Modeling of multicomponent flour mixtures for bakery products using software

N A Berezina¹, A V Artemov¹, I A Nikitin², E V Khmeleva¹, V A Kozlova¹ and N A Makarova¹

¹Orel State University named after I.S. Turgenev, 95, Komsomolskaya st., Orel, 302026, Russian Federation
²K.G. Razumovsky Moscow State University of Technologies and Management (The First Cossack University) 73, Zemlyanoy Val st., Moscow, 109004, Russian Federation

E-mail: jrdan@yandex.ru

Abstract. Rational proportion of food constituents in recipes of rye-wheat bakery products taking into account the basic principles of food combinatorics while simultaneously obtaining the final product with high consumer properties is a relevant objective. Modern tools for implementation of this task is computer-aided modeling using mathematical apparatus that involves information technologies application to automate the process. The article presents an integrated approach to optimization of the multicomponent mixture composition for rye-wheat bakery products taking into account the chemical composition and technological properties of food constituents of the mixture. Applying of the automated calculation module made it possible to obtain multicomponent flour mixtures with balanced composition where proteins, fats and carbohydrates ratio is 1.0:0.8:3.9-4.8, calcium, phosphorus and magnesium ratio is 1:0.5-0.6:1.2-1.5 due to the use of food and technological potential of unconventional raw materials for baking. At the same time, the protein content in rye-wheat bakery products made from multicomponent mixtures is by 1.7-2.3% higher than that of the analog, lipids content – by 1.5-3.5% higher, the amount of digestible carbohydrates decreased by 7.5 – 9.5%, the amount of fiber increased 5.0-8.5 times, the amount of calcium increased 5.0-6.6 times, the amount of phosphorus increased 1.3-1.6 times, and the amount of magnesium increased 1.4-1.8 times.

1. Introduction
The tempo of modern living, the development of food-processing industry, and the deterioration of the environment have created the worldwide problem of human diet correction. A scientific approach to solving this problem is possible taking into account the results of recent scientific research in the field of digestive physiology, food biochemistry, microbiology, and the laws of rational nutrition [1]. In addition, sedentary lifestyle causes the need to revise the standards for the amount of daily consumed food in the direction of its reduction [2], which in turn makes it necessary to increase the digestibility of products by improving their composition balance.

At the current development stage of products recipes optimization, balanced in accordance with physiological needs, state-of-the-art tools to the implementation of this task is computer-aided modeling using mathematical apparatus [3]. In order to simplify product design automation, the
properties of raw ingredients in recipes should be systematized and formalized [4]. Automated calculation of recipes will allow responding flexibly to changing consumer preferences, taking into account adjustments for variable properties of raw ingredients, as well as optimizing and simplifying the development of food products with specified indicators of typical values.

Popular types of rye-wheat bakery products satisfy the body's energy needs [5], but have a high imbalance in the ratio of the main nutrients – proteins, fats, carbohydrates, as well as calcium, phosphorus, magnesium, contain a low amount of dietary fiber and have insufficient biological value. Despite the high significance of rye-wheat bakery products which are among food staples, a considerable reduction in their consumption has been observed in the Russian Federation in recent decades [6]. The situation can be compensated by the development of products with increased nutritional value, when a portion contains a balanced combination of basic nutrients, mineral composition, increased biological value and concentration of useful components.

The modern food industry has the opportunity to use a wide range of raw ingredients of different chemical composition, which have various properties, both organoleptic and physico-chemical. The research results of Russian and foreign scientists show that to enrich food products, including bakery products, with useful substances various types of non-traditional raw materials for baking can be used: secondary raw materials (products of grain, fruits, vegetables, pseudocereals processing) [7], various grain crops [8], as well as dried fruit and vegetable powders [9], and others.

The purpose of the work is modeling of multicomponent flour mixtures for rye-wheat bakery products with specified indicators of typical values using automated calculation.

2. The purpose of the study
The purpose of the work is modeling of multicomponent flour mixtures for rye-wheat bakery products with specified indicators of typical values using automated calculation.

