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Research Article

Simulation of formulation composition of the enriched spelt cereal products

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Abstract

The article deals with the simulation issues of the formulation composition of the enriched spelt crisp bread and green tea extract. The use of spelt and green tea extract as a raw material in the production of new functional crisp bread is substantiated. In order to optimize the formulation composition of new products, the response surface technique was used. Simulation and processing of experimental data was performed in the environment of Statistica 10 software package (StatSoft, Inc.). On the basis of mathematical simulation methods the optimum mass fractions of green tea extract and table salt – 0.47 and 1.01% respectively were substantiated as components of crisp bread. The enriched crisp bread made on the basis of previously calculated formulation are characterized by the improved organoleptic properties, have the normalized physical and chemical indicators, are characterized by high nutritional and biological values. Prospects for further research are: expansion of the range and scientific and practical substantiation of formulations of new functional crisp bread; production of these products and their comprehensive assessment of quality indicators; development of set of measures for the effective production of new functional cereal products to the consumer market. Practical applications: The proposed method of calculating the optimum composition of new functional cereal products on the example of crisp bread will be useful for representatives of the food industry and can be used in the development of enriched products of different groups of food products.

Keywords: functional product, crisp bread, spelt, green tea extract, optimization, formulation, response surface

Abbreviations: BAS - biologically active substances; BM - bulk mass; Cgte - green tea extract; CQI - complex quality index; Cts - table salt; Mi - weight coefficient; L - linear effect; OE - organoleptic evaluation; Q - quadratic effect; QFD – quality function deployment; SD - swelling degree

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Introduction

Among the various environmental factors affecting the human body nutrition is of paramount importance for its life, adaptation and stress resistance and, finally, determines the duration of not only life, but also active human activity. Unfortunately the quality of the population's nutrition has deteriorated significantly in recent years and this trend continues (Doronin et al. 2009). The consequences of such a nutrition is a violation of the nutritional status of a modern human being, the emergence of hypovitaminosis, reduced immunity, deterioration of physical development, the growth of cardiovascular disease, diseases of the gastrointestinal tract and other non-infectious diseases of alimentary nature (Annual report on the health of the population of Ukraine 2016). One of the reasons for this imbalance is the production of food products by the food industry, which do not meet the recommended standards of rational nutrition in terms of food and biological value. According to analysts the main global trends in the development of food production will be the transition to the development and production of enriched products. The use of only natural ingredients in their production, the maximum extraction of chemical additives from their composition while ensuring high quality and safety. The combination of these characteristics is a prerequisite for high competitiveness of products, its popularity among consumers. In this regard one of the most promising ways of the development of food industry is the production of products with a given chemical composition due to the enrichment with extraction food substances, a wide range of which is contained in natural raw materials of plant, animal and microbiological origin (Moskalenko et al. 2009). The perspective line in the development of manufacture of functional products is creation of the enriched products on the basis of cereals. At the same time ready-to-eat products – crisp bread are of particular interest among consumers, which have good consumer properties, increased shelf life, they are convenient for transportation and consumption, are in demand among different segments of the population. However, not enough attention is paid to the studies aimed at the formation of consumer

properties of functional crisp bread in order to better meet the needs of the target category of consumers. In this regard, taking into account consumer properties, technological capabilities, as well as on the basis of marketing research of the potential consumers and the use of QFD methodology (Mardar et al. 2016), we decided to perform research on the development of new functional crisp bread. Spelt was used as the main raw material for the production of crisp bread. Spelt is a type of soft wheat, which, unlike traditional wheat, is characterized by a high content of proteins, dietary fibers, minerals, vitamins and other biologically active substances (BAS). The content of carbohydrates in spelt is less than in ordinary wheat. But it should be noted that it contains a special type of soluble carbohydrates – mucopolysaccharides, which are able to strengthen the immune system, reduce cholesterol and regulate blood clotting. The protein content in spelt can reach 19.5%, while its digestibility of proteins is 80.1% (for comparison: the digestibility of wheat proteins – 78.9%). A significant advantage of spelt in comparison with genetically close to its soft wheat is much lower content of gluten, which causes celiac disease in humans, to which almost one percent of people is sensitive. Compared to wheat spelt has on average about 30-60% higher content of Fe, Cu, Mg, P, K, Zn, Se. It contains B vitamins, E vitamin and niacin (Hospodarenko et al. 2016; Escarnot et al. 2012; Suchowilska et al. 2012). All this is the evidence of the expediency of development of new functional spelt products. The main objective of the development of the enriched food products is to fill with them the deficit of essential nutrients and BAS, which is observed in the human body. First of all, we have analyzed the actual nutrition of the population of Ukraine, identified its shortcomings and identified the deficit of nutrients and BAS observed in the nutrition of the population. It was established (Annual report on the health of the population of Ukraine 2016; Moskalenko et al. 2009) that there is a shortage of minerals, vitamins and other BAS in the nutrition of the population of Ukraine. Based on this fact it was decided to introduce green tea extract into the composition of

crisp bread. This extract is characterized by a high content of polyphenols – 25-30% (including catechins 10-14%), organic acids (citric, malic, succinic) – 0.5%, amino acids – 6,0%, alkaloids (caffeine, theobromine, theophylline) and 2.5% of carbohydrates (glucose, fructose, sucrose) – 7%, pectin – 4%, it contains B vitamins, ascorbic acid, macroelements (potassium – K₂O, sodium – Na₂O, calcium CaO, magnesium MgO) – 7-10%, microelements: Fe – 130 µg. kg⁻¹, C – 41 µg. kg⁻¹, Zn – 11 µg. kg⁻¹, Mn – 1062 mg. kg⁻¹ (Zhamukova 2016). The use of green tea extract as a vitamin and mineral supplement will regulate the chemical composition of crisp bread in accordance with the modern requirements of the science of nutrition and thus creates competition for food products, which include chemically synthesized food coloring agents and flavors.

