# УНИВЕРСИТЕТ ИТМО

# MINISTRY OF SCIENCE AND HIGHER EDUCATION OF THE RUSSIAN FEDERATION

ITMO UNIVERSITY

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# SCIENCE-BASED DESIGN FOR FOODS COMPOSITION

RECOMMENDED FOR USE AT ITMO UNIVERSITY for master students of all forms of education, studying in the program of training: 19.04.01 "FoodTech" and 19.04.02 "Food Quality and Safety"



Saint-Petersburg 2021

### МИНИСТЕРСТВО НАУКИ И ВЫСШЕГО ОБРАЗОВАНИЯ РОССИЙСКОЙ ФЕДЕРАЦИИ

УНИВЕРСИТЕТ ИТМО

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# НАУЧНО-ОБОСНОВАННОЕ ПРОЕКТИРОВАНИЕ ПИЩЕВЫХ КОМПОЗИЦИЙ

УЧЕБНО-МЕТОДИЧЕСКОЕ ПОСОБИЕ

### РЕКОМЕНДОВАНО К ИСПОЛЬЗОВАНИЮ В УНИВЕРСИТЕТЕ ИТМО

по направлению подготовки 19.04.01, 19.04.02 в качестве Учебно-методическое пособие для реализации основных профессиональных образовательных программ высшего образования магистратуры

УНИВЕРСИТЕТ ИТМО

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This allows the student understand the manual to methodological principles of designing the composition of multicomponent products, considering the quality indicators of raw materials and finished products. This course will provide an overview of knowledge of nutritional science, in particular of the latest advances in food science in the field of active and healthy longevity and also advanced technologies of the modern manufacturing industry. Studying this course will allow students to gain skills in development of recipes and technologies for the production of specialized foods for various population groups. As a result of studying the discipline students will know how to design a science-based food composition with desirable properties for specialized nutrition.

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## УНИВЕРСИТЕТ ИТМО

Университет ИТМО национальный \_ исследовательский университет, ведущий вуз России в области информационных, фотонных и биохимических технологий. Альма-матер победителей международных соревнований по программированию – ІСРС (единственный в мире семикратный чемпион), Google Code Jam, Facebook Hacker Cup, Яндекс.Алгоритм, Russian Code Cup, Topcoder Open и др. Приоритетные направления: IT, фотоника, робототехника, квантовые коммуникации, Sciences. Art&Science. трансляционная медицина, Life Science Communication. Входит в ТОП-100 по направлению «Автоматизация и управление» Шанхайского предметного рейтинга (ARWU) и занимает 74 место в мире в британском предметном рейтинге QS по компьютерным наукам (Computer Science and Information Systems). С 2013 по 2020 гг. – лидер Проекта 5-100.

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### **INTRODUCTION**

Currently, in the field of healthy nutrition there is a trend for the production of products with a multicomponent composition, which includes not only macronutrients, but also vitamins, minerals, and biologically active substances necessary for the body. The production of such food products is relevant, since a large number of components in their composition allows the most complete provision of the human body with important nutrients in the amount necessary for normal life and functioning. These types of products are designed to maintain human health and reduce the cost of its restoring it.

In the modern world, the optimization of any industry requires increasing production efficiency, saving raw materials, and improving technological processes. To improve the food production industry, computer systems are applied in the design of multicomponent food products. Computational methods have acquired a particular importance due to developing digital systems of computer mathematics. Computational methods mainly include mathematical methods for solving extremum problems, which arise in planning and organization of food production.

#### Computational-practical work 1

#### Determining the balance level of a daily ration for the military in the Russian Federation

According to the World Health Organization (WHO), the health of the population depends on lifestyle and social conditions by 50-55%, on genetic factors by 20-22%, on the environment by 19-20%, on the level of the healthcare system and the quality of medical care by 7-10%. Thus, the most significant factor in human health is lifestyle, in particular, nutrition.

The purpose of this computational-practical work is to assess the balance of the daily ration for the Russian Federation (RF) military, taking into account one of the ration options presented in Annex 1. The work is carried out in a team of students, 3-4 students per team.

#### <u>Work order</u>

1. A team of students are given the task to analyze the daily ration for the RF military based on the specification of individual rations (Annex 1).

2. Fill in the names of the products of the ration selected in table 2, distributing them by meals throughout the day (three meals per day).

3. Present the chemical composition of all products based on a portion of every product, using the reference book "Chemical composition of food products" by I. M. Skurikhin or the information and reference system - the database on the chemical composition of the products available at the link: <u>http://www.intelmeal.ru/</u> [1, 2].

3. Calculate the total content of macronutrients by food cycles and the daily diet as a whole.

4. Calculate the energy value for food cycles and daily ration as a whole, using the coefficients of the energy value of nutrients (table 1).

5. Discuss the data obtained and draw conclusions taking into account the norms of physiological needs for energy and nutrients for the RF military, choosing the target audience by physical activity group and gender (Annex 2 and 3) [3].

The military should eat at least 3 times a day, with ith the distribution of the energy value of their diet corresponding to the following ratios:

- breakfast - 20–35%;

- lunch - 40-50%;

- dinner - 25-30%.

Foods containing animal proteins are recommended to be consumed in the morning.