3. Materials and methods
To design multi-component flour mixtures, the following raw ingredients were used: breadmaking flour – medium rye flour according to GOST R 52809-2007, light wheat flour according to GOST R 52189-2003, soy flour according to GOST 3898-56, lentil flour according to TU 9293-009-89751414-10 (TU- Commodity Specification), sesame seeds according to GOST 12095-76, shelled sunflower seeds according to TU 9729-233-01597945-05, skimmed milk powder according to GOST 33629-2015, dried whey according to GOST 33958-2016, sugar-containing potatoes powder according to TU 9166-293-02069036-2012 «Sugar-containing potatoes powder», food sugar beet powder according to TU 9112-304-02069036 Food sugar beet powder «Sugar beet fibers» extruded, dried pregelatinized millet flour according to TU 9113-325-02069036 Dried pregelatinized flours «Pseudocereals».

In accordance with the design goals, the chemical composition and quality indicators were determined in the raw ingredients. The mass fraction of moisture was determined by drying using the SESH-3M device (electrical drying cabinet), reducing substances - according to GOST 8756.13-87, lactose in dairy products - according to GOST 34304-2017, the total protein content -according to the Kjeldahl method, starch - by volumetric method based on obtaining a complex compound with iodine, with subsequent oxidation of starch with bichromate and iodometric accounting of the latter, lipids - by a method based on determining the refractive indices of lipids and α-bromo-naphthalene, lignin – according to the method based on its precipitation by acid hydrolysis, holocellulose (a mixture of cellulose and hemicellulose) - by weight method after aliquot delignification, pectin substances - by calcium pectate, ash mass fraction - according to GOST 32933-2014, phosphorus content - according to GOST 32904-2014, 51420-99, calcium - according to GOST 26657-97, 26570-95, falling number - according to GOST 30498-97. The research results are shown in table 1.

The amino acid composition of raw ingredients was determined by chromatographic method using the AAA-339 analyzer in accordance with GOST 32192-2013. The research data are presented in table 2.
Table 1. Chemical composition and quality indicators of raw ingredients for multicomponent mixtures

