The Method of Computer-Aided Design of a Bread Composition with Regard to Biomedical Requirements

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***Abstract*—A method for efficient software implementation of bread optimized multicomponent mixtures has been developed. These polycomposite mixtures have a chemical composition that meets the modern physiological standards of nutrition for the elderly people. To implement the developed algorithm a high-level programming language Object Pascal was used using the IDE Borland Delphi 7.0. An unconventional raw material was selected, which allows to provide necessary requirements to the quality indicators of the finished bread in all modeled mixtures. Modeling the composition of flour mixtures for gerodietic nutrition using the software made it possible to obtain compositions with a specific ratio of prescripted components, balanced in accordance with the intended purpose.**

***Keywords*—Modeling; polycomposite mixture; bread; gerodietic nutrition; quality**

I. Introduction

The approach to creation of technologies of multicomponent products with a chemical composition [1] that is regulated in accordance with modern physiological nutritional standards predetermined the intensive development of research, united by the concept of "design" of consumer food products. The problem of creating food with a given level of nutritional adequacy has been formed for a long time [2] and is highly relevant at the present time. First of all, this is due to the increasing complexity of the composition of modern food products and the emergence of new knowledge about the effect of the components they contain on human health [3], expanding the range of new types of food ingredients.

The development of a new product range and technologies of bread with a complex raw material composition currently occupies an important place in the development of bakery production. The use of new and non-traditional raw materials has high prospects in the food industry, as it allows you to get bulk food with high nutritional value, preventive and therapeutic properties.

The principles of the food products composition design are based on standards and criteria for optimizing the quality of food, based on modern knowledge of biology, medicine and food chemistry. The solution of the problem of optimizing the compositions of polycomposite food products, including rye-wheat bread, is possible using indicators that can be described mathematically. As a result of research of domestic and foreign scientists in the field of biology and medicine [4], the concept of a balanced diet was formulated. According to the concept proportions of individual substances causing the sum of exchange reactions that underlie human life were determined [5].

The numerical values [6] of the optimal nutrient ratios, given in the balanced nutrition formula, make it possible to use them as formal optimization criteria for creating polycomposite mixtures with given levels of nutritional adequacy by analytical combining the main prescription component of breadmaking-flour in combination with new and unconventional raw materials.

To date, various software products have been developed and are being actively used to automate technological calculations of food recipes of various groups.

The most common instrument for creating such programs for calculating and optimizing recipes is the spreadsheet MS Excel. The initial data for calculations is entered into the corresponding cells of the spreadsheet, and the calculation formulas are entered into the others. The advantage of this shell is the prevalence [7], simplicity of calculations and a lot of methodological and reference literature on its use. In addition, it has a number of built-in modules to simplify routine procedures for finding a solution, correlation and regression analysis, etc. The disadvantage of using MS Excel is the lack of automated input of initial data and calculated dependencies, as well as obtaining a single solution for solving optimization problems using standard tools.

The program for calculating the chemical composition of food for catering in high school institutions [8] is designed to calculate the energy and nutritional value of a school food. The program allows you to evaluate the chemical composition of the school food ration according to 28 indicators, including the calculation of proteins and fats by origin, carbohydrates by molecular weight, vitamins A, B and E by their equivalents. The disadvantage of the program is the lack of possibility to optimize the diet for nutritional adequacy.

The optimization of parameters of the product under development by modeling the formulation using the integral balance criterion for a wide range of indicators was used in developing theoretical prerequisites for computer-aided design of food products for the elderly people. At the same time, a qualimetric multiplicative model was used [9], which allows to bring relative complex and simple individual quality indicators of different origin into one form, ensuring the independence of the properties of each indicator. This approach has a disadvantage inherent in combining many contradictory factors into one criterion. The resulting solution is unstable and very empirical.