Table 1. Coefficients of energy value of food macronutrients

Nutrients	kcal / g	kJ / g
Proteins	4.00	16.7
Fats	9.00	37.7
Carbohydrates	4.00	15.7

Ration	Product	Weight, g	Mass fraction, g				Energy value,
			water	proteins	fats	carbohydrates	kcal
1st meal (breakfast)							
2nd meal (lunch)							
3rd meal (dinner)							
Total							

## Table 2 The daily diet (ration) of the military RF (men or women)

#### **Computational-practical work 2**

# Assessment of the macronutrient composition of foods based on, taking into account the quantitative macronutrient classification

When designing specialized food products, it is necessary to assess their chemical composition taking into account the quantitative macronutrient classification. For example, in the case of a high protein product, protein is assessed as the dominant macronutrient, which requires quantitative confirmation. Regardless of animal or vegetable origin, the group of high-protein products include products, which have the mass fraction of protein (P) in dry matter at least 75%. By analogy, the groups of high-fat and high-carbohydrate foods are estimated, for which the mass fractions of fat (F) or carbohydrates (C) in terms of dry matter are not less than 75%. The group of protein-fat products includes the products, for which the following inequalities are true:

$$75\% \ge P > 50\%$$
 and  $50\% \ge F > 25\%$ 

The group of protein-carbohydrate products includes products that fulfill the following inequalities:

$$75\% \ge P > 50\%$$
 and  $50\% \ge C > 25\%$ 

The group of protein-fat-carbohydrate products includes those, for which the following inequality is fulfilled:

$$75\% \ge P > 50\%$$
 and  $50\% \ge (F + C) > 25\%$  and  $12.5\% > C \ge 0\%$ 

In relation to protein-carbohydrate-fat products, these restrictions are as follows:

$$75\% \ge P > 50\%$$
 and  $50\% \ge (C + F) > 25\%$  and  $12.5\% > F \ge 0\%$ 

The group of fat-protein products includes products, for which the following inequality is fulfilled:

$$75\% \ge F > 50\%$$
 and  $50\% \ge P > 25\%$ 

For the group of fat-carbohydrate products, the inequalities take the form:

$$75\% \ge F > 50\%$$
 and  $50\% \ge C > 25\%$ 

By analogy with the previous reasoning, the group of fat-protein-carbohydrate products includes those, for which the following inequalities are true:

$$75\% \ge F > 50\%$$
 and  $50\% \ge (P + C) > 25\%$  and  $12.5\% > C \ge 0\%$ 

The group of fat-carbohydrate-protein products includes such types of products, for which the following inequality is fulfilled:

$$75\% \ge F > 50\%$$
 and  $50\% \ge (C + P) > 25\%$  and  $12.5\% > P \ge 0\%$ 

The group of carbohydrate-protein (a) or carbohydrate-fat (b) products includes such types of products, for which inequalities are true:

a)  $75\% \ge C > 50\%$  and  $50\% \ge P > 25\%$ 

b) 
$$75\% \ge C > 50\%$$
 and  $50\% \ge F > 25\%$ 

The group of carbohydrate-protein-fatty products includes the products described by the following inequalities:

$$75\% \ge C > 50\%$$
 and  $50\% \ge (P + F) > 25\%$  and  $12.5\% > F \ge 0\%$ 

The group of carbohydrate-fat-protein foods includes foods, for which the following inequalities are applied:

$$75\% \ge C > 50\%$$
 and  $50\% \ge (F + P) > 25\%$  and  $12.5\% > P \ge 0\%$ 

It should be understood that meat raw materials, taking into account their chemical composition, can be attributed to such classification groups as protein, protein-fat, fat-protein or fat.

#### Work order

1. Following the teacher's instructions, select the main source of protein of animal or plant origin, using the reference data. Evaluate the protein source based on the quantitative macronutrient classification, providing evidence for its belonging to a certain group.

2. In order to correct the product in relation to one of the selected groups of macronutrient classification, various types of raw materials of animal or vegetable origin should be offered as additional ingredients. Evaluate them taking into account the quantitative macro-nutrient classification, proving their belonging to a particular group of raw materials. Fill in the blank cells of Table 3 in each row.

3. Present the composition of the product to be developed (based on 100 g of the finished product), taking into account the use of at least five additional raw ingredients from Table 3. Use Table 4 to present the calculation results.

4. Calculate the mass fraction of protein or other macronutrient in the product composition according to Formula (1):

$$s_p = \frac{\sum_{i=1}^n x_i s_i}{\sum_{i=1}^n x_i}, (1)$$

where

 $S_p$ - mass fraction of protein or other macronutrient in the product,%;

X<sub>i</sub>- mass fraction of the i-th component in the recipe,%;

 $S_i$ - mass fraction of protein or other macronutrient in the i-th component of the formulation,%.

5. Make a conclusion about the meeting of daily requirements for macro nutrients and energy when using a portion of the developed product for a certain population group, presenting the calculation data in Table 5.

Table 3 Classification of additional raw ingredients of the recipe

Classification group	Raw ingredients		
protein			
fatty			
carbohydrate			
protein-fatty			
protein-carbohydrate			
protein-fat-carbohydrate			
protein-carbohydrate-fat			
fat-protein			
fat-carbohydrate			
fat-protein-carbohydrate			
fat-carbohydrate-protein			
carbohydrate-protein			
carbohydrate fat			
carbohydrate-protein-fatty			
carbohydrate-fat-protein			

#### Table 4. Formulation of developed product

Name of the ingredients of the recipe of developed product	Mass fraction of ingredients per		
	100 g	portion	
1			
2			
3			
4			
5			
TOTAL	100 g		

Table 5. Satisfaction of the daily requirement for macro-nutrients through the use of a portion of the developed product

Macro-nutrient	Consumption	Mass fraction of macro-	The degree of satisfaction
names	rates, g / per day	nutrients in a portion of the	of the daily requirement,%
		product, g	
Proteins			
Fats			
Carbohydrates			

#### **Computational-practical work 3**

#### Determination of the biological value of the protein component in the product

To express the biological value of protein products, the amino acid composition of a test product is compared with the one of a reference protein. To analyze the biological value of a protein component, generally accepted is the amino acid (chemical) method.