| Indicators | Names | medium rye flour | light wheat flour | sugar-containing | extruded flour seeds | soya | lentil | sesame | sunflower | instant skimmed milk powder | dried whey | dried pregelatinized millet flour |
|------------|-------|------------------|-------------------|------------------|----------------------|-----|-------|--------|----------|--------------------------|----------|-----------------------------|
| Total protein, % | | 9.9 ±0.02 | 12.5 ±0.02 | 9.2 ±0.02 | 2.1 ±0.1 | 27.3 ±0.5 | 17.8 ±0.5 | 32.2 ±0.5 | 13.2 ±0.5 | 35.2 ±0.5 | 12.1 ±0.5 | 7.7 ±0.5 |
| Weight fraction of reducing sugar, % on a dry basis | | - | 50.0 ±0.5 | 5.35 ±0.5 | 6.2 ±0.5 | 2.0 ±0.5 | - | 2.0 ±0.5 | - | - | 8.7 ±0.5 | - ±0.5 |
| Starch, % | | 73.0 ±0.5 | 70.8 ±0.5 | 16.0 ±0.5 | 41.5 ±0.5 | 3.5 ±1.0 | 36.0 ±1.0 | 11.2 ±1.0 | 3.4 ±1.0 | - | - | 35.1 ±1.5 |
| Weight fraction of lipids, % on a dry basis | | 1.6 ±0.01 | 1.3 ±0.01 | 0.4 ±0.01 | 1.3 ±0.01 | not detected | not detected | 48.0 ±0.5 | 52.0 ±0.5 | 1.2± | 1.5± | 3.2± |
| Food fibre , % including: Holocellulose (cellulose+ hemicellulose) | | 1.2 ±0.01 | 0.2 ±0.01 | 5.6 ±0.01 | 29.5 ±1.5 | 1.3 ±0.5 | 3.7 ±0.5 | 2.3 ±0.5 | 5.0 ±0.5 | - | - | 5.1 ±0.01 |
| Lignin, % | | - | - | - | 3.0 ±0.2 | - | - | - | - | - | - | - |
| Pectin substances (water-soluble pectin / protopectin), % | | - | 0.4/1.5 | 1.1/3.8 | - | - | - | - | - | - | - | - |
| Ash, % on a dry basis | | 0.7 ±0.01 | 1.2 ±0.01 | 2.8 ±0.05 | 1.2 ±0.05 | 6.1 ±0.05 | 2.9 ±0.05 | 11.9 ±0.05 | 3.4 ±0.05 | 6.2 ±0.05 | 6.2 ±0.05 | 1.5 ±0.01 |
| Major mineral elements content, mg on a dry basis | | 34.0 ±0.01 | 32.0 ±0.01 | 24.4 ±0.01 | 47.5 ±0.01 | 26.5 ±0.01 | 27.2 ±0.01 | 171.4 ±0.01 | 299.0 ±0.01 | 1155.0 ±0.01 | 1100.0 ±0.01 | 18.8 ±0.01 |
| Calcium | | 186.0 ±0.01 | 184.0 ±0.01 | 225 ±0.01 | 26.5 ±0.01 | 645.0 ±0.01 | 325.0 ±0.01 | 683.0 ±0.01 | 325.0 ±0.01 | 920.0 ±0.01 | 1200.0 ±0.01 | 232.0 ±0.01 |
| Magnesium | | 60.0 ±0.01 | 73.0 ±0.01 | 98.0 ±0.01 | 53.0 ±0.01 | 145.0 ±0.01 | - | 540.0 ±0.01 | 317.0 ±0.01 | 160.0 ±0.01 | 150.0 ±0.01 | 86.7 ±0.01 |
| Mass fraction of moisture, % | | 12.0 ±0.05 | 12.0 ±0.05 | 13.5 ±0.05 | 11.0 ±0.05 | 13.5 ±0.05 | 8.5 ±0.05 | 8.5 ±0.05 | 7.5 ±0.05 | 3.5 ±0.05 | 4.5 ±0.05 | 14.5 ±0.05 |
| Falling number, c | | 166 ±10 | 244 ±10 | 456 ±10 | 460 ±10 | 62 ±10 | 238 ±10 | 210 ±10 | 220 ±10 | 62 ±10 | 62 ±10 | 310 ±10 |
Table 2. Amino acid composition of raw ingredients for multicomponent mixtures

| Amino Acid Name | Content, % | medium rye flour | light wheat flour | sugar-containing potatoes | food sugar beet powder extruded | soya | lentil | sesame | sunflower | instant-skimmed milk powder | dried whey | dried pregelatinized millet flour |
|-----------------|------------|------------------|------------------|--------------------------|-------------------------------|------|-------|--------|-----------|-----------------------------|-----------|----------------------------------|
| Lysine          | 0.34       | 0.30             | 0.27             | 0.09                     | 1.86                          | 1.33 | 0.89  | 0.56   | 2.29                   | 0.34                       | 0.16       |
| Threonine       | 0.36       | 0.24             | 0.44             | 0.28                     | 1.16                          | 0.70 | 1.25  | 0.58   | 1.14                   | 0.27                       | 0.25       |
| Methionine+     | 0.43       | 0.35             | 0.29             | 0.05                     | 0.52                          | 0.29 | 0.81  | 0.41   | 0.97                   | 0.13                       | 0.40       |
| Cystine         | 0.63       | 0.67             | 0.43             | 0.14                     | 1.21                          | 0.76 | 1.29  | 0.54   | 1.74                   | 0.28                       | 0.52       |
| Leucine         | 0.36       | 0.35             | 0.27             | 0.1                       | 1.70                          | 1.13 | 1.94  | 0.81   | 1.74                   | 0.28                       | 0.52       |
| Isoleucine      | 0.74       | 0.85             | 0.67             | 0.06                     | 2.61                          | 1.46 | 3.05  | 1.25   | 2.70                   | 0.23                       | 0.69       |
| Phenylalanine+  | 0.13       | 0.12             | 0.05             | 0.01                     | 0.32                          | 0.15 | 0.52  | 0.19   | 0.35                   | 0.08                       | 0.12       |
| Tyrosine        | 0.46       | 0.41             | 0.40             | 0.17                     | 1.24                          | 0.80 | 1.65  | 0.64   | 1.39                   | 0.21                       | 0.33       |
| Valine          | 3.45       | 3.29             | 2.82             | 0.9                      | 10.62                         | 6.62 | 11.4  | 4.98   | 12.32                  | 1.82                       | 2.99       |
| Total essential |             |                  |                  |                          |                              |      |       |        |                       |                       |            |

