ORIGINAL ARTICLE

Neural Network and Regression Analysis of the Dependence of the Ranking Score of Organoleptic Characteristics on the Food System Composition

Maria S. Koneva, Sergey V. Usatikov, Natalia A. Bugaets, Maya Yu. Tamova

Department of Public Catering and Service, Kuban State Technological University, 2 Moskovskayast, Krasnodar 350072, Russian Federation

Abstract

Aim: The aim of this research is to develop the technology for producing antianemic smoothie for pregnant women based on the optimization of the composition and organoleptic characteristics of the final product. **Methods and Materials:** The relationship of organoleptic criterion with the quantitative composition of the formulation is identified by neural network and regression analysis of the ranking score of organoleptic characteristics. The model parameters are obtained by means of "Statistica" software package. Convolution of balancing index and sensory evaluation is proposed in the form of a multiplicative function of desirability. The weight optimizing problem of the smoothie composition was solved by means of MathCAD scripts. **Results and Discussion:** At that, wheatgrass juice is an alternative source of iron supplement in the recipe of the smoothie. When modeling the weight composition of the developed product, particular attention was paid to the physiological need of pregnant women in nutrients and their content in food sources such as kiwi, grapes, yogurt, wheat germ juice, and honey. Mathematical optimization model of the smoothie composition for pregnant women needs to take into account the organoleptic characteristics of the combined product. The sensitivity of the network was the main criterion for the selection of ingredient composition that maximally contributes to sensory evaluation when mixing a smoothie. **Conclusion:** We came up to the conclusion that the most important components of the smoothie mix (in the context of organoleptic characteristics) are wheatgrass juice and yoghurt. In consequence of the research, we have developed the methodology of mathematical modeling of the smoothie composition for pregnant women, which meets most fully the following requirements: Optimal content of feedstuff with antianemic properties, and high organoleptic characteristics of the final product.

Key words: Balanced chemical composition, iron deficiency anemia, regression models

INTRODUCTION

The Russian Federation, as other advanced countries, has established a system of multilevel monitoring of the nutritional status of the population. Despite the fact that recent years are characterized by positive trends in changing food consumption structure by increasing consumption of vegetables and fruit, meat and dairy products, as well as fish, the nutritional status of the Russian population still seriously deviates from the healthy eating.

The priority role of nutrition in maintaining the health of the population is enshrined in the most important policy decisions: "The Foundations of State Policy of the Russian Federation in the Field of Healthy Nutrition of the Population for the Period through 2020," approved by the Decree of the Russian Federation Government dated 25.10.2010 No.1873-p, in the context of the implementation of the Decrees of the President of the Russian Federation "On Measures to Implement the Demographic Policy of the Russian Federation" dated 07.05.2012 No. 606, "On Improvement of State Policy in the Field of Public Health" dated 07.05.2012 No. 598, and "National Strategy for Action on Children for 2012-2017."

Address for correspondence:
Maya Yu. Tamova, Kuban State Technological University, 2 Moskovskayast, Krasnodar 350072, Russian Federation. E-mail: koneva_mr@bk.ru

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The major tasks of the state policy in the field of healthy nutrition of the Russian population include the preservation and strengthening of health of the population and prevention of diseases caused by inadequate and unbalanced nutrition through a number of activities, including:

- Production development of food enriched with essential components, specialized baby food, functional food, dietary (medical and preventive) food products, and nutritional supplements to food;
- Ensuring priority development of fundamental research in the field of modern biotechnological and nanotechnological production methods of new food sources and biomedical assessment of their quality and safety.[1]

The problem of healthy eating of pregnant women still remains a subject of sighting the attention of obstetricians-gynecologists and neonatologists and has no tendency to decrease its relevance. The adequacy of food security of pregnant women, and further, a newborn breastfed baby underlies not only child's survival but also ensures a high level of his health.[2]

A balanced diet, acquiring a number of features is a key determinant of health and well-being of the future mother. Thus, the needs of women in nutrients (proteins, vitamins, minerals, etc.) during pregnancy significantly increase, especially in the second and third trimesters of pregnancy. This is due to the fact that food and caloric content of diets in this period should satisfy the requirements of both the woman and the developing fetus.

The diets of pregnant and lactating women often experience shortage in caloric content and nutrilites that adversely affect their health condition, pregnancy, fetal development, and formation of lactation.

Iron deficiency leads to the development of iron deficiency anemia (IDA). The relevance of the prevention and treatment of this pathology is due to its high frequency of occurrence in women during pregnancy and the severity of possible complications. The presence of IDA in pregnant women increases the risk of miscarriage, premature birth, and disorders of placental circulation.

According to the analysis of the research performed by the World Health Organization, more than half of the worldwide population suffers from IDA. In emerging countries, its frequency among pregnant women is 56%. Russia also preserves the trend of increasing in number of women suffered with IDA.[3,4]

Over the past 10 years, the prevalence of anemia among pregnant women has increased significantly and ranges from 21% to 80%. At that, from 75% to 90% of pregnant women suffer from IDA.[3]

IDA is a disease characterizing by the reduced iron content in serum, bone marrow, and depot. This disrupts the formation of hemoglobin that results in hypochromic anemia and trophic disorders in the tissues. IDA remains a serious problem in obstetrics because the incidence of this disease is not reduced.