In 1973, the joint expert committee of the Food and Agriculture Organization at the United Nations (FAO) and the World Health Organization (WHO) proposed the use of a reference protein containing 8 essential amino acids with the following quantitative characteristics: isoleucine - 40 mg, leucine - 70 mg, lysine - 55 mg, methionine + cystine - 35 mg, phenylalanine - 28 mg, threonine - 40 mg, tryptophan - 10 mg, valine - 50 mg per gram (Table 6). In 2011, according to the latest data from FAO and WHO, the reference protein quantitative and qualitative composition was revised (Table 7). To calculate the amino-acid (chemical) score, the content of each essential amino acid in a test product is compared with its content in the reference protein by the Formula (2):

Amino-acid score=  $A_x / A * 100, \%$  (2),

Where

 $A_x$  - the mass fraction of the essential amino acid in the test product, g / 100g of protein; A - the mass fraction of an essential amino acid in the "reference" protein, g / 100g of protein. An amino-acid with that has a scorerate of less than 100% is called limiting. In the presence of several limiting amino- acids in the composition of the product, the amino- acid with the lowest aAmino-acid score is isolated and, which is called the "first limiting amino acid".

An amino-acid with a score less than 100% is called limiting. In the presence of several limiting amino-acids in the composition of the product, the amino-acid with the lowest amino-acid score is isolated and called the "first limiting amino acid".

#### <u>Work order</u>

1. Provide data on the composition of essential amino acids of the product in g / 100g of protein using the reference book I.M. Skurikhin "Chemical composition of food products".

2. Determine the biological value for the protein component of the product by the amino- acid (chemical) method according to the WHO and FAO from 1973 and 2011.Fill the calculation results in Tables 6 and 7.

3. Draw conclusions.

Table 6. Biological value of the protein component of the product relative to FAO and WHO, 1973

Essential amino acids $(E \land \land)$	Mass fraction of EAA,		Mass fraction of EAA,		Amino-acid score,
	FAO / WHO, investigated product		70		
Valin Isoleucine					
Leucine					

Lysine		
Methionine + cystine *		
Threonine		
Tryptophan		
Phenylalanine		

\* the need for one amino-acid can be covered by the presence of another, then the pairs are summed up

Table 7. Biological value of the protein component of the product relative to FAO WHO, 2011

Essential amino acids	Mass fraction of EAA,		Amino-acid score,
(EAA)	g / 100	g protein	%
	FAO / WHO,	investigated	
	2011	product	
Histidine	2.00		
Isoleucine	3.20		
Leucine	6.60		
Lysine	5.70		
Methionine + Cysteine *	2.70		
Phenylalanine + Tyrosine *	5.20		
Threonine	3.10		
Tryptophan	0.85		
Valine	4.30		

\* the need for one amino acid can be covered by the presence of another, then the pairs are summed up

#### **Computational-practical work 4**

# Evaluation of the biological value of the protein component within a multicomponent product

The production of multicomponent products provides opportunities to reduce the shortage of traditional raw materials, especially during the period of seasonal supplies, as well as expand the range of products with replaced components. It should be noted that in 2007and 2011 a joint expert committee of organizations such as the Food and Agriculture Organization at the United Nations (FAO) and the World Health Organization (WHO) revised the amino acid composition of the **reference protein** (data are presented in Table 8).

The calculation is performed step by step with the initial choice of a specific recipe for a multicomponent product. A protein component is selected. It has to contain essential amino acids, taking into account milk as a reference product.

#### <u>Work order</u>

1. Based on the recipe composition, the percentage (mass fraction) of the protein-containing ingredient and the amount of protein in it, calculate the mass fraction of protein in the complete composition according to Formula 3:

$$S_p = \frac{\sum_{i=1}^n x_i s_i}{\sum_{i=1}^n x_i},$$
 (3)

where

 $S_p$ - mass fraction of protein in the combined mixture,%;

 $x_i$ - mass fraction of the i-th component in the formulation;

 $S_i$  - mass fraction of protein in a specific i-th component of the recipe,%.

2. After determining the total protein content in the mixture, evaluate its qualitative composition. To do this, calculate the quantitative content of each of the essential amino-acids in the combined mixture according to Formula 4:

$$A_{j} = \frac{\sum_{i=1}^{n} x_{i} s_{i} m_{ij}}{\sum_{i=1}^{n} x_{i} s_{i}}, (4)$$

where

 $A_j$  - the content of a specific essential amino-acid in the total protein component of the formulation,%;

 $S_i$  - mass fraction of protein in this component,%;

 $x_i$  - mass fraction of the i-th component in the formulation,%;

mij - mass fraction of a specific EAA in this component,%.

3. Fill in the obtained results in Table 8. Draw conclusions.

Table 8. Biological	value of the	protein com	ponent of a	developed	product
0		1	1	1	1

Essential amino	Mass fraction of EAA,					Amino acid
acids (EAA)		g /	100g protei	n		rate of the
	FAO /	ingredient	ingredient	ingredient	developed	product,%
	WHO,	1	2	3	product	
	2011					
Histidine	2.00					
Isoleucine	3.20					
Leucine	6.60					
Lysine	5.70					
Methionine +						
Cysteine *	2.70					
Phenylalanine +						
Tyrosine *	5.20					
Threonine	3.10					
Tryptophan	0.85					
Valine	4.30					

#### **Computational-practical work 5**

# Estimated indicators characterizing qualitative composition of the protein component in the product

Rogov I.A. and Lipatov N.N., the academicians of the Russian Academy of Agricultural Sciences, proposed fundamental criteria to assess the biological value of protein components for the nutritional balance of raw material. The assessment of protein components includes: coefficients of differences of amino-acid score (CDAAS), rationality of amino-acid composition (Rp), comparable redundancy (G) and biological value (BC). In particular, the CDAAS (%) shows the average excess of the amino acid score of essential amino-acids in comparison with the lowest score of any essential amino-acid (excess amount of essential amino-acids is not used for plastic needs). CDAAS is determined by Formula 5:

$$CDAAS = \frac{\sum \triangle DAAS}{n}, (5)$$

where

 $\Delta$ DAAS - the difference between the amino-acid score calculated according to Formula 6; n - the number of essential amino acids.

$$\triangle DAAS = C_i - C_{min} , (6)$$

where

 $C_i$ - the score of the i-th essential amino acid,%;

 $C_{min}$  - the minimum score of essential amino-acids,%.

