter near the limits will correspond to the sharp change in desirability.

The dimensionless parameter \( y_i \) is to be calculated according to the following formula:

\[
y_i = \frac{2y_i - y_{\text{max}} + y_{\text{min}}}{y_{\text{max}} - y_{\text{min}}}.
\]
The exponent \( n \) is to be calculated by specifying the value \( d \) (preferably in the range of \( 0.6 \leq d \leq 0.9 \)) followed by the calculation of \( y_i \) according to the expression (4). Then the exponent is to be calculated according to the following formula:

\[
    n = \ln \frac{1}{d_i} \frac{\ln d_i}{\ln y_i}. \tag{5}
\]

The conversion of the values of dimensional (physical) indicators \( y \) of the product quality into the dimensionless indicators \( y \) in a linear relationship there between can be carried out according to the following formula:

\[
    y = a_0 + a_1x, \tag{6}
\]

where \( a_0 \) and \( a_1 \) are the equation coefficients.

Having taken the logarithm of the equation (2) for the second time, we will obtain as follows:

\[
    \ln \frac{1}{d_i} = -y, \text{ or } y = \ln \frac{1}{\ln \frac{1}{d_i}}. \tag{7}
\]

Let us substitute the values of \( y \) (7) into the equation (6):

\[
    a_0 + a_1x = \ln \frac{1}{\ln \frac{1}{d_i}}. \tag{8}
\]

Let us set up a system of equations for the boundary values of the desirability indicators \( d_1 \) and \( d_2 \) (a distinct and satisfactory value):

\[
    \begin{align*}
    a_0 + a_1x_1 &= \ln \frac{1}{\ln \frac{1}{d_1}}, \\
    a_0 + a_1x_2 &= \ln \frac{1}{\ln \frac{1}{d_2}}.
    \end{align*} \tag{9}
\]

The values of the partial desirability indicators \( d_1 \) and \( d_2 \) are to be chosen independently (for example, a distinct value equal to \( d_1 = 0.8 \); and a satisfactory value \( d_2 = 0.37 \)). By simultaneously solving the system of equations (9), the values of the \( a_0 \) and \( a_1 \) coefficients are to be found.

The obtained solution should result in the equation of linear dependence between the studied indicator \( x \) and the dimensionless values \( y \). By using this equation, the value of \( y \) can be found for any value of \( x \), followed by the calculation of the partial indicator of desirability \( d \) according to the formula (2) and of the generalized indicator of desirability \( D \) according to the formula (1).

According to the authors, the major challenge in using the Harrington’s desirability function when solving a problem concerning the choice of the product formulation out of the set of possible alternatives of the optimized formulations is the lack of a common approach and, therefore, the subjectivity in selecting the nomenclature and numeric values of the physical quality indicators of the compared product alternatives. The following describes the authors’ approach to solving this problem.

RESULTS AND DISCUSSION

For a clear understanding of the properties of the object studied (a multicomponent food product), it is necessary to identify the relations between the elements of such an object. The aggregate of the elements’ interrelations ensuring the integrity of the system is called the system structure. The model of the structure of a designed product is a list of the relations being essential for the solution of a specific problem. For example, generally, when optimizing the formulation of a multicomponent product, the raw material wasted while moving through the pipelines is not taken into account, though such losses exist. At the same time, the loss of the nutritional value of a raw material during the mechanical or thermal treatment can be considered. It is possible to construct the block diagrams, wherein only the elements and their interrelations as well as the difference between the elements and the relations are marked. Such diagrams are called graphs.

The diagram demonstrating the interrelations between the elements of the designed product with a specified composition is shown in Fig. 2 in the form of a planar composition with 7 elements and 6 relations. This interrelation determines the energy, nutrition, and biological value of a multicomponent product. The change in values (mass fractions) of one of the formulation mixture elements leads to the change in values of the interrelated elements. For example, the vitamins-related optimization of a product will lead to the change in its energy value as well as in the formulation-based, mineral, fatty acid, and amino acid composition.

In its general view, the design of a multicomponent product formulation involves the implementation of the stages shown in Fig. 3. This article observes only the fourth stage.

The implementation of the third stage is possible both by using the following computer programs developed by the authors: "Minimum-Maximum" (Certificate of Registration No. 2010612628 of April 15, 2010), "Ideal Protein" (Certificate of Registration No. 2010616153 of September 17, 2010), "Design of Formulations" (Certificate of Registration No. 2011611470 of February 14, 2011), and through any other automated means for calculating and optimizing the formulations, which are currently known in a sufficient quantity.

As known, a diet should contain such an amount of energy and nutrients, which corresponds to a daily rate of the physiological standard for a certain group of the population. The content of a micro- and macronutrient, both below and above the permissible rates, indicates the unbalanced state of the diet. The problem of formulation optimization consists in choosing the components and determining their ratios, which ensure the maximum conformance of the nutrients’ mass fractions with a physiological standard.
Fig. 2. A planar graph of the formulation design of a multicomponent food product: R – the macronutrient composition of the designed product; A – the amino acid composition of the product; F – the fatty acid composition of the product; C – the cost of the product; E – the energy value of the product; V – the vitamin composition of the product; M – the mineral composition of the product.