A common drawback of existing software systems is the lack of a recipe optimization subsystem, based on a set of criteria for food, biological and mineral value, as well as finding a single solution that is optimal in terms of specified parameters. In addition, this approach does not allow to predict consumer properties of the product, which does not allow to speak about the possibility of its full launch on an industrial scale.

However, modeling of polycomposite mixtures for baking, based only on the analytical combination of the quantitative and qualitative component of the nutrients contained in them, has a very significant imperfection associated with the lack of guarantees of obtaining the final product of sufficient consumer dignity.

Combining the nutrient composition of mixtures for baking without taking into account the technical-functional properties of the final variants of mixtures makes the use of improvers a prerequisite for their use. It increases the cost of the final product, and also narrows the choice from a variety of analytical calculations of recipes at the raw set stage. As a result, the final choice of a polycomposite mixture is possible only after direct testing of mixtures and this fact greatly complicates and lengthens their development.

This shows the urgency of the task of developing time-efficient formalized methods for optimizing flour polycomposite mixtures for rye-wheat bread of high nutritional value with specified technological properties. Solving the problem is possible by modeling the technological and nutrient adequacy of baking mixtures. The approach is based on an analytical assessment of partial qualities of individual components of the mixture and designing a quantitative and qualitative nutrient composition of the polycomposite mixture for rye-wheat bread with the increased nutritional value. And their physical and chemical interaction with the main raw material ingredient (flour) must be taken into account.

The aim of this work is to develop a method of effective software implementation of the nutritional value and technological adequacy of rye-wheat bread, based on an innovative model of optimal composition and simulation algorithms.

II. Methodological Approach of Quantitative and Qualitative Evaluation of the Composition of a Polycomposite Mixture for Rye-Wheat Bread

On the basis of the methodological approach of quantitative and qualitative assessment of the nutrient composition of the polycomposite mixture was the principle of separation as the key component of the protein part of the mixture. This is largely due to the fact that proteins, being an evolutionary-conditioned dominant of the diet, in general, determine the nature of nutrition. The satisfaction of a body with this component at a physiologically necessary level allows the body to display the functions of other nutrient components of food [10].

When considering the optimization of the amino acid composition of multicomponent products, the principles of Mitchell-Block [11] were recommended as principles for calculating quality, based on the interrelation of protein quality with its biological value.

Without a doubt, the computational method for determining the biological value of a baking mix composition has a number of drawbacks inherent in all computational methods [12], since it does not take into account the difference in protein digestibility in the various components that are included in the mixture. However, for practical purposes in computer design, the calculation method is currently only acceptable for the following reasons: biological methods are extremely complex [12], lengthy and expensive; when designing multicomponent mixtures, the priority is not the absolute value of the biological value, but the finding of such a ratio of prescripted components which ensures its maximum value [13].

The modeling of the nutrient composition of the model compositions of rye-wheat bread of a gerodietic orientation was carried out taking into account the basic medical and biological requirements for this group of products [14].

Modeling the technological adequacy of the flour mixture, which ensures a stable quality of the final product, was carried out by introducing the flour technological indicator called the “drop number”, calculated using the Perten formula [15].

In order to develop a time-efficient and accurate algorithm for calculating the composition of the mixture in general, the task is formulated as follows: simulate the component composition of the mixture for gerodietic bread with a biological value of at least 60%, providing the “protein:fat:carbohydrate” ratio close to 1.0:0.8:3.5, “Ca:Mg:P” - 1:0.6:1.3, fiber - not less than 0.2 g per 100 g of finished bread, the “drop number” of the mixture is 200-240 s. The calculation algorithm is shown in Fig. 1.