The main reasons for development of anemia in pregnant women are the hemodilution caused by an increase in blood volume and the true deficit of dietary iron.

The average human diet should contain at least 20 mg of iron, while 30 mg - for pregnant women. The woman consumes daily with food on average from 2000 to 2500 kcal, which contain from 10 to 20 mg of iron. At the same time, a woman loses every day about 1 mg of iron. In addition, the losses of iron increase substantially during pregnancy, childbirth, and during lactation. Thus, often in pregnancy, the demand for iron exceeds the capacity of absorption of iron from food.[4]

Izmukhanbetov[4] draws attention to environmental pollution from chemicals, pesticides, and high mineralization of drinking water as the major circumstances impeding the absorption of iron from food.

The IDA is divided into the "anemia of pregnancy" and "anemia in pregnant women," implying in the first case, the disease that develops during pregnancy, while in the second case - anemia, which existed even before the gestational process. "Anemia of pregnancy" is more severe because woman's organism has adapted to the disease which started before pregnancy, while the "anemia in pregnant women" is a complication similar to gestational toxicosis. In the second half of pregnancy, anemia is diagnosed almost 40 times more often than during the first weeks.[4]

Anemia complicates pregnancy, childbirth and the postpartum period. Oxygen starvation (hypoxia) of the fetus resulting in delayed fetal development occurs at the background of placental insufficiency. In severe cases, this leads to acute hypoxia, which threatens the life of the fetus. As a result, the child may be born immature, with low weight and will subsequently be susceptible to infections.[4]

Iron deficiency and a lack of its deposition in antenatal life contribute to the development of IDA in newborn infants. This leads to changes in metabolism of cell structures, the violation of hemoglobin formation, delayed mental and motor development, occurrence of chronic fetal hypoxia, and imbalances in the immune system of the mother during pregnancy. Some of these abnormalities may be irreversible.[3,4]

Given this high frequency of anemia during pregnancy, the need of preventive measures for all pregnant women becomes evident. Prevention of IDA in pregnant women is required to create iron depot in the newborn infant that in turn prevents the development of anemia in children.

Healthy eating of pregnant woman with additional vitamin and mineral provision contributes to preventing the development of anemia in the mother, avoids problems with teeth, eases morning sickness, and reduces the risk of infectious diseases.

One of the most important approaches to improve the nutritional status of pregnant women is an introduction to their daily diet of special food that contains essential nutrients in the quantities which can largely satisfy the needs of women in this important period of life.

One of the ways to compensate nutritional deficiency is introduction into the diet of enriched and specialized food products, i.e., food having a medical and functional purpose. Best practices and domestic experience show that the most effective and affordable way of providing the population with essential food substances is enrichment of mass consumption product with nutrilites.

These products allow intake of nutrients, required for women, with a limited amount of food in proportions adequate to the optimal development of the fetus, as well as provide long-lasting and high-quality lactation.

At present, prescribing iron preparations is the main treatment of IDA. Although the prevention of iron deficiency conditions or their integrated treatment is possible through the correct nutrition. This needs developing and introducing in the diet of pregnant women of specialized food products, allowing for non-pharmacological prevention of IDA that will exclude the possible negative effects of the additive agents used in drugs.

The aim of this research is to develop the technology for producing antianemic smoothie for pregnant women based on the optimization of the composition and organoleptic characteristics of the final product.

Innovative technologies allow developing the production of specialized food products enriched with non-traditional components, which include essential nutrients.

An alternative source of active iron is wheatgrass juice, which contributes to the normalization of the blood formation. The juice from wheatgrass is a source of polyphenols and chlorophyll. Chemical formula of chlorophyll resembles blood ferriheme, which is a component of hemoglobin [Figure 1] and plays a major role in oxygen transport.

The positive effect of chlorophyll on the functioning of vital organs such as the heart, intestines, uterus, liver, lungs, and vascular system is well known. Chlorophyll strengthens the blood function.

MATERIALS AND METHODS

Evaluation of the mass fraction of proteins was performed by Kjeldahl method; carbohydrates, including mono and disaccharides were measured by permanganate and photocolorimetric methods; dietary fiber was calculated as the sum of the mass fractions of pectin, protopectin, hemicellulose, and cellulose measured by titrimetric method.

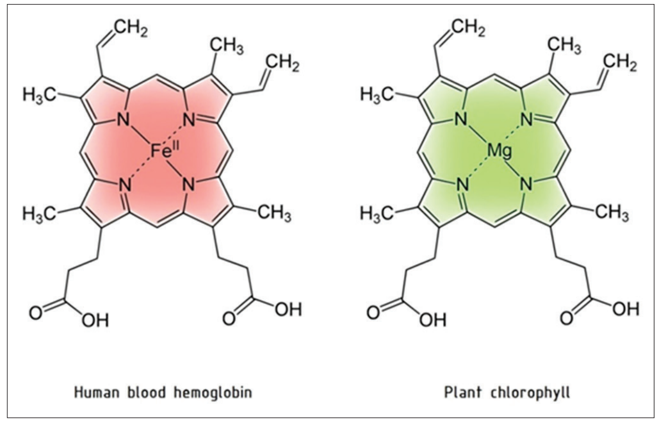

Figure 1: Hemoglobin and chlorophyll structures

Analysis of minerals was performed with the use of physicochemical methods – optical and electrochemical techniques. Determination of iron content in the product was carried out by colorimetric method. The method is based on the change in color intensity of a solution of coordination compound of bivalent iron with red ortho-Phenanthroline. The test was conducted with the application of photoelectric colorimeter using a filter with λ_{max}= (490±10) nm.