The main postulates of the amino acid balance modeling of food products using the amino acid score are presented in the works of N. N. Lipatov. In the work [10], devoted to the aspects of the amino acid balance modeling of food products, an approach is applied, according to which when designing the amino acid composition of a recipe mixture, the content of some components is constant, while others are reduced as a result of replacing by the third ones. This design technique is the most appropriate for bread-making mixes. Preliminary studies have found that the amount of flour in the bread-making mix should be at least 70 % to ensure an acceptable quality of the finished rye-wheat bread.

To implement the possibility of automated calculation of a multicomponent flour mixture with a balanced composition, formalization was carried out that takes into account the mutual balance of essential amino acids in the mixture in accordance with the FAO/WHO standard.

After the amino acid score designing, the biological value indicator of the bread-making mix designed was calculated in accordance with the Mitchell-Block approach. The calculation of the technological criterion for the designed mixture was carried out using the Perten empirical formula [11]. When designing the multicomponent mixtures, the optimization problem took into account the ratio of proteins and carbohydrates (1:4), Ca:P:Mg (1:1.5:0.5).

In connection with the multitask designing goal of a multicomponent flour mixture with unconventional raw materials for rye-wheat bakery products, a software with a flexible interface was developed "Software for calculating and analyzing the optimal composition of a multicomponent flour mixture" (certificate of state registration ECM no. 2019619374/ ECM № 2019619374). The example of how the software works is shown in figure 1.

Bakery products were made from model multicomponent flour mixtures in an accelerated way using the Lezisauer acidifier. Then the following indicators of bakery products were studied: the mass fraction of moisture – in accordance with GOST 21095-75, titrated acidity – in accordance with GOST 5670-51, grain of bread – in accordance with GOST 5669-51, specific volume and organoleptic evaluation [12]. The determination of the digestibility of bakery products made from flour multicomponent mixtures was carried out in vitro by incubating a 20% bread suspension in a pepsin solution in a glycine buffer, and in a trypsin solution in a phosphate buffer and determining the optical density of extracts using a color density meter.
4. Discussion of the results
More than 40 model flour mixtures were generated using the software. After analyzing the calculated data, 3 mixtures with a biological value of at least 75% were selected. The quantitative and qualitative characteristics of the mixtures are shown in table 3. For comparison, as a reference sample, the characteristic of the bread-making mixture consisting of medium rye flour and light wheat flour is given.

| Ingredients and Indicators Names | Multicomponent Flour Mixtures |
|----------------------------------|-------------------------------|
|                                  | Control sample | Sample 1 | Sample 2 | Sample 3 |
| Light wheat flour                | 50.0            | 28.0     | 22.0     | 20.0     |
| Medium rye flour                 | 50.0            | 54.1     | 50.0     | 50.0     |
| Lentil flour                     | -               | -        | -        | 5.0      |
| Soya flour                       | -               | 3.0      | 3.0      | 4.0      |
| Milk powder                      | -               | 0.2      | 0.2      | -        |
| Dried whey                       | -               | 0.3      | -        | -        |
| Food sugar beet powder extruded  | -               | 6.4      | -        | -        |
| Sugar-containing potatoes powder | -               | -        | 13.8     | -        |
| Pregelatinized millet flour      | -               | -        | -        | 5.0      |
| Sesame seeds                     | -               | -        | 1.0      | 6.0      |
| Sunflower seeds                  | -               | 8.0      | 10.0     | 10.0     |
| Total of the mixture components  | 100.0           | 100.0    | 100.0    | 100.0    |
| Biological value, %              | 62.0            | 75.4     | 77.1     | 78.8     |
| Falling number, c                | 206.0           | 200.5    | 210.7    | 207.6    |
| Protein, g/100 g                 | 11.2            | 13.3     | 13.7     | 13.9     |
| Lipids, g/100 g                  | 1.45            | 6.4      | 6.3      | 4.9      |
| Carbohydrates (monodisaccharides + starch), g/100 g | 71.9 | 57.7 | 59.8 | 53.9 |
| Food fibers, g/100 g             | 0.3             | 2.6      | 1.7      | 1.5      |
| Calcium, mg/100 g                | 33.0            | 159.8    | 141.5    | 178.92   |
| Phosphorus, mg/100 g             | 186.5           | 205.5    | 215.5    | 241.1    |
| Magnesium, mg/100g               | 66.5            | 89.5     | 91.6     | 109.1    |