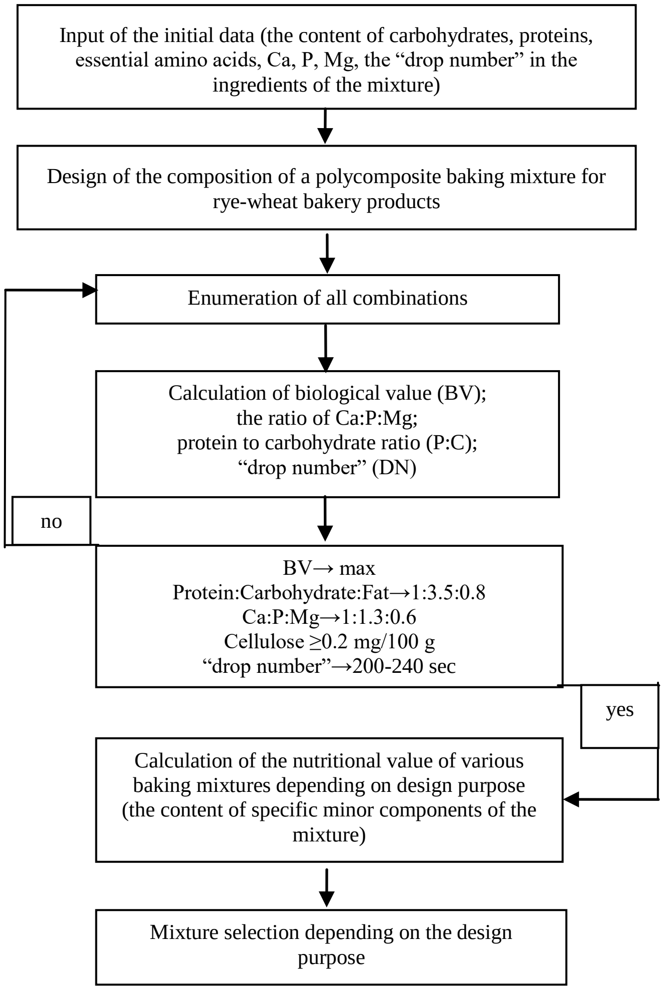

Fig. 1. Algorithm for Calculating Polycomposite Mixtures for Rye-Wheat Bakery Products of High Nutritional Value with Specified Technical-Functional Properties.

On the basis of the proposed algorithm for calculating a polycomposite mixture in a high level programming language Object Pascal using IDE Borland Delphi 7.0 a software for calculating the optimized composition of a model mixture for breads with a gerodietic orientation has been developed. An example of the software is shown in Fig. 2.

III. Materials and Methods

The chemical composition of raw materials and the "drop number" are shown in Table 1 as determined experimentally.

Analysis of the Table 1 data shows that selected raw ingredients have a rich chemical composition compared to bread flour, which will balance the composition of model mixtures for calcium, phosphorus and magnesium, increase fiber content and other components for balanced nutrition of the elderly. In addition, each of the ingredients has a special composition that in a mixture allows to obtain a product with a wide positive spectrum of health effects. Flax and sunflower seeds containing increased amount of fats will enrich model mixtures with polyunsaturated fatty acids, dry wheat gluten consisting mainly of protein will help balance the ratio of proteins and carbohydrates. The same role is played by ingredients with increased protein content - skimmed milk powder, soy flour, lentil flour, sunflower seeds. All types of raw materials have a higher fiber content than bread flour, which has a wide positive spectrum of effects on the body. Amaranth flour will allow to enrich model mixtures for bakery products with the strongest antioxidant - squalene, and buckwheat flour - with a routine that has anti-sclerotic and anti-hypertensive effects. Barley flour contains a large amount of β-glucan polysaccharide, which has a cholesterol-lowering effect and a lipid-lowering effect.

Practically all the ingredients will enrich model compositions with calcium, necessary for the prevention of osteoporosis, reduction of bone fragility and thyroid gland activity, and recommended for some muscle diseases. Calcium lactate, used as one of the components of the mixture, is widely used in the food industry not only as a source of calcium. It also has the functions of a flavor enhancer, flour and bread improver. The quality assessment of the calculated polycomposite mixtures was carried out by analyzing the chemical composition and balance of bread main nutrients from the mixtures by indicators of the mass fraction of moisture, specific volume, porosity, yield, organoleptic rate and Invitro digestibility using the enzyme pepsin [16].