The determination of copper and zinc in foods was performed by atomic absorption method employing atomic absorption spectrometer “Quantum-Z. ETA” with the wavelength for Cu - 324 nm and for Zn - 285.9 nm. The method is based on the ability of free atoms of the elements to absorb light energy of the flame gases at a wavelength characteristic for each element.

Determination of calcium was performed by the capillary electrophoresis method employing “Capel - 103” system. The method is based on the migration and separation of cations under the effect of an electric field due to their different electrophoretic mobility. Identification and quantitative determination of the analyzed cations were performed using indirect method, by registering the UV absorption at a wavelength of 254 nm. Processing of results was performed using the “Multichrome” software.[5]

To identify phenol carbonic acids, we used the method of complex mixtures analysis, which is based on electrokinetic phenomena (electromigration of ions and other charged particles and electro-osmosis) for the separation and determination of components, namely, capillary electrophoresis. These phenomena occur in solutions when placed in an electric field, predominantly, of high voltage. If the solution is placed in a thin capillary, made of quartz, for example, the electric field imposed along the capillary causes inside the movement of charged particles and passive flow of liquid, whereby the mixture is separated into individual components since the parameters of electromigration are specific to each kind of charged particles. At the same time, disturbing factors (diffusive, sorptive, convective, gravitative, etc.) in the capillary are substantially weakened. This provides record efficiency of separations.[5]

Analysis of phenolic compounds was performed using the "Capel-105M" system of capillary electrophoresis (group of "Lumex" company) with quartz cupellation 60 mm in length with an inner diameter of 75 µm. Borate buffer solution (pH = 9.2) was used as the leading electrolyte. The injection of a sample was carried out at a pressure of 30 mbar for 5 s. Spectrophotometric detection was conducted at a temperature of 24.9°C, an operating voltage of 23 kV, and a wavelength of 280 nm during 860 s. System management, data acquisition and processing were performed using specialized "Elforan" software.

Determination of antioxidant activity in the analyzed sample was performed with the use of a liquid chromatography "Color Jauza-01-AA" (NPO "Khimavtomatika"). The mass concentration of antioxidants was measured by means of the calibration curve of the signal output versus the concentration of gallic acid.

Quantitative analysis of amino acid composition of proteins in wheatgrass juice was performed employing the capillary electrophoresis system of "Capel - 105M" (group of "Lumex" companies) with the "Multichrome" data processing software ("Ampersend", Russia). Effective capillary length up to the detector was 35 cm. A buffer solution containing 25 mM of sodium dodecyl sulfate, 1.8 mM of sodium tetraborate, and 10.7 mM of sodium dihydrogen phosphate was used as the leading electrolyte for all electrophoretic separations. The injection of the sample was carried out under a pressure of 20 mbar for 10 s. Spectrophotometric detection was conducted at a temperature of 30°C, operating voltage of the electric field of 25 kV, and the detector wavelength of 254 nm.

For the development of a design methodology of antianemic multicomponent food products with due consideration of the organoleptic characteristics and the conditions for the optimal balance of nutrients, we used a mathematical optimization model of the weight composition of the final product, which is based on the methods of mathematical programming and regression analysis, including neural network regression model. Neural network and regression analysis of the dependence of the ranking score of organoleptic characteristics on the prescription composition of the product is performed using the "Statistica" software package. The solution to the problem of multicriterial optimization of the product's organoleptic characteristics evaluation and the balancing index is proposed based on convolution of criteria according to the multiplicative model of Harrington's desirability functions and reduction to the problem of mathematical programming, which is solved by means of scripts of the MathCAD problem-solving environment.

RESULTS

A wide range of pharmacological effect of wheatgrass juice is due to the presence of bioactive substances: Minerals, polyphenols, amino acids, polysaccharides, organic acids, vitamins, and other essential nutrients [Tables 1-4].

DISCUSSION

When developing formulations of antianemic food products, we have based on the principles of food combinatorial calculus,[6] taking into account the possibility of chemical interaction between ingredients, selected such combinations, application, and processing methods, which ensured their maximum safety during production and storage, as well as improved bioaccessibility.