Fig. 3. The stages of a multicomponent product design.

I Setting partial problems of designing
II Ranking the problems by their priority
III Solving the problems
IV THE CHOICE OUT OF THE VARIETY OF THE OPTIMIZED FORMULATION ALTERNATIVES
V Practical implementation (working with the formulations, applying them in the production)
All the developed countries provide the recognized norms of such physiological standards. For example, in the United States, the Food, Nutrition and Consumer Services Division established in the U.S. Department of Agriculture and its agencies (www.cnpp.usda.gov, www.fns.usda.gov) are engaged in dealing with these issues. In Russia, there are the "Standards of Physiological Needs of the Energy and Nutrients for Various Groups of the Population of the Russian Federation" approved in 2008 by the Federal Service for Supervision of Consumer Rights Protection and Human Welfare. The "Standards" are the effective national regulations that define the values of the standard rates of consumption of the essential nutrients and energy sources, which are physiologically substantiated by the modern science of nutrition. The World Health Organization also regularly publishes the recommendations on diet and health [12].

The theoretical calculations and practical experiments show that in most cases it is impossible to achieve simultaneously by all indicators the standard level of balance when designing the multicomponent food products. This complicates the task of choosing one or more multicomponent products out of the variety of formulation alternatives optimized according to a certain partial indicator or even a set of indicators. Therefore, we suggest reasserting the problem of choice as the problem of assessing the degree of the product’s composition conformance with the recommended physiological standards.

To make a scientifically substantiated choice out of the variety of the optimized formulation alternatives of the multicomponent food products, it is proposed to use the following 6 criteria:

- A balanced state index of the product’s macronutrient composition BNCI (will be denoted in the formulas as $U_n$);
- A balanced state index of the vitamin composition BVCI ($U_v$);
- A balanced state index of the mineral composition BMCI ($U_m$);
- A balanced state index of the amino acid composition BACI ($U_a$);
- A balanced state index of the fatty acid composition BFCI ($U_f$);
- A balanced state index of the energy value BEVI ($U_e$).

These partial criteria allow us to comprehensively assess the level of the formulation balanced state of a product designed for a specific group of the population.

The criteria calculation is carried out as the geometric mean. Thus, a partial criterion for assessing the balanced state of the BNCI macronutrient composition is to be calculated according to the following formula:

$$U_n = \sqrt[3]{P \frac{N_j}{N_{ej}}}$$

(10)

where $N_j$ is the content of the $j$-th macronutrient (fat, protein, carbohydrate) in the formulation of a product, $g$; $N_{ej}$ is the standard of physiological needs of the $j$-th macronutrient, $g$; $3$ is the number of standardized macronutrients (proteins, fats, carbohydrates).

The balanced state index of the vitamin composition is to be calculated according to the following formula:

$$U_v = \sqrt[3]{P \frac{V_j}{V_{ej}}}$$

(11)

where $V_j$ is the content of the $j$-th vitamin in the formulation of a product, mg; $V_{ej}$ is the standard of physiological needs of the $j$-th vitamin, mg; $n$ is the number of standardized vitamins (the list depends on a group of the population).

The balanced state index of the mineral composition BMCI is to be calculated according to the following formula:

$$U_m = \sqrt[3]{P \frac{M_j}{M_{ej}}}$$

(12)

where $M_j$ is the content of the $j$-th mineral substance in the formulation of a product, mg; $M_{ej}$ is the standard of physiological needs of the $j$-th mineral substance, mg; $n$ is the number of standardized mineral substances (the list depends on a group of the population).

The balanced state index of the amino acid composition BACI is to be calculated according to the following formula:

$$U_a = \sqrt[8]{P \frac{A_j}{A_{ej}}}$$

(13)

where $A_j$ is the content of the $j$-th essential amino acid in the formulation of a product, mg/g of protein; $A_{ej}$ is the content of the $j$-th essential amino acid in 100 g of ideal protein, mg/g of protein; $8$ – is the number of essential amino acids.

The balanced state index of the fatty acid composition BFCI is to be calculated according to the following formula:

$$U_f = \sqrt[3]{P \frac{F_j}{F_{ej}}}$$

(14)

where $F_j$ is the content of the $j$-th fatty acid in the formulation of a product, mg%; $F_{ej}$ is the physiologically substantiated standard of the $j$-th fatty acid, mg%; $n$ is the number of the taken into account fatty acids.

A partial criterion for assessing the balanced state of the product formulation according to the energy value:
where $E_i$ is the energy value of 100 g of a product, kcal; $E_{ij}$ is the desired level of the energy value of 100 g of a product, kcal.