The biological value (BV) of the protein component is determined by Formula 7:

$$BV = 100 - CDAAS, \%, (7)$$

The coefficient of rationality of the j-th essential amino-acid  $-a_j$ , characterizing the possibility of utilization of amino-acids by the body, is predetermined by the minimum speed of an essential amino-acid and is calculated by the Formula 8:

$$a_j = C_{min}/C_j, (8)$$

The coefficient of rationality of the amino-acid composition, Rp numerically characterizes the balance of essential amino-acids in relation to the physiologically necessary standard. In the case when  $\text{Cmin} \leq 1$  (in fractions of units), the coefficient of rationality of the amino-acid composition is calculated based on the Formula 9:

$$R_p = \frac{\sum_{j=1}^{k} (a_j A_j)}{\sum_{j=1}^{k} A_j}, (9)$$

The indicator of comparable redundancy in the content of essential amino-acids (EAAs), G, characterizes their total mass. Due to the amino-acid composition imbalance, EAAs are not used for anabolic needs in such an amount of protein in the product evaluated that is equivalent to EAAs amount in 100 g of the reference protein in terms of the content of potentially utilized EAAs. Determination of G is carried out according to the Formula 10:

$$G = \frac{\sum_{j=1}^{n} (A_j - C_{min} A_{ej})}{C_{min}}, (10)$$

where

 $A_j$  - the mass fraction of the j-th essential amino-acid in the raw material, g / 100g of protein;  $A_{ej}$  - the mass fraction of the j-th essential amino-acid corresponding to the physiological needs, g / 100g of protein.

In 1840, a German chemist Justus von Liebig (1803-1873), who is considered one of the founders of modern agrochemistry, formulated the ecological and economic law of the minimum, which is also known as Liebig's law (Fig. 1). The law states that it is the scarcest resource (a limiting factor) that dictates the growth. For example, a limiting factor for the amino-acid composition of a protein may be the absence or low amount of an essential amino-acid. Liebig's Law can be applied to calculate a number of biological value indicators in a product. Then, Lisin P.A. [13, 14] proposed to evaluate the biological value of the protein component using the amino-acid composition index (UA) according to Formula 11:

$$U_A = \sqrt[m]{\prod_{i=1}^m d_{A_j}}, (11)$$

given that:

$$d_{A_j} = (rac{A_j}{A_{rj}})$$
, если  $A_j \leq A_{rj}$   
 $d_{A_j} = (rac{A_{rj}}{A_j})$ , если  $A_j \geq A_{rj}$ 

where

 $A_j$  - the mass fraction of an essential amino-acid in the test sample, g / 100g of protein;  $A_{rj}$  - mass fraction of an essential amino-acid in reference protein, g / 100g of protein.



Figure 1. The law of the minimum proposed by Justus von Liebig

We have proposed a formula for calculating a complex balance indicator of the protein component in a product, which allows to assess the qualitative composition of the protein component according to three calculated indicators (Formula 12).

$$\mathbf{D} = \sqrt[n]{\prod_{i=1}^{m} U_i} = \sqrt{U_A \cdot U_{bv}} \cdot U_R , (12)$$

where

 $U_A$  - the amino-acid composition index;

 $U_{bv}$  - the index of the biological value of the composition;

 $U_R$  - the index of rationality of the composition.

To analyze the calculated data, which tend to "1", the Harrington's function, known as the desirability scale, should be applied. The desirability scale is divided in the range from 0 to 1 by 27 five subranges: [0-0.2] - "very bad", [0.2-0.37] - "bad", [0.37-0.63] - "satisfactory", [0.63-0.8] - "good" and [0.8-1] - "very good".

#### <u>Work order</u>

1.Calculate the indicators characterizing the qualitative composition of the protein component in a product using the data previously obtained (the results of computational practical work 3 or 4)

2. Fill in the obtained results in Table 9.

3. Draw conclusions about the biological value of the protein component in the investigated product taking into account the Harrington's function.

Table 9 Indicators of the biological value of the protein component in the product

Product	Protein mass fraction,%	Number of limiting EAAs	E	stimated	indica	ators		
			KPAC, %	BV, %	Rp	G	Ua	D

#### **Computational-practical work 6**

#### Fatty acid analysis of the product lipid composition

The following factors should be considered when the fat composition of the combined product is developed:

• the ratio between the main groups of fatty acids (saturated: monounsaturated: polyunsaturated fatty acids);

• the ratio of the two main families of polyunsaturated fatty acids, namely omega - 6 and omega - 3 fatty acids.

Based on the values of physiological needs in energy and nutrients for various groups of the population in the Russian Federation, it is possible to formulate a set of initial requirements for the complete composition of fat, providing the necessary set of fatty acids in optimal ratios for various groups of the population (Table 10).