Dosage of iron in a specialized product for pregnant and lactating women can be set at the level of 50-60%

Table 1: Chemical composition of wheatgrass juice

Indicator name	Indicator value
Mass fraction, %	
Proteins	1.74
Carbohydrates	2.77
Including	
Monosaccharide's	1.51
Disaccharides	1.26
Pectin	0.19
Protopectin	0.30
Hemicellulose	N/A
Cellulose	0.1
Dietary fiber	0.59

Table 2: Composition of bioactive substances of wheatgrass juice

Bioactive substance name	Content of bioactive substance
Macroelements, mg/l	
Potassium	1283
Sodium	48.36
Magnesium	125.50
Calcium	25.01
Microelements, mg/l	
Iron	154.00
Copper	1.40
Zinc	0.17
Vitamins and provitamins, mg %	
Vitamin C	4.71
R-active substances	265.00

of science-based standards of its recommended total consumption during pregnancy. The effectiveness of this dosage may increase by its combination with vitamins C, B_2, B_6, B_{12}, and folic acid, which are necessary for the successful absorption and utilization of iron in the human body.[3] We have considered also the availability of demineralizing factors that reduce the absorption of iron. These include oxalic acid, phytin, tannins, caffeine, and ballast substances [Table 5].[7]

In this work, we used the generalized criterion to model the multicomponent products formulations with the specified interval boundaries of adequate and acceptable consumption for each of the indicators.[8]

Table 3: Composition of phenolic compounds of wheatgrass juice

Indicator name	Retention time, min	Indicator value, mg/l
Rutin	6.840	91.53
Lilac	7.627	29.14
Ferulic	7.740	33.67
Salicylic	8.055	57.73
Benzoic	8.147	56.50
p-coumaric	8.405	15.58
Vanillic	8.502	62.08
Quercetin	8.728	12.92
4-hydroxybenzoic	9.143	3.526
Coffee-colored	10.048	8.978
Gallic	11.080	10.45
3.4 -dihydroxybenzoic	11.513	18.81

Table 4: Amino acid composition of proteins of wheatgrass juice

Amino acid name	Content, mg/dm³
Essential amino acids	
Arginine	67.91
Valine	87.97
Histidine	125.4
Isoleucine	8.462
Leucine	49.94
Lysine	2.622
Methionine	86.1
b-phenylalanine	25.63
Nonessential amino acids	
A-alanine	40.01
Glycine	10.75
Proline	450.80
Serine	47.65
Tyrosine	17.16

A team under the leadership of Academician Lipatov *et al*.[9] has conducted research on the design of products and diets with specified nutritional value based on computer modeling. The initial stage of development of theoretical bases and specific implementation methods of the balanced foods design principles was associated with formalization of qualitative and quantitative representation of rational use of essential amino acids in the adequate exstrophy technology.

The formalization takes into account mutual balance between the essential amino acids. The following was proposed on the basis of the Mitchell Block principle: The utilization coefficient of essential amino acids; the utility coefficient of amino acid composition in the product g/100 g of protein; the amino acid composition coefficient, which characterizes the balance of essential amino acids relative to the physiologically required norm (standard); comparable redundancy indicator of the content of essential amino acids that characterizes the total mass of essential amino acids which are not used for anabolic purpose. It should be noted that despite the theoretical soundness, experimental verification of mutual balance of amino acids involves the study of metabolism in the human body that is a very complicated problem.

Lipatov *et al*. discusses the design methodology of multicomponent food products formulations, which includes three stages:

- Modeling of protein amino acid composition of designed food product and the choice of values satisfying criterion to the maximum extent;
- Evaluation of fatty acid composition of the designed product;
- Calculation of the caloric content of designed food products.

The main idea put forward by Ivashkin *et al*.[10] is the complexity of decision-making, ensuring stable quality of the generated product, and at the same time the need for creating objective rations and diets, which are subject to probabilistic variations in the characteristics and properties of the original biological raw food. Adequate decisions in each particular case are associated with the adjustment of the composition of the rations and food products depending on the physiological needs of the human body (sex, age, place of residence, etc.).

Information basis of this system consists of a database, structurally showing the physicochemical parameters of the animal-vegetable products, optimization criteria, and assessment of adequacy.

A compilation of the optimal diet is reduced to the development of an interactive algorithm for determining the composition of products, their quantities and limitations with regard to certain sets of criteria. Next step consists in the assessment and optimization of existing diet.

Table 5: Antinutrients and possible ways of eliminating their influence

Inhibitor (antinutrient factor)	Food source (action conditions)	Method of eliminating negative effect
Oxalic acid	Spinach, sorrel, and rhubarb	The increased consumption of digestible iron sources: Meat and fish products; organic acids (ascorbic, citric, malic, and tartaric): Juices of fruit and berries without pulp; vitamins a and of b group
Dietary fiber	Bran, brown bread, many cereals, vegetables, and fruits (in case of excessive intake)	
Tannins	Tea, coffee, quince, persimmon, chokeberry, blueberry, cocoa, and chocolate	
Calcium	Dairy products	
Phytic acid	Soy, legumes, grains, and except sprouted grains	Heat treatment

As the target function, we use the hierarchy of quadratic criteria of minimum deviation from the reference structure of a variety of food indicators and/or bioavailability, presented in the generalized form as the goodness of fit:[10]

$$\sum_{k=1}^{n}\left(B_k^o-\sum_{j=1}^{m}b_{ki}y_i\right)^2 \rightarrow \min, \qquad (1)$$

Where,
B_k^o - is the normative content of the k^{th} element in the diet;
b_{ki} - is the specific content of the k^{th} element of the chemical composition in the j^{th} product;
y_i - is the mass fraction of the j^{th} product in the diet.
According to the total volume of the daily ration V:

$$\sum_{k=1}^{m} y_j = V \qquad (2)$$

According to acceptable limits of mass fraction (volume) change of the j^{th} product in the diet:[10]

$$y_j^{min} \le y_i \le y^{max}; \quad j=\overline{1,m} \qquad (3)$$

The optimization procedure continues until all the possible redistributions of mass fractions of components are exhausted resulting in obtaining the alternative diet with a minimum deviation of the k^{th} element from the set standard value in the structure of adequate nutrition.