Theoretically, the ideal formulation will be the product formulation with all indices equal to "1": $U_a = 1$, $U_i = 1$, $U_m = 1$, $U_f = 1$, $U_a = 1$, $U_f = 1$. Thus, we propose to perform the calculation of the generalized Harrington's desirability function ($D_i$) as the geometric mean of the partial balanced state indices:

$$D_i = \sqrt[6]{P_i} = \sqrt[6]{U_a \cdot U_i \cdot U_m \cdot U_f \cdot U_a \cdot U_f}.$$  \hspace{1cm} (16)

The ideal balanced state of the formulation is achieved at $D_i = 1$. Since the criteria calculation is carried out basing on the daily rate of the physiological needs of nutrients and energy, then theoretically, the "1" can be achieved only by analyzing a daily human diet for its balanced state. When assessing the balanced state of the formulation alternatives, the conclusions should be made according to the comparison of the relative degree of conformance of the $D_i$ value with the standard, and not of the absolute value of the generalized desirability function.

Let us consider a specific example. The task is to design the formulation of a dish for the out-of-school feeding of the children aged 7-11 years – cottage cheese with fresh berries. The "Standards of Physiological Needs of the Energy and Nutrients for Various Groups of the Population of the Russian Federation" are taken as a standard of the children’s needs. The initial stage of designing is the calculation of the nutritional composition, i.e. the substantiation of the a priori information on the ingredients content of the designed nutrient compositions, their content is based on the nutritional compositions, % (without losses).

Table 1. Formulation alternatives

| Ingredients                          | Variants of nutritional compositions, % (without losses) |
|--------------------------------------|--------------------------------------------------------|
|                                      | 1            | 2               | 3         | 4      | 5          |
| Low-fat cottage cheese               | 75.0         | 95.9            | 60.0      | 85.0   | 60.0       |
| Fresh berries                        | 25.0         | 1.3 (cowberry) + | 9.4 (bilberry) + | 8.1 (cowberry) + | 2.7 (bilberry) + |
|                                      |              | 1.5 (bilberry) + | 30.6 (black currant) | 6.9 (cranberry) | 37.3 (black currant) |
| BMCI                                 | 0.027        | 0.022           | 0.027     | 0.023  | 0.027      |
| BEVI                                 | 0.034        | 0.036           | 0.032     | 0.033  | 0.033      |
| BACI                                 | 0.090        | 0.044           | 0.112     | 0.055  | 0.108      |
| BMCI                                 | 0.065        | 0.041           | 0.063     | 0.049  | 0.068      |
| BACI                                 | 1.570        | 1.900           | 1.320     | 1.640  | 1.350      |
| Generalized desirability function $Di$| 0.097        | 0.077           | 0.096     | 0.078  | 0.098      |
The difficulty of choosing out of five variants consists in the fact that the formulations appear to be balanced according to different indicators – one composition is better in vitamin content, another – in mineral, etc.; there is no evident leader. Using out methodology, it is possible to substantiate the choice of a specific formulation out of the number of alternatives. The calculation of the generalized Harrington's desirability function taking into account the proposed by us partial criteria (balanced state indices) has shown that the integral level of the formulation balance according to the fifth variant is the maximum out of the variants analyzed: 0.098. Of course, this figure is far from "1", but, nevertheless, now the choice among the variety of alternatives becomes objective and substantiated.

Such a nutritional composition contains 0.5% of fat, 11.4% of protein, 7.0% of carbohydrates, and 76.5 kcal per 100 g. The ratio in the composition of the polyunsaturated fatty acids, monounsaturated fatty acids, and saturated fatty acids is 1.0 : 0.6 : 0.1. One portion of the product (200 g) according to the fifth variant satisfies the daily demand of a schoolboy/schoolgirl aged 7–10 years for vitamin A by 20.6%, C – by 226.0%, B3 – by 95.4%, B2 – by 24.2%, and B6 – by 17.4%: for micro- and macro-elements such as potassium – by 42.6%, calcium – by 16.8%, phosphorus – by 24.6%, magnesium – by 18.8%, and iron – by 10%. There is no shortage of any of the essential amino acids.

Thus, when designing the formulations for the out-of-school feeding of the children aged 7–11 years, it can be recommended to take as a basis the composition of the low-fat cottage cheese with the addition of the fresh bilberry and black currant as well as of the stevioside, a natural sweetener, according to one’s taste. It should be noted herein that the given example observes only the initial stage of the formulation designing – the nomenclature and the ratio of ingredients are substantiated. However, this does not mean the end of formulation designing. Although such a composition is considered to be balanced according to the nutritional content, it is still required to complete the rest stages of the formulation designing before making a final decision. In particular, it is necessary to assess the organoleptic characteristics of the dish (it is possible that the ratio of 60% of cottage cheese and 40% of berries would fail the tasting assessment), the technological compatibility of ingredients, the need for the additional preparation of the vegetable raw materials and its influence on the raw material content, the stage and the form of adding the fruit fillers, the storage capabilities of the product, etc.

However, the purpose specified by the authors has been reached – the choice out of the variety of the formulation alternatives optimized according to any criterion becomes understandable and is based on the formalized clear scientific data.

CONCLUSION

The universal approach, proposed by the authors, to the choice out of the variety of the optimized formulation alternatives allows us to eliminate the subjectivity when selecting the nomenclature and the quantitative values of the physical indicators of quality of the compared variants of products, to integrally assess the efficiency of optimization, and to scientifically substantiate the choice of a specific formulation out of several variants being optimal according to different criteria.

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