T 1' /	Category of population			
Indicator	Children under 1	Chosen category of the population		
	year old	of the Russian Federation		
Fatty acid content, % of lipids or				
g / 100 g of lipids:				
Saturated (SFA)	41.78			
Monounsaturated (MUFA)	43.03			
Polyunsaturated (PUFA),	12.42			
in particular:				
Linoleic acid (n - 6)	10.85			
Linolenic acid (n - 3)	0.62			
Arachidonic acid	0.95			
n-3 : n-6 ratio	?			

Table 10. Physiological needs for various groups of population

The requirements for biologically complete fat constitute the basis of a mathematical model considering the dependence of the content of EFA, MUFA, and PUFA on the composition of the fat mixture.

The fatty acid content in the mixture can be calculated using Formula 13:

$$C_{mj} = \frac{\sum_{i=1}^{n} (C_i L_i)}{\sum_{i=1}^{n} C_i}$$
, (13)

where,

 $L_i$  - the content of fatty acids of any type in the mixture, %; (for example, SFA);  $C_i$ - content of the component in the mixture, %; (for example, palm oil);  $L_{ci}$  - content of fatty acids of this type in the Ci component, % (for example, saturated fatty acids in palm oil). Fatty acid balance of potential fat-containing ingredients in a product for particular nutritional purposes can be assessed using the Fatty Acid Balance Factor (RL) according to Formula 14:

$$R_L = \sqrt[m]{\prod_{i=1}^m d_{L_i}} \quad , \quad (14)$$

given that:

$$d_{L_i} = \frac{L_i}{L_{ni}}, if \ L_i \le L_{ni}$$

$$d_{L_i} = (\frac{L_i}{L_{ni}})^{-1}$$
, if  $L_i \le L_{ni}$ 

where,

 $L_i$  - the mass fraction of the i-th fatty acid in a developed product, g/100 g of lipids;

 $L_{ni}$  - the mass fraction of the i-th fatty acid corresponding to the physiological needs, g/100 g of lipids;

i = 1 corresponds to  $\sum EFA$ ,  $i = 2 - \sum MUFA$ ,  $i = 3 - \sum PUFA$ , i = 4 – linoleic (n - 6), i = 5 – linolenic (n - 3), i = 6 – arachidonic fatty acid (for baby nutrition only). <u>Work order</u>

1. Fill in the missing values in Table 10, then analyze them.

2. Develop a recipe for a multicomponent product, considering its fatty acid composition, using the above formulas.

3. Evaluate the qualitative composition of the lipid component of the developed product using the coefficient of fatty acid compliance considering the Harrington's function, fill in Table 11 with the results obtained.

4. Draw conclusions about promising types of raw materials to produce multicomponent food products and suggest approaches to increase their fatty acid balance.

Harrington's function is divided in the range from 0 to 1 into five subranges: [0-0.2] - "very bad", [0.2-0.37] - "bad", [0.37-0.63] - "satisfactory", [0.63-0.8] - "good", [0.8-1] - "very good". Specific parameters of comparative systems are distributed on a scale according to the requirements in the interval of effective values of the scale special indicators.

The use of the Harrington's function allows for an integrated balance assessment of the designed food products, a comparative evaluation of the nutritional and energy value of food products and the development of product catalogs (card indices) with a nutrient composition.

Sample(s)		Fatty acids	s, g / 100	g lipids	5	Fatty acid balance factor, RL		
	SFAMUFAPUFA $n - n - 6$ $n - 3$ $i = 1$				<i>i</i> = 3	<i>i</i> = 5		
Physiological needs						-	-	

Table 11. Biological value of the lipid component of a developed product

Developed product				
$d_{L_i}$			-	-

**Computational-practical work 7** 

#### **Evaluation of the functionality of an ingredient in a product formulation**

The daily requirements for nutrients and energy are presented in the Methodical recommendations MP 2.3.1.2432 -08 [3].

#### <u>Work order</u>

1. A team of students are given the task to recalculate the norms of consumption of nutrients for the nutrition of a certain category of population following the teacher's instructions (according to Annex 2 and 3).

2. Fill in Table 12 with the data from the original source and the data obtained as a result of recalculation.

3. Analyze the product to be enriched with the proposed functional ingredient - kelp, per 100 g of product and a portion of the product (students obtain this information on their own). Fill estimated data in table 12.

4. Analyze the chemical composition data for the functional ingredient - kelp (Table 13).

5. Design the composition of the developed product with kelp and calculate the micronutrients, including iodine. Fill the calculation results in Table 14.

6. Draw conclusions about the functionality of kelp as part of the developed product.

Conversion of weight units to international units:

Vitamin A - 1 mg = 3300 IU

Vitamin D - 1 mcg = 40 IU

Vitamin E - 1 mg = 1.21 IU

Substances	Require		Mass fraction, per	100 g	Mass	fraction, per	portion	Satisfying the daily micronutrient			
	ments *							requirer	nents		
		Based product	Additional ingredient (AI)	Complex product (CP= BP + AI)	BP, g	AI, g	CP,g	Portion of CP, %	Additional ingredient (AI) in portion of CP, %		
Fibers, g	20.00										
Vitamin A, IU	2970										
Vitamin B2, mg	1.80										
Vitamin B6, mg	2.4										
Vitamin PP, mg	20.00										
Calcium, mg	1000.00										
Magnesium, mg	400.00										
Sodium, mg	5000.00										
Phosphorus, mg	800.00										

Table 12. Approved calculation of functionality regarding to BV of carbohydrate, vitamin or mineral componens

Indicator	Content
Moisture, %	6.51
Crude protein, %	8.65
Crude fiber, %	11.29
Crude fat, %	0.48
Crude ash, %	48.90
Calcium, %	0.69
Phosphorus, %	0.38
Sodium, %	4.10
Manganese, mg / kg	97.00
Iron, mg / kg	740.00
Copper, mg / kg	13.50
Zinc, mg / kg	128.00
Cadmium. mg / kg	1.00
Fluorine, mg / kg	3.40
Iodine, mg / kg	1250.00

Table 13 Chemical composition of kelp species Laminaria Digitata

When calculating, it is necessary to take into account the loss of iodine during heat treatment in the amount of 65% of the initial amount of micronutrient in the product (kelp). Evidencebased calculation makes it possible to judge the declared functionality of the product developed when it is used in a certain amount. The data in Table 14 allows to assess the replenishment degree of the daily requirement for iodine using a portion of the product under development.