The choice of optimum alternative from the set of found Pareto - optimal solutions corresponds to the minimum value of the goodness of fit, which assesses the total residual variance of obtained structure of the indicators of the diet relative to the regulatory option on a scale from 0 to 1.

If in consequence of the structural - parametric optimization, parametric differences are not minimized to an acceptable level, a new selection of necessary and desired products from the database is carried out.

The inclusion of additional products in the current diet is associated with finding in its new composition of most scarce k^{th} element or superfluous l-element with the maximum residual deviation from the norm. Further, in the case of a deficiency, the $n+1^{th}$ product with the highest possible content of the k^{th} element is revealed to be included in the diet by reducing the mass fraction of p^{th} product with a minimum specific content of this element.

According to the authors,[11] it is expedient to carry out the development of new recipes of combined food products based on the mathematical modeling method with respect to the minimizing criterion of caloric content, by selecting raw food with specified limits of the function value and adjustable parameters.

In this case, the objective function is limited by the caloric content of the designed product:[10]

$$F = C_1 X_1 + C_2 X_2 + C_3 X_3 + \ldots + C_n X_n = \min \qquad (4)$$

Where,
$C_1, C_2, C_3, \ldots, C_n$ - are the caloric values of the corresponding component of the composition, kcal;
$X_1, X_2, X_3, \ldots, X_n$ - are the relative contents of the raw components in the composition, % wt.

Limitations on adjustable indicators in the projected composition can be written as:[7]

$$K_1 X_1 + K_2 X_2 + K_3 X_{3+} \ldots + K_n X_n = Y_n \qquad (5)$$

Where,

$K_1, K_2, K_3, \ldots, K_n$ - are the average values of the relative content of the regulated indicator in a particular component;

Y_n - is the value of the controlled indicators in the final product.

Solution of these equation systems is carried out using the software packages for the optimization of food products formulations through their mathematical processing that allows determining the relative content of raw material components as well as the caloric content of the designed compositions.

A possible design option is the optimal selection of the diet composition conducted based on the maximum values of the utility coefficient and a minimum value of comparable redundancy indicator at the amino acid score approaching unity.

The problem of choosing the optimal formulation of a given product can be reduced to finding such a product composition (mixture) in which the ratio of quality indicators would be as close to the standard as possible:[10]

$b_1:b_2:b_j:\ldots:bm = e_1:e_2:e_j:\ldots:e_m$

Where,

b_j, e_j - are appropriate quality indicators of the designed product (mixture) and a standard.

Optimization of the food products formulations can be carried out using the known simplex method, which is a numerical method of solving a linear programming problem that allows finding the optimal solution, i.e., the extreme point of a linear objective function at linear constraints on the sought variables. The decision-making process based on the use of the simplex method transforms from informal to formalized method. The adoption of formalized solutions is based on two main methods: Logical modeling and optimization. Optimal solutions have the following basic components: Mathematical model, solution algorithm of concerned problem, and the original data. The optimization problem is solved based on the selected indicators (e.g., chemical composition, vitamin and mineral compositions, and caloric content). It makes sense to use simplex lattice planning of experiment when studying the effect of mixture compositions on their properties.

To calculate a mathematical model of the formulations, we use the original output information. The calculations involve the target function, restrictions on nutrients content, and boundary conditions for some variables.

The disadvantage of this approach is that the resulting solution is often at the border of the admissible application domain of sought variables, i.e., the problem is fully or partially degenerate. When solving the formulation optimization problem in this way, it is impossible to take into account several optimization and nonlinearity criteria, which can take place at the interaction of desired variables.

According to Shazzo *et al*.'s study,[8] it is possible to establish the relationship between quality indicators of a mixture at different types of used ingredients, based on a comprehensive assessment of the organoleptic characteristics of the products depending on the mixture composition. We have developed the optimization criteria of the multicomponent mixtures composition.

When solving the formulated problems based on the objective functions using the optimization programs we determined nominal proportions of the product modeling: Organoleptic characteristics, content of basic nutrients, and compliance with the content of trace elements in the mixture.

When carrying out multicriteria optimization of the mixtures composition, the optimization of quality parameters of the final product was carried out for a wide range of products.

The obtained data confirm the effectiveness of the proposed methods for the optimization of mixtures consumer qualities.

Similar results were obtained for other types of products. This confirms the effectiveness of the proposed method for evaluation of the organoleptic characteristics of the products depending on the composition of the mixture.

We have revealed the mixing regularities of different ingredients according to their quality indicators not obeying the additivity law: The content of nutrient in the raw material and organoleptic characteristics of the final product.

The article presents the theoretical justification of improved computer optimization method of the mixtures composition and organoleptic characteristics which are based on the application of objective functions, characterizing the rational use of natural resources, ensuring maximum output and high consumer performance of the final product, as well as suggests the multicomponent mixtures formation method.