TABLE I. THE CHARACTERISTIC OF RAW MATERIALS' CHEMICAL COMPOSITION

Name of raw materials	**proteins**	**lipids**	**Carbohydrates**		**Calcium**	**Phosphorus**	**Magnesium**	**"drop number", sec**
			mono- and disaccharides	**cellulose**				
	g/100g				***mg/100 g***			
rye flour	9.9	1.7	73	0.3	34	189	60	150
wheat flour	12.5	1.2	70.8	0.2	32	184	73	210
flax seeds	18.9	42.16	28	27.3	255	642	392	450
barley flour	10.2	1.2	71	6.9	80	175	63	520
amaranth flour	9.5	3.9	67.8	1.1	179	620	229	320
buckwheat flour	12.4	3.2	73.7	1.9	23.9	264.3	147	320
skimmed milk powder	48.2	1.2	48.2	0	1155	920	160	60
soy flour	48	0.2	9.7	1.3	212	198	145	60
lentil flour	24	0.2	38	3.7	83	294	0	60
sunflower seeds	20.7	52	3.4	27.3	530	317	220	210
dry wheat gluten	78	0	15	0.6	142	260	25	450
calcium lactate	0	0	0	0	16000	0	0	-

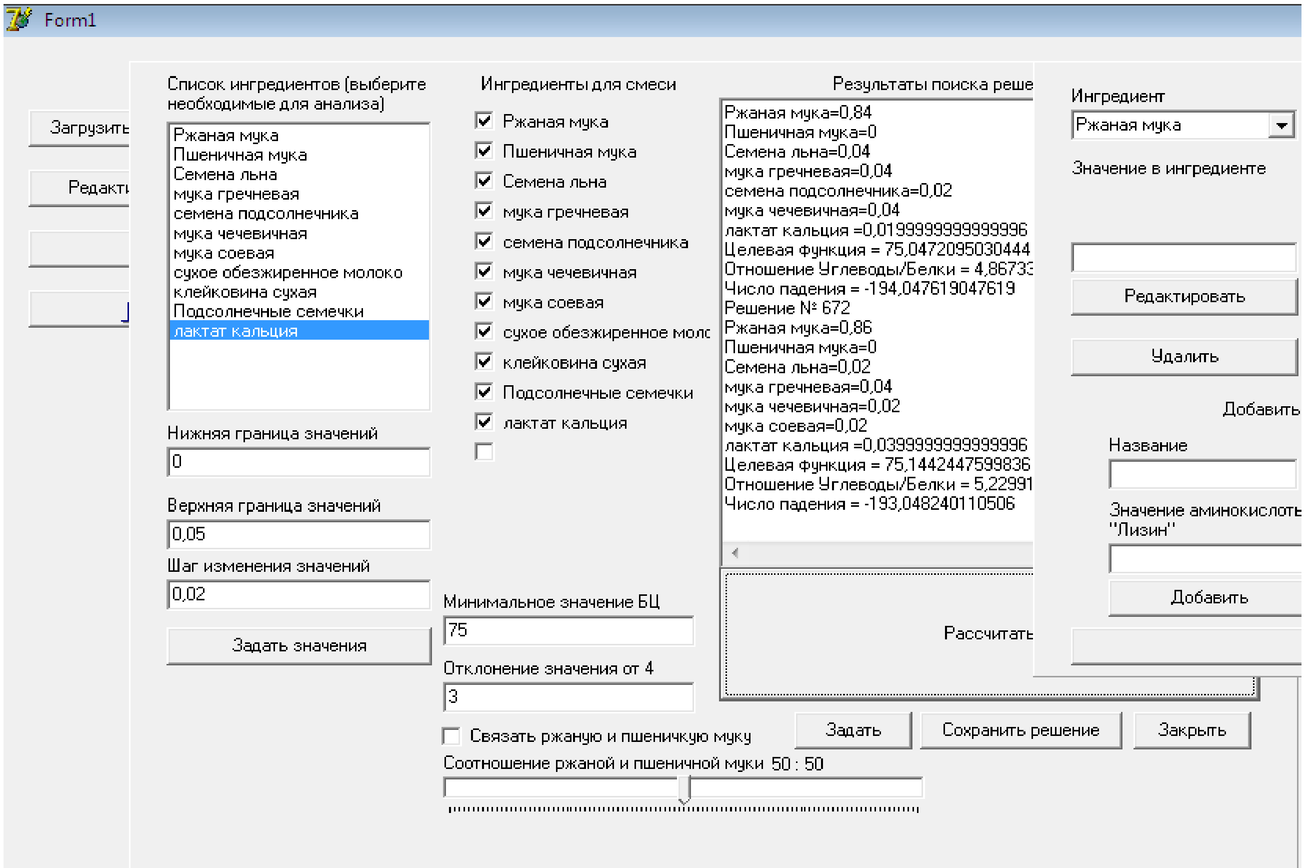

Fig. 2. Software Interface Example.

IV. Results and Discussion

As a result of the software work (Fig. 2), more than 40 model flour mixtures were generated. After analyzing the calculated data, 6 mixtures were selected with a biological value of at least 75%. The research results are grouped in Table 2. For comparison, the characteristics of bread flour mixtures are given.

The data in Table 2 shows that modeling of the flour mixtures composition for gerodietic nutrition using the software allowed us to obtain compositions with a ratio of prescripted components balanced in accordance with the intended purpose.