Micro-	Consumption	Content in 100	)g of product	Content per	Replenishment of
nutrient,	rate for an	due to kelp	taking into	serving of	the daily
units of	adult in the	at 5% of its	account the	product (	requirement for
measure	Russian	introduction	loss of	g), taking	micronutrients by
	Federation		iodine	into	consuming a
			during heat	account	portion of the
			treatment (-	losses	product,%
			65%)		
Iodine,	150-200	minimum	minimum	minimum	
mcg					

Table 14 Evaluation of the iodine content in the developed product

#### **Computational-practical work 8**

#### **Optimization of foods recipe using Microsoft Excel**

Biochemical, physicochemical, and microbiological processes, which are operated by a biotechnological engineer during, depend on many factors. To correctly respond to changes in these factors, a biotechnological engineer should know their influence on the parameter and optimization criterion and possess the process modeling skills. In this case, it becomes possible to correct the technological process using automatic control systems.

Modern computer technology approaches play an important role in improving the technology of products with a complex raw material composition and methods of economic

analysis. There are many formulation options available for the development of a multicomponent product. However, the task for a specialist in this field is to select a recipe with specified parameters from a variety of options (for example, with a minimum cost price, high quality indicators, maximum use of raw materials).

At the first stage of creating a new food product, the primary task is to design the formulation of the product to be developed in such a way that it meets all the consumer's needs. When developing multicomponent food products with several limiting factors, it is difficult to accomplish this task without computer technology. For instance, Microsoft Excel provides various options for recipe calculations of multicomponent food systems.

The most popular tool for solving optimization problems is the standard Microsoft Excel Find Solution Add-in that is included in Microsoft Office. This Add-in allows to effectively solve recipe tasks, and the presentation of results in the form of tables provides information convenient for accounting and reporting. Moreover, the Excel Search Add-ins are as functional as those of special mathematical programs such as MathCAD. All other things being equal, the generally recognized advantage of Excel is the simplicity of the interface and accessibility to the user.

#### Work Order

1. Design a recipe of a product for feeding young children using a Microsoft Excel spreadsheet. The indicators of Table 15 should be used as the initial data for designing the formulation of the infant formula.

Ingradiants	$\mathbf{v}$		Cost rub /kg			
ingredients	$\Lambda_i$	fat	Protein	carbohydrate	water	Cost, Tub./Kg
Skimmed milk	$\mathbf{X}_{1}$	0.1	2.0	4.8	93.1	73
Powdered milk whey	$X_2$	0.3	14.0	67.0	18.7	80.4
Vegetable oils	$X_3$	99.9	0	0	0.1	62
Lactose	$X_4$	0	0	100.0	0	160
Prebiotic dietary fiber	$X_5$	0	0	100.0	0	91.4
Probiotic culture	$X_{6}$	0	75.5	22.5	2.0	113.8
Vitamin complex	$X_7$	0	0	0	0	476.3
Trace elements	$X_{s}$	0	0	0	0	399.1
Stabilizer (0.01%)						
Infant Formula Standard		27.7	10.6	53.9	7.8*	

Table 15 Initial data for the development of the formulation of the infant formula

\* The water content in the infant formula will be: 100 - (27.7 + 10.6 + 53.9) = 7.8%.

2. Using Microsoft Excel, make a table as shown in Figure 2 (with the chemical composition data for the compound formulation components of the mixture. Uncertain factors are the mass fractions of the raw material components of the formulation, which must be determined taking the objective function and several restrictions. In this case, the prime cost of the finished product is selected as a purpose function.

	А	В	С	D	E	F	G	Н
3	Ingredient	x	Mass, kg	fat	Protein	carbohydrate	water	Cost, rub/kg
4	skim milk	X1		0,1	2	4,8	93,1	73
5	dry milk w	X2		0,3	14	67	18,7	80,4
6	Vegetable	Х3		99,9	0	0	0,1	62
7	Lactose	X4		0	0	100	0	160
8	Prebiotic dietary fiber	X5		0	0	100	0	91,4
9	Probiotic culture	X6		0	75,5	22,5	2	113,8
10	Vitamin complex	х7		0	0	0	0	476,3
11	Trace elements	X8		0	0	0	0	399,1
12	Stabilizer (0.01%)		0,01					
13				27,7	10,6	53,9	7,8*	
14								
15	Total:		0,01					
16								
	Infant							
	Formula							
17	Standard	ndard						
18	Target functions, rub						0	
19	Entering ba	alance equa	ations	0	0	0	0	

Figure 2. Initial data for optimizing the formulation of infant formula in Excel

3. In cell C15, present the calculation of the total mass of all components for the mixture according to the following formula: = SUM (C4: C13). In line 19, enter the balance equations, in cells D19 to G19, calculate the mass fractions of fat, protein, carbohydrates and water in 100 kg of the infant formula. For example, the formula in cell D19 will look like this:

= SUMPRODUCT(\$C\$4:\$C\$11;D4:D11)/100

4. Fill the cells E19, F19, G19 by analogy

5. In cell H18, calculate the cost of 100 kg of the mixture as the sum of the products of the mass for a particular type of raw material in terms of its price. Then the formula in the cell takes the form:

= SUMPRODUCT(C4:C11;H4:H11)

6. In line 17, indicate the standard indicators of the infant formula, namely, the content of fat, protein, carbohydrates, and water.