This approach has a disadvantage inherent to the combination of many conflicting factors into a single criterion. The resulting solution is unstable and is highly empirical. Similar disadvantages are inherent to the approach of Ivashkin *et al*.[10] when developing expert system of adequate nutrition at designing of food products, where the authors propose to carry out optimization procedure for each selected criterion by pairwise comparison and quality evaluation of the resulting product with respect to an independent quality functional and the desirability scales.

The analysis of literary sources showed that the problem of designing food products is resolved in the framework of the chosen direction, for example, mineral or vitamin composition, or caloric content. At that, great attention is paid to the design of combined products, which is understood as the process of creating rational formulas providing a specified level of adequacy.

At that, little attention is paid to the balanceness of the organoleptic characteristics of the final product based on the mixture composition. Thus, the desire of consumers when choosing ingredients used for the production of final product is not taken into account. Furthermore, it is necessary to consider the daily body's need for certain nutrients when designing products that do not carry the side effects and are produced without the use of unpermitted technologies.

In the domestic market, a range of additional specialized nutrition for pregnant and lactating women is presented in the form of dry mixtures for preparing drinks and cocktails, usually imported. Thus, the production of domestic food products for special purpose is very important.

It is necessary to develop an optimization algorithm, which would allow modeling products with a given organoleptic characteristics providing an optimal balance of nutrients (micronutrients and major mineral elements). For this purpose, we employ multicriteria optimization of the balancing index and sensory evaluation of the smoothie composition, as well as mathematical programming methods, implemented by means of mathematical software environments "Statistica" and MathCAD.

When simulating composition of designed products, we took into account the daily requirement of a pregnant woman in nutrients and acceptable norms of their content in the optimal formulation. Adequate and tolerable upper levels of nutrient intake were determined on the basis of MR 2.3.1.2432, Table 6.[12]

Data on the chemical composition of the products used for the preparation of designed food system are given in Table 7.[13]

The weight composition of the products was developed using mathematical programming methods. The weight optimization problem of the smoothie composition is solved by means of MathCAD scripts.[14]

Mathematical optimization model of the smoothie composition for pregnant women needs to take into account the organoleptic characteristics of the combined product. The solution of the concerned problem was found by the expert evaluation method, in which the organoleptic characteristics are determined based on the ranking of the expert estimates at a pairwise comparison of the proposed samples.

Psychologists have proved that the pairwise comparison is behind any selection (i.e., when choosing products, they are compared pairwise), however, the ordinal scale (non-ordered series) with fixed supporting (reference) points, which are called scores, is often compiled in advance.

Expert estimates often arise in practice, for example, when tasting food. When using an expert method for quality evaluation one often uses ordinal scale. The comparison is solved based on the principle of "better - worse" and "more - less". At that, more detailed information concerning how many times a certain product is better or worse than the other one often is not required.

Table 8 presents the data related to just one ranking option of 14 samples of smoothies based on the pairwise comparison.

Table 6: Permissible levels of nutrients in the final product

Nutrients	Daily nutrition	Level	
		Minimum	Maximum
Carbohydrates, g	348	257	586
Iron (Fe), mg	33	4	45
Copper (Cu), mg	1.1	0.9	5
Calcium (Ca), mg	1300	500	2500
Vitamin B_1 (thiamine), mg	1.7	0.3	6.7
Vitamin B_9 (folic acid), mcg	600	150	1000
Vitamin C (ascorbic acid), mg	100	45	700
Vitamin A (retinol), mcg	1000	500	3000

This result is obtained by just one expert, who evaluated the samples in a certain way. The preference of one object over another is designated by 1, while the reverse situation corresponds to 0.

The array (scale of order) of objects, whose comparative evaluation is given in Table 8, would be:
$Q_9 = Q_{13} < Q_4 = Q_{12} < Q_1 = Q_2 = Q_6 = Q_7 < Q_{10} = Q_{12} < Q_3 = Q_{11} < Q_5 < Q_8.$

For obtaining more accurate result, we used estimates of several experts.

When designing food products, the optimization problem is usually simplified by reducing it to a single criterion problem. Therefore, in most cases, just one product parameter is selected for further optimization of product composition.

The combined use of neural network and linear regression estimation of organoleptic characteristics will allow modeling products, which can have perfectly balanced composition as well as optimal organoleptic characteristics.

At that, regression problems require predicting the value of a variable, which, as a rule, possesses continuous numeric values: Sensory evaluation, food composition balance, etc. In such cases, just a single numeric variable is required as the output value.

In turn, the neural network can solve simultaneously several problems of regression and/or classification, though usually is used to solve only one task. Thus, in most cases, the neural network will have only one output variable; the case of classification problems with many conditions may require several output elements (at that, post-processing stage is responsible for converting the information from output elements into an output variable).

The number of input and output elements is determined by the problem conditions. Doubts may arise as to which output values should be used and which not. It is assumed that the input values are chosen intuitively and that all of them are significant. In a first approximation, we can take just one intermediate layer with the number of elements in it equal to the half-sum of the numbers of input and output elements.[15]

Network elements are arranged into a layered topology with a direct signal transmission. Such a network can be easily interpreted as "input-output" model, in which the weights and the threshold values (bias) are the free parameters of the model. This network can simulate the function of virtually any degree of complexity, at that, the complexity of the function is determined by the number of layers and the number of elements in each layer. Determination of the number of intermediate layers and the number of elements in them is an important factor when choosing a network.