Bakery products were made from the model multicomponent flour mixtures in an accelerated way using an acidifier, compressed yeast and salt in amount of (% of the mixture mass): 2.0, 2.2 and 1.5, respectively. Quality indicators of finished products are shown in table 4. A bakery product from a chain store – the rye-wheat bread «Spassky» baked according to TU 1091451-006-48363077-2016 (JSC «Orlovsky Khlebocombinat» («Oryol Bakery Complex») was used as a reference sample.
Figure 1. Example of an operating step of the «Software tool for calculating and analyzing the optimal composition of a multicomponent flour mixture»

Table 4. Quality indicators of bakery products made from multicomponent flour mixtures

| Ingredients and Indicators Names | Rye-wheat bread «Spassky» reference sample | Multicomponent Flour Mixtures Sample 1 | Sample 2 | Sample 3 |
|---------------------------------|------------------------------------------|-------------------------------------|----------|---------|
| Mass fraction of moisture, %    | 49.5±0.5                                 | 49.5±0.5                            | 49.5±0.5 | 50.0±0.5|
| Specific volume, g/cm           | 1.7±0.1                                  | 1.8±0.1                             | 1.7±0.1  | 1.5±0.1 |
| Grain of bread, %               | 50.5±1.0                                 | 55.0±1.0                            | 52.5±1.0 | 48.5±1.0|
| Acidity, degree                 | 9.0±0.2                                  | 9.0±0.2                             | 9.0±0.2  | 9.0±0.2 |
| Organoleptic evaluation, scores point | 65.0±2.0                                 | 65.0±2.0                            | 70.5±2.0 | 69.5±2.0|

The quality indicators of bakery products made from multicomponent mixtures were determined to be close to those of the reference sample from the chain store.

The results of determining the digestibility of bakery products made from multicomponent flour mixtures in vitro are shown in figure 2.
Figure 2. Digestibility of bakery products made from multicomponent flour mixtures

The in vitro digestibility of bakery products made from multicomponent flour mixtures was found to be more intense than that of the reference sample bread «Spassky» due to the large number of water-soluble proteins in their composition, which are more susceptible to proteolytic cleavage [13].

The calculation of the basic nutritional ingredients content in 100 g of the developed bakery products was made in accordance with the guidelines [14]. The calculation results are shown in table 5. For comparison, the chemical composition of rye-wheat bread «Spassky» was calculated.

Table 5. Chemical composition of 100 g of bakery products made from multicomponent flour mixtures

| Ingredients and Indicators Names | Rye-wheat bread «Spassky» reference sample | Characteristics of rye-wheat bakery products |
|----------------------------------|--------------------------------------------|------------------------------------------|
|                                   | Sample 1 | Sample 2 | Sample 3 |
| Protein, g/100 g                  | 7.1      | 8.8      | 9.3      | 9.4      |
| Lipids, g/100 g                   | 2.7      | 4.2      | 4.7      | 6.2      |
| Carbohydrates (monodisaccharides + starch), g/100 g | 43      | 35.2     | 35.5     | 33.5     |
| Calcium, mg/100 g                 | 18.3     | 105.7    | 95.8     | 121.2    |
| Phosphorus, mg/100g               | 105.1    | 135.9    | 145.9    | 163.3    |
| Magnesium, mg/100g                | 41.7     | 59.2     | 62.0     | 73.9     |
| Food fibers, g/100 g              | 0.2      | 1.7      | 1.2      | 1.0      |
| Caloric content, kcal             | 214.5    | 218.2    | 226.4    | 232.3    |
| Biological value, %               | 62.2     | 75.4     | 77.1     | 78.8     |