The flour mixtures modeled by the software complex were used to make bakery products using the methods adopted in baking. The bread quality indicators are given in Table 3. Loafs of bread baked only from rye-wheat and wheat flour were control samples.

The determination of the digestibility of bakery products for gerodietic nutrition was carried out "in vitro" by incubating a 20% bread suspension in a solution of pepsin in glycine buffer. Bakery products from the trading network were used as control samples: the "Nareznoy" loaf made from wheat flour and the rye-wheat bread "Spassky". The research results are presented in Fig. 3.

It was determined that quality indicators of bread baked of model mixtures for gerodietic nutrition were not lower than control samples, and thier "in vitro" digestibility even exceeded the digestibility seen in samples of "Spassky" bread and "Nareznoy" loaf. It is due to the large amount of water-soluble proteins in their composition, which are susceptible to proteolytic cleavage. This proves the high digestibility of the developed products. The result is important for the nutrition of older people, whose metabolism is slower than at a young age.

The calculation of the content of basic nutrients in 100 g of developed bakery products for gerodietic nutrition in accordance with methodological recommendations is made [17]. The results of the calculation are shown in Table 4. For comparison, the chemical composition of the "Nareznoy" loaf and the "Spassky" rye-wheat bread was calculated.

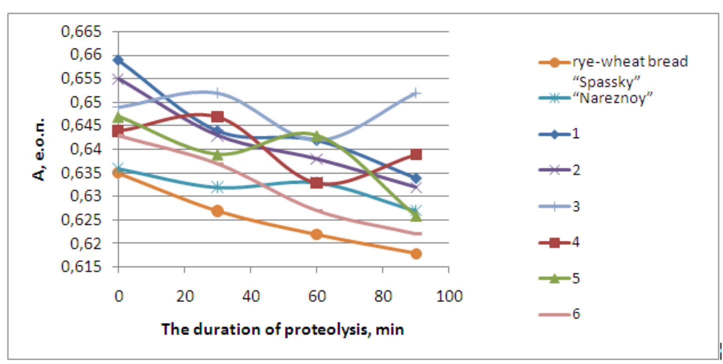

Fig. 3. Digestibility of Bakery Products From model Mixtures for Gerodietic Nutrition.