7. After filling in the initial table with the formulas recording, start the Search for solutions function (Menu  $\rightarrow$  Tools  $\rightarrow$  Search for solutions) (Figure 3). A dialog box "Search for solutions" will appear on the screen, in it you will need to select the cell of the objective function (cell H18) - the prime cost of the mixture without considering the cost of the stabilizer - and set it equal to the minimum value. The stabilizer is not taken in the calculation of the cost of the mixture since this ingredient is a constant parameter in the product production.

		А	В	с	D	E	F	G	Н
1									
2						Massanas	2000 V		
3	V	Параметры поиска решения					×	Вода	Цена, руб/кг
4	C							93,1	73
5	C	Оптимизировать целевую ф	VHKUMO: SH\$18				1	7 18,7	80,4
6	Р		511510				-	0,1	62
7	Л	До: О Максимум 🔘	Миниму 🔘 <u>З</u> начен	ния: 0	)			) 0	160
8	п							) 0	91,4
9	п	Изменяя ячейки переменны	IX:					i 2	113,8
10	в	\$C\$4:\$C\$11					<b>1</b>	) 0	476,3
11	Ν							) 0	399,1
12	C	в <u>с</u> оответствии с ограничен	иями:						
13		\$C\$4:\$C\$11 >= 0				<u>До</u> бавит	ь		
14		\$D\$17 = \$D\$19 \$E\$17 = \$E\$10				Измания			
15	V	SFS17 = SFS19				измени	0		
16						⊻далить			
17	C							7,8	r
18	∎					Сбросит	ь		0
19	в							) 0	
20	-				<ul> <li>✓ <u>3</u></li> </ul>	агрузить/сох	ранить		
21		Сделать переменные без	ограничений неотр	ицательными					
22	-	Выберите Поиск ра	ашания налинайных з			-			
25		метод решения:	CELETINA TROUMERTEN	ладач шетодо		Параме	тры		
24									
25		Метод решения							
27		Для гладких нелинейных за ОПГ для динейных задан	адач используйте пои	іск решения н йных задач с	нелинейных	задач метод	ом		
28		негладких задач - эволюци	онный поиск решени	ипах задач с 1я.	imititeee-me	годоні, а для			
29									
30									
31		Справка		Найти	решение	Зак	рыть		
32	μL						_		

Figure 3. Screenshot of the Search for solutions window in Excel

Next, you need to select the changing cells - these are cells containing the masses of certain types of raw materials (C4: C11).

Then, denote the limitations of the function, for example:

• the content of skim milk in the mixture must be greater than or equal to 15% (C4> = 15);

• the content of certain types of ingredients must be greater than or equal to zero (C4: C11 > = 0);

• mass fractions of fat, protein, carbohydrates, and water in 100 kg of the finished product must be equal to the standard values (D17 = D19; E17 = E19; F17 = F19; G17 = G19).

After entering all the parameters, you should activate the "Execute" button in the "Search for solutions" window and obtain the formulation for baby food, optimized according to the prime cost (Figure 4).

	А	В	С	D	E	F	G	Н	
3	Ingredient	x	Mass, kg	fat	Protein	carbohydrate	water	Cost, rub/kg	
4	skim milk	X1	15	0,1	2	4,8	93,1	73	
5	dry milk w	X2	1	0,3	14	67	18,7	80,4	
6	Vegetable	X3	27,70971	99,9	0	0	0,1	62	
7	Lactose	X4	1	0	0	100	0	160	
8	Prebiotic dietary fiber	X5	48,48218	0	0	100	0	91,4	
9	Probiotic culture	X6	13,45695	0	75,5	22,5	2	113,8	
10	Vitamin complex	Х7	1	0	0	0	0	476,3	
11	Trace elements	X8	1	0	0	0	0	399,1	
	Stabilizer								
12	(0.01%)		0,01						
13									
14									
15	Total:		108,6588						
16									
17	Infant Formula Standard			27,7	10,6	53,9	7,8*		
18	Target fun	ctions, rub						9891,47486	
19	Entering ba	alance equa	ations	27,7	10,6	53,9	14,44885		

Figure 4. Results of optimization of the formula for the infant formula in Excel

As a result, cell H18 will automatically calculate the lowest product cost that can be obtained using all the listed food components, considering the specified restrictions. The "Search for a solution" Microsoft Excel can be used for a targeted and prompt calculation the optimal cost of the formula for feeding young children with certain restrictions to the components of the formula of the mixture, as well as for calculating its nutritional and biological value.

### ANNEX 1

### Combined diet for RF military

Product name	Quantity for 1 person per day (g)
Bread from a mixture of peeled rye and	350
wheat flour, 1st grade	
White bread from wheat flour 1 grade	400
Wheat flour 2 grade	10
Various groats	120
Pasta	40
Meat	200
Fish	120
Animal fats, rendered, margarine	20
Vegetable oil	20
Cow butter	30
Cow's milk	100
Chicken eggs	4 pieces per week
Sugar	70
Salt	20
Tea	1,2
Bay leaf	0.2
Pepper	0.3
Mustard powder	0.3
Vinegar	2
Tomato paste	6
Potatoes and vegetables, total:	900
potatoes	600
cabbage	130
beet	30
carrot	50
onion	50
cucumbers, tomatoes, roots, herbs	40
Fruit and berry juices	50
Jelly concentrate	30
Multivitamin preparation "Hexavit"	1