The protein content in bakery products made from multicomponent flour mixtures was found to be by 1.7-2.3 % higher than that of rye-wheat bread «Spassky», lipids – by 1.5-3.5 % higher, the amount of carbohydrates decreased by 7.5 – 9.5%, the amount of fiber grew 5.0-8.5 times larger, the amount of calcium grew 5.0-6.6 times larger, phosphorus – 1.3-1.6 times larger, and magnesium – 1.4-1.8 times larger. At the same time, the biological value increased by 13.2-16.6 % in the developed bakery products, the ratio of proteins:fats:carbohydrates is one that corresponds to the optimal absorption of these nutrients - 1:0.8:3.9-4.8, the ratio of minerals such as Ca:Mg:P corresponds to 1:0.5-0.6:1.2-1.5. Calculations show that the developed bakery products have a balanced composition.

5. Conclusion

Modeling of multicomponent flour mixtures for bakery products using software made it possible to increase the biological value of rye-wheat bakery products, to optimize the content of basic nutrients (proteins, fats, carbohydrates) in a ratio favorable for absorption, to increase the content of minerals and ensure their optimal ratio.

6. Acknowledgment

The work was carried out with the financial support of the Russian Foundation for Basic Research in the framework of grant No. 19-016-00049 «Software system development for automated calculation of the flour mixtures composition for functional and dietary nutrition».

References

[1] Tutelyan V A 2010 Laws of nutrition science Modern medical technologies 4 98-99
[2] Nikolaeva M A 2018 Rational norms of food consumption and compliance with the actual consumption of food products in Russia Commodity science of food products 3 34-40
[3] Karpov V I, Portnov N M, Nikitin I A, Sidorenko Y I, Zavalishin I V, Petrov S M, Podgornova N M, Sidorenko M Y and Sheterman S V 2019 Automated Methodology for Optimizing Menus in Personalized Nutrition International Journal of Advanced Computer Science and Applications 10 (11) 317-322 DOI: 10.14569/IJACSA.2019.0101144

[4] Musina O N and Lisin P A 2015 An approach to the choice of alternatives of the optimized formulations Foods and Raw Materials 3 (2) 65–73

[5] Kourkouta L et al. 2017 Bread and Health Journal of Pharmacy and Pharmacology 5 (11) 821-826

[6] Danilchuk Yu V and Suslova N K 2014 State of the market, formation of the range of rye-wheat bread Merchandiser of food products 10 51-56

[7] Kurek M and Wyrwisz M 2015 The Application of Dietary Fiber in Bread Products Food Process Technol 6 (5) 1-4

[8] Tarasenko N A 2017 Prospects for the use of secondary products of vegetable raw materials processing in the recipes of protein-carbohydrate enrichers Proceedings of higher educational institutions. Food technology 2-3 (356-357) 10-13

[9] Nilova L P, Malyutenkova S M, Kaigorodtseva M S and Evgrafov A A 2018 The formation of quality and antioxidant properties of bakery products with cloudberry powder Proceedings of the Voronezh State University of Engineering Technologies 80 (2) 138-143 https://doi.org/10.20914/2310-1202-2018-2-138-143

[10] Lipatov N N 1990 Principles and methods of food recipes designing for balancing diets Proceedings of higher educational institutions. Food technology 6 5-10

[11] Falling Number instrument. Excerpts from Manual. File access mode http://www.soctrade.in.ua/upload/Instrukcii/VyderzhkiizinstrukciiFallingNumber1900.pdf

[12] Labutina N V, Koryachkina S Ya, Berezina N A and Khmeleva E V 2009 Raw materials, semi-finished products and finished bakery products monitoring: study guide (Moscow: DeLi)

[13] Pokrovskiy A A and Minakov I D 1965 Food attack by proteolytic enzymes in vitro Nutrition issues 3 33-44

[14] Kosovan A P, Dremucheva G F and Polandova R D 2008 Study guide for determining the chemical composition and energy value of bakery products (M.: Moscow printing house № 2)