TABLE II. QUANTITATIVE-QUALITATIVE CHARACTERISTICS OF FLOUR MIXTURES

Component Name	Quantitative-qualitative characteristics of model mixtures							
	A mixture of rye and wheat flour (control 1)	*Rye flour (control 2)*	*1*	*2*	*3*	*4*	*5*	*6*
rye flour	50	100	-	-	-	30.0	30.0	70.0
wheat flour	50	-	50.0	60.0	60.0	35.0	35.0	-
buckwheat flour	-	-	5.0	5.0	5.0	8.0	10.0	-
lentil flour	-	-	9.3	9.0	6.8	4.2	9.3	9.3
amaranth flour	-	-	9.5	8.3	10.0	9.1	4.3	8.0
barley flour	-	-	9.8	-	-	-	-	-
flax seeds	-	-	5.0	-	-	-	-	-
soy flour	-	-	10.0	5.0	5.0	10.0	7.7	9.0
sunflower seeds	-	-	-	10.0	6.0	-	-	-
skimmed milk powder	-	-	-	-	5.0	-	-	-
dry wheat gluten	-	-	0.6	2.2	1.8	3.0	3.0	3.0
calcium lactate	-	-	0.8	0.5	0.4	0.7	0.7	0.70
The sum of the components of the mixture	100	100	100	100	100	100	100	100
Biological value,%	62.0	62.5	79.0	80.0	81.2	80.5	83.3	84.7
Drop number, s	200	150	210	220	230	230	200	200
Calcium, mg/100g	33.0	34.0	212.8	190.6	211.8	181.2	172.4	181.1
Phosphorus, mg / 100 g	186.5	189.0	280.0	251.8	288.2	240.3	226.3	234.8
Magnesium, mg / 100 g	66.5	60.0	102.7	92.16	95.15	86.85	75.46	74.12
Cellulose, mg/100 g	0.3	0.2	2.86	1.20	0.94	0.67	0.81	0.69
Protein g / 100 g	11.2	9.9	16.69	16.13	16.96	17.04	16.95	17.18
Lipids, g / 100 g	1.45	1.7	3.52	6.73	4.77	1.74	1.63	1.54
Carbohydrates (mono-disaccha-rides), g / 100 g	71.9	73	58.94	57.36	60.51	62.09	62.03	60.93
The ratio of components								
Calcium	1.0	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Phosphorus	5.7	5.6	1.32	1.32	1.36	1.33	1.31	1.30
Magnesium	2.0	1.8	0.48	0.48	0.45	0.48	0.44	0.41
Protein	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Lipids	0.1	0.2	0.21	0.42	0.28	0.10	0.10	0.09
Carbohydrates	6.4	7.4	3.53	3.56	3.57	3.64	3.66	3.55

TABLE III. QUALITY INDICATORS OF BREAD MADE OF MODEL MIXTURES

The name of indicators	Characteristics							
	A mixture of rye and wheat flour (control 1)	*Rye flour (control 2)*	*1*	*2*	*3*	*4*	*5*	*6*
Moisture content, %	44.3 ±0.5	50.0 ±0.5	43.5±0.5	44.8±0.5	44.6±0.5	49.5±0.5	50.0±0.5	50.0±0.5
Specific volume, g / cm	1.5 ±0.1	1.5 ±0.1	1.5±0.1	1.6±0.1	1.6±0.1	1.4±0.1	1.6±0.1	1.5±0.1
Porosity,%	55.0 ±1.0	48.5 ±1.0	52.5±1.0	55.0±1.0	55.5±1.0	48.2±1.0	48.5±1.0	48.5±1.0
Output, %	148.2±0.5	149.9±0.5	148.2±0.5	147.7±0.5	148.4±0.5	148.8±0.5	147.9±0.5	150±0.5
Organoleptic evaluation score, points	70.5 ±2.0	70.5 ±2.0	70.5±2.0	65.0±2.0	70.5±2.0	72.0±2.0	71.5±2.0	69.5±2.0