We used the ST neural network batch function.[9,15]

The data of the organoleptic test of the product conducted with the control test panel served source data to produce regression model for the sensory evaluation of the smoothie.

This resulted in multiple versions of compositions close to the specified parameters, from which we selected the most balanced sample not only in terms of chemical composition but also in terms of organoleptic characteristics. These data are shown in Table 9.

To carry out analysis, we chose the neural network of the multilayer perceptron type with an inner layer of 6 neurons (5 input neurons and 1 output neuron), which interpolates these data by a monotonous surface.

Table 7: Chemical composition of recipe ingredients of the smoothie

Nutrients	Products				
	Kiwi fruit	Grapes	Natural yoghurt with a fat mass fraction of 3.2%	Honey	Wheatgrass juice
Carbohydrates, g/g	81×10^{-2}	154×10^{-1}	35×10^{-2}	835×10^{-1}	277×10^{-3}
Iron (Fe), g/g	8×10^{-6}	6×10^{-6}	1×10^{-5}	8×10^{-5}	154×10^{-4}
Copper (Cu), g/g	15×10^{-6}	8×10^{-7}	1×10^{-7}	6×10^{-7}	14×10^{-6}
Calcium (Ca), g/g	34×10^{-4}	3×10^{-4}	12×10^{-3}	14×10^{-3}	25×10^{-4}
Vitamin B_1, g/g	3×10^{-7}	5×10^{-7}	4×10^{-7}	1×10^{-7}	129×10^{-5}
Vitamin B_9, g/g	25×10^{-7}	4×10^{-8}	1×10^{-8}	15×10^{-7}	8×10^{-8}
Vitamin C, g/g	18×10^{-3}	6×10^{-5}	6×10^{-6}	1×10^{-9}	47.1×10^{-9}
Vitamin A, g/g	8×10^{-8}	3×10^{-8}	21×10^{-7}	1×10^{-8}	375×10^{-5}

Table 8: Ranking of the 14 samples by pairwise comparison

	Sample number														Evaluation of organoleptic characteristics
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
1	x	0	0	1	1	0	1	0	1	1	0	0	1	0	6
2	1	x	1	0	0	1	1	0	0	0	1	1	0	0	6
3	1	0	x	0	1	0	1	0	1	1	1	1	1	0	8
4	0	1	1	x	0	1	0	0	1	0	0	0	0	1	5
5	0	1	0	1	x	1	0	0	1	1	1	1	1	1	9
6	1	0	1	0	0	x	1	1	0	0	0	0	1	1	6
7	0	0	0	1	1	0	x	1	1	0	0	1	0	1	6
8	1	1	1	1	1	0	0	x	1	0	1	1	1	1	10
9	0	1	0	0	0	1	0	0	x	1	0	0	1	0	4
10	0	1	0	1	0	1	1	1	0	x	1	1	0	0	7
11	1	0	0	1	0	1	1	0	1	0	x	1	1	1	8
12	1	0	0	1	0	1	0	0	1	0	0	x	1	0	5
13	0	1	0	1	0	0	1	0	0	1	0	0	x	0	4
14	1	1	1	0	0	0	0	0	1	1	0	1	1	x	7

The sensitivity of the network was the main criterion for the selection of ingredient composition that maximally contributes to sensory evaluation when mixing a smoothie. Under the sensitivity of the neural network, we understand the maximal possible appearance of one and the same attribute at the network output. At frequent repetitions, this attribute (numerical evaluation of this attribute) has the greatest impact on the final result of the analysis in comparison with all the other attributes [Table 10].[15]

Thus, we came up to the conclusion that the most important components of the smoothie mix (in the context of organoleptic characteristics) are wheatgrass juice and yoghurt. Grapes, kiwi, and honey, according to the sensitivity analysis of neural network, have smaller values of sensitivity. Therefore, there is a possibility of their expulsion from the arguments of the regression model of the sensory evaluation of the mixture composition [Tables 11 and 12].

In this case, the multiple correlation coefficients is R=0.9 [Table 11]. Square of fixed correlation index coincides with the first digit of R^2 [Table 11]. This means that the number of observations is sufficient to estimate the significance of regression. In the Fisher criterion, *P* is practically equal to zero; therefore, the regression is significant [Table 11].

The linear regression formula [Table 12] has the form:

$$S = 0.9+(0.14\times X_1)+(-0.27\times X_2) \qquad (7)$$

Where,

X_1, X_2 - are the contents of the yoghurt and wheatgrass juice in the mixture, respectively, in grams.

Neural network analysis has shown that the use of yogurt and wheatgrass juices have the greatest effect on the organoleptic characteristics of the mixture. Neural network and linear regression analysis have shown that the dependence on the quantitative status of the test mixture is monotonic. Nevertheless, the linear regression may not be appropriate for this situation, because it does not guarantee that the score of estimated organoleptic indicator in the form of desirability function will fall within the range from 0 to 1. We propose the following regression model of the desirability function of sensory evaluation [Figure 2]:

$$S(X) = 1 - \exp\left[-\sum_{i=1}^{n} a_i X_i^2\right] \qquad (8)$$

Where,

$X = \{X_1, X_2, \ldots, X_n\}$ - is the percentage composition vector of the mixture consisting of n ingredients %.