### Norms of physiological needs for energy and nutrients for men

	Indicators, (per day)					Ι	Physical ac	tivity grou	p, (coeffici	ent of phys	sical activit	y)					Men over 60
			I (1.4)			II (1.6)			III (1.9)			IV (2.2)			V (2.5)		
								•	Age group	S				•			1
		18-29	30-39	40-59	18-29	30-39	40-59	18-29	30-39	40-59	18-29	30-39	40-59	18-29	30-39	40-59	-
			-					E	nergy and r	nacronutri	ents					<u>.</u>	
	Energy, kcal	2450	2300	2100	2800	2650	2500	3300	3150	2950	3850	3600	3400	<4200	3950	3750	2300
2	Protein, g	72	68	65	80	77	72	94	89	84	108	102	96	117	111	104	68
	Including animal, g	36	34	32.5	40	38.5	36	47	44.5	42	54	51	48	58.5	55.5	52	34
3	Fat, g	81	77	70	93	88	83	110	105	98	128	120	113	154	144	137	77
4	Carbohydrates, g	358	335	303	411	387	366	484	462	432	566	528	499	586	550	524	335
	Dietary fiber, g									20							
									Vita	mins							
	Vitamin C, mg								Ģ	90							
	Vitamin B1, mg								1	.5							
	Vitamin B2, mg								1	.8							
	Vitamin B6, mg								2	2.0							
	Niacin, mg								-	20							
	Vitamin B12, mcg								3	3.0							
	Folate, mcg								4	00							
	Pantothenic acid, mg								5	5.0							
	Biotin, mcg								4	50							
	Vitamin A, mcg								9	00							
	ret.eq.																
	Beta-carotene, mg								5	0.0							
	Vitamin E, mg current. Equiv. fifteen																
	Vitamin D, mcg		10									15					
	Vitamin K, mcg		120														

-			
		Minerals	
	Calcium, mg	1000	1200
	Phosphorus, mg	800	
	Magnesium, mg	400	
	Potassium, mg	2500	
	Sodium, mg	1300	
	Chlorides, mg	2300	
	Iron, mg	10	
	Zinc, mg	12	
	Iodine, mcg	150	
	Copper, mg	1.0	
	Manganese, mg	2.0	
	Selenium, mcg	70	
	Chromium, mcg	50	
	Molybdenum, mcg	70	
	Fluorine, mg	4.0	

\* For people working in the Far North, energy consumption increases by 15% and proportionally increases the need for proteins, fats and carbohydrates.

### ANNEX 3

## Norms of physiological needs for energy and nutrients for women

	Indicators, (per day)	Physical activity group, (coefficient of physical activity)													
		I (1.4)			II (1.6)			III (1.9)			IV (2.2)				
		Age groups													
		18-29	30-39	40-59	18-29	30-39	40-59	18-29	30-39	40-59	18-29	30-39	40-59		
		Energy and macronutrients													
	Energy, kcal	2000	1900	1800	2200	2150	2100	2600	2550	2500	3050	2950	2850		
2	Protein, g	61	59	58	66	65	63	76	74	72	87	84	82		
	Including animal, g	30.5	29.5	29	33	32.5	31.5	38	37	36	43.5	42	41		
	% of kcal	12	12	12	12	12	12	12	12	12	12	12	12		
3	Fat, g	67	63	60	73	72	70	87	85	83	102	98	95		
	Fat,% of kcal	30	30	30	30	30	30	30	30	30	30	30	30		
	MUFA,% of kcal			•		•		10		•	•			•	
	PUFA,% of kcal	6-10													
	Omega-6,% of kcal	5-8													
	Omega-3,% of kcal	1-2													
	Phospholipids, g	5-7													
4	Carbohydrates, g	289													
	Sugar,% of kcal	<10													
	Dietary fiber, g							20							
		Vitamins													
	Vitamin C, mg							90							
	Vitamin B1, mg							1.5							
Vitamin B2, mg 1.8															
	Vitamin B6, mg	2.0													
	Niacin, mg	20													
	Vitamin B12, mcg	3.0													
	Folate, mcg	400													
	Pantothenic acid, mg							5.0							
	Biotin, mcg							50							

Vitamin A, mcg	900	
ret.eq.		
Beta-carotene, mg	5.0	
Vitamin E, mg	15	
current. Equiv.		
fifteen		_
Vitamin D, mcg	10	15
Vitamin K, mcg	120	
	Minerals	
Calcium, mg	1000	1200
Phosphorus, mg	800	
Magnesium, mg	400	
Potassium, mg	2500	
Sodium, mg	1300	
Chlorides, mg	2300	
Iron, mg	18	
Zinc, mg	12	
Iodine, mcg	150	
Copper, mg	1.0	
Manganese, mg	2.0	
Selenium, mcg	70	
Chromium, mcg	50	
Molybdenum, mcg	70	
Fluorine, mg	4.0	

\* For people working in the Far North, energy consumption increases by 15% and proportionally increases the need for proteins, fats and carbohydrate

#### REFERENCES

- 1. Skurikhin I.M. Tables of the chemical composition and caloric content of Russian food products. M .: DeLiprint, 2007 .-- 275 p.
- 2. Database of the chemical composition of food products: access mode: <u>http://www.intelmeal.ru/</u>
- 3. Norms of physiological needs for energy and nutrients for various groups of the population of the Russian Federation, approved by G.G. Onishchenko dated 12/18/2008 (see Methodological recommendations MP 2.3.1.2432 -08) (in electronic form at link 43:http://narod.ru/disk/start/38.dl36sfnarod.yandex.ru/37395018001/h25bf3a908f248f c90a18b5fe3165f039/Normy2008.pdf

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## Science-based design for foods composition

Учебно-методическое пособие

В авторской редакции Редакционно-издательский отдел Университета ИТМО Зав. РИО Н.Ф. Гусарова Подписано к печати Заказ № Тираж Отпечатано на ризографе

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