TABLE IV. CHEMICAL COMPOSITION OF BAKERY PRODUCTS FROM MODEL MIXTURES FOR GERODIETIC NUTRITION

Name of food substances	**Estimated composition**							
	"Nareznoy" loaf	***"Spassky" rye-wheat bread***	***1***	***2***	***3***	***4***	***5***	***6***
Proteins, g	7.1	7.6	11.3	10.9	11.5	11.5	11.5	11.6
Fat, g	2.7	1.0	9.0	8.7	9.2	9.2	9.2	9.3
Carbohydrates, g	49.1	48.6	39.8	38.8	40.9	42.0	41.9	41.2
Dietary fiber, g	0.2	0.2	1.9	0.8	0.6	0.5	0.5	0.5
Calcium, mg	18.3	22.3	143.8	128.8	143.1	122.5	116.5	122.4
Phosphorus, mg	105.1	126.0	189.2	170.2	194.7	162.4	152.9	158.7
Magnesium mg	41.7	44.9	69.4	62.3	64.3	58.7	51.0	50.1
Potassium, mg	101.7	110.5	277.4	225.9	245.1	226.2	209.0	239.4
Sodium, mg	5.7	9.1	31.0	37.6	51.4	26.9	22.5	29.0
Omega-6, g	2.2	-	4.2	1.7	3.4	5.6	5.7	5.8
Vitamin E, mg	2.2	-	4.1	4.4	4.8	5.3	5.3	5.2
Energy value, kcal	249.1	210.4	256.9	249.4	263.2	267.1	266.8	265.4
Biological value,%	66.5	62.2	79.0	80.0	81.2	80.5	83.3	84.7

Calculation of the food substances chemical composition of developed bakery products (100 g) made of model mixtures for gerodietic nutrition showed that the protein content in them is 1.5-1.6 times higher than that in the control samples - "Nareznoy" loaf and "Spassky" rye-wheat bread. The fat content is 3.2-3.4 times higher, the amount of carbohydrates decreased by 19.3-20.5%, the level of dietary fiber is 2.5-9.5 times higher, the amount of calcium is 2.5-9.7 times higher, phosphorus - 6.7-7.9 times higher, magnesium - 1.5-1.8 times higher, potassium - 1.2-1.7 times higher, sodium - 2.1-2.4 times higher, the content of omega-6 - 0.8-2.6 times higher, vitamin E - 1.9-2.4 times higher.

At the same time the developed bakery products have the increased biological value by 16.8-19.0 %. Proteins, fats and carbohydrates are in a ratio corresponding to the optimal absorption of these nutrients in gerodietic products - 1.0:0.8:3.5. The ratio of mineral substances Ca:Mg:P corresponds to 1:0.6:1.3, and the content of polyunsaturated fatty acids and fiber is at least 1.0 g and 0.2 g, respectively. Calculations show that the developed bakery products correspond well to requirements for products recommended for gerodietic nutrition.

V. CONCLUSION

A software has been developed for calculating the optimized composition of a model mixture for gerodietic bread according to biological value. This was achieved by mathematical formalization of the problem, taking into account the "drop number" of the mixture as well as the limitations on the optimal content of unconventional raw materials and the number of amino acids that are deficient in bakery products, the ratio of proteins:fats:carbohydrates, Ca:Mg:P, fiber content.

Bakery products prepared from flour mixes modeled with the program complex differed by a higher protein content - 1.5-1.6 times, higher fats content - 3.2-3.4 times, the decrease of carbohydrates amount by 19.3-20.5%. At the same time, the bread had quality indicators that are traditional for this type of product.

As a further task for the study, it would be advisable to develop an integrated large-scale replenishable database of the chemical composition of raw ingredients for broader opportunities in the preparation of flour mixtures. It would also be important to be able to use different optimization criteria when composing flour mixes depending on the tasks.

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