In this case (8) takes the form:

$$V(x) = 1 - \exp\left[-\left[a\left(\frac{100x_2}{m(x)}\right)^2 + b\left(\frac{100x_4}{m(x)}\right)^2\right]\right] \qquad (9)$$

Where,

$x = \{x_2; x_4\}$ - is the weight of the mix components (wheatgrass juice and yogurt), g.

The parameters of the regression model (9) a and b (where a and b are the values of the organoleptic characteristics of the mixture composition made of yoghurt and wheatgrass juice, respectively) are obtained by means of "Statistica" package.

The correlation index for the 8 is R=0.44. Therefore, technically, the given regression model is worse than 7, though it is more adequate to the situation of the organoleptic indicators.

The final result of the sensory evaluation of the smoothie composition can be represented in the form of regression model:

$$v(x)=1-\exp\left[-\left[0.971\times 10^{-3}\left(\frac{x_2\times 100}{m(x)}\right) + \left(-0.52\times 10^{-4}\left(\frac{x_4\times 100}{m(x)}\right)\right)\right]^2\right] \qquad (10)$$

Thus, 10 gives the Harrington desirability function for the sensory evaluation of the smoothie mixture composition.

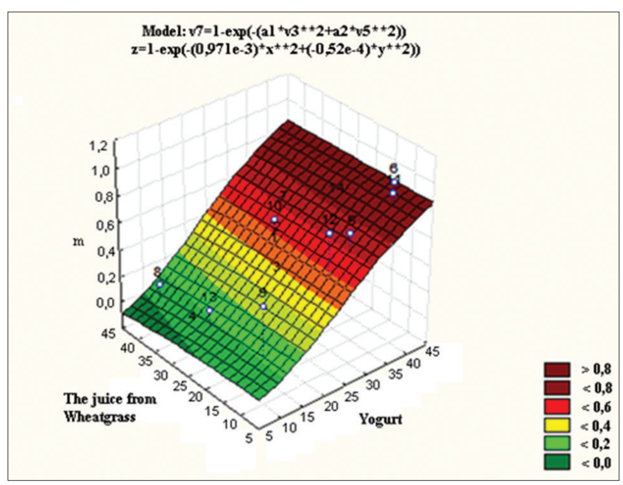

Figure 2: Regression model of the desirability function of sensory evaluation depending on the content of the components in the mixture (x - wheatgrass juice, %; y - yogurt, %)

Table 9: The data of organoleptic characteristics

Sample number	Case No. 1						
	Kiwi	Grapes	Yogurt	Honey	Wheatgrass juice	Evaluation (1-14) of organoleptic characteristics	S
1	25	25	25	9	25	7	0.461538462
2	10	30	30	10	30	6	0.384615385
3	30	10	30	11	30	2	0.076923077
4	30	30	10	10	30	1	0
5	30	30	30	10	10	11	0.769230769
6	10	40	40	10	10	14	1
7	10	10	40	10	40	5	0.307692308
8	40	10	10	10	40	3	0.153846154
9	40	40	10	10	10	8	0.538461538
10	10	40	25	10	25	10	0.692307692
11	25	25	40	10	10	13	0.923076923
12	40	25	25	9	10	12	0.846153846
13	25	40	10	10	25	4	0.230769231
14	25	10	40	11	25	9	0.615384615

Table 10: Sensitivity analysis of neural network

Networks	Sensitivity analysis of neural network score (1-14) of organoleptic characteristics (scores - option 1) samples train				
	Kiwi	Grapes	Yogurt	Honey	Wheatgrass juice
2. MLP 5-9-1	1.810654	3.66825	15.09518	1.738548	12.91648
3. RBF 5-7-1	3.580387	11.56319	24.42835	4.178110	28.01699
5. MLP 5-7-1	1.791926	2.47219	9.67867	1.772295	12.24720

Table 11: The calculation results of “Statistica” batch function of the linear multiple regression

Multiple regression results		
Dependent: Score (1-14)	**Multiple R=0.90261086**	**F=24.18262**
	R^2=0.81470636	**df=2.11**
Number of cases: 14	Adjusted R^2=0.78101661	*P*=0.000094

Standard error of estimate: 1.957602943, intercept: 9.906470331, standard error: 1.866757, t (11)=5.3068, *P*=0.0002, yogurt: β=0.426; Wheatgrass juice, β=−0.73

Table 12: Calculation results of the linear multiple regression parameters in the “Statistica” batch function

n=14	Regression summary for dependent variable: Score (1-14), R=0.90261086, R^2=0.81470636, adjusted R^2=0.78101661, F (2, 11) = 24.183, *P*<0.00009 standard error of estimate: 1.9576					
	β	Standard error of β	β	Standard error of β	*t* (11)	*P*-level
Intercept			9.906470	1.866757	5.30678	0.000250
Yogurt	0.425808	0.131718	0.148961	0.046079	3.23272	0.007977
Wheatgrass juice	−0.726536	0.131718	−0.275192	0.049891	−5.51584	0.000182

CONCLUSION

In consequence of the research, we have developed the methodology of mathematical modeling of the smoothie composition for pregnant women, which meets most fully the following requirements: Optimal content of feedstuff with antianemic properties, and high organoleptic characteristics of the final product.

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