Objective and task of research. The objective of the research was to optimize the component composition of spelt crisp bread with the inclusion of green tea extract and table salt. The following tasks were solved for the objective to be achieved:

- 1) To optimize the formulation composition of crispbread with the inclusion of green tea extract, table salt and spelt;
- 2) On the basis of a pre-calculated formulation to assess the quality of the enriched crisp bread (organoleptic, physico-chemical parameters and nutritional value).

Materials and Methods

Materials

Object of study – spelt crisp bread with the inclusion of green tea extract and table salt.

Methods of analysis

Calculation of the optimum composition of new crisp bread was performed in the environment of Statistica 10 software package (StatSoft, Inc., USA). Basically the existing models of formulation optimization are reduced to the problem of linear programming. The objective function is the requirements of the maximum value of the organoleptic evaluation and the output of a single

component, the need for the content of the component of at least the planned value and some additive criterion that takes into account the cumulative effect of several criteria with different weight rates. To optimize the formulation composition of crisp bread, response surface technique was used (Myers et al. 2016). This technique is a set of mathematical and statistical techniques aimed at simulation processes and finding combinations of experimental series of predictors to optimize the response function $\hat{y}(x, b)$, which is generally described by the following polynomial:

$$\hat{y}(x, b) = b_0 + \sum_{i=1}^n b_i x_i + \sum_{k=1}^n b_k x_k^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^n b_{ij} x_i x_j \quad (1)$$

$$BM = b_0 + b_1 \cdot C_{ts} + b_{11} \cdot C_{ts}^2 + b_2 \cdot C_{gte} + b_{22} \cdot C_{gte}^2 + b_{12} \cdot C_{ts} \cdot C_{gte} \quad (2)$$

where – x - change vector, b – parameter vector.

Simulation and processing of experimental data was performed in the environment of Statistica 10 software package (StatSoft, Inc.).

The mass fraction of green tea extract (C_{gte}) and table salt (C_{ts}) was varied in the formulations of the enriched crisp bread. Additives were subjected to screening, magnetic cleaning and dosage. Spelt was previously subjected to peeling under mild conditions (Yegorov et al. 2017) and then to screening, magnetic cleaning and dosage of the prepared dry ingredients, water was added and mixed for 5 minutes until a homogeneous mass was obtained. The obtained mixture was sent to a special device for the production of wholegrain swollen grains, where it was thermally and mechanically processed at a pressure of 2.5...5.0 MPa for 8 seconds. As a result the bread was obtained from spelt with the addition of green tea extract in the form of round briquettes (Fig. 1). Bulk mass (BM, kg/m³), swelling degree (SD, cm³.g⁻¹) were determined in the finished products and organoleptic evaluation (OE, points) was performed. Complex quality index (CQI) which takes into account the cumulative impact of bulk

density, organoleptic characteristics, degree of swelling and weight coefficient (Mi) of the single indicators was also used on calculations. Organoleptic evaluation of crisp bread was performed according to a 20-point scale, which was developed by the authors and set out in methodology (Mardar et al. 2015); volume mass – according to (GOST 15113.1-77); swelling degree – according to (Ostrov et al. 2004).

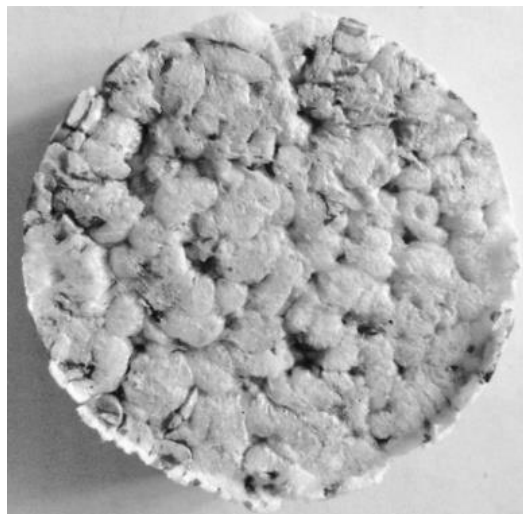


Figure 1. Example of crisp bread with green tea extract

Results and Discussion

Response function was chosen for simulation of bulk mass (BM, kg/m³), swelling degree (SD, cm³·g⁻¹), organoleptic evaluation (OE, points) and complex quality index (CQI), which has the form of a second-degree polynomial:

$$SD = b_0 + b_1 \cdot C_{ts} + b_{11} \cdot C_{ts}^2 + b_2 \cdot C_{gte} + b_{22} \cdot C_{gte}^2 + b_{12} \cdot C_{ts} \cdot C_{gte} \quad (3)$$

$$OE = b_0 + b_1 \cdot C_{ts} + b_{11} \cdot C_{ts}^2 + b_2 \cdot C_{gte} + b_{22} \cdot C_{gte}^2 + b_{12} \cdot C_{ts} \cdot C_{gte} \quad (4)$$

$$CQI = b_0 + b_1 \cdot C_{ts} + b_{11} \cdot C_{ts}^2 + b_2 \cdot C_{gte} + b_{22} \cdot C_{gte}^2 + b_{12} \cdot C_{ts} \cdot C_{gte} \quad (5)$$

where: BM – bulk mass, kg/m³;

SD – swelling degree, cm³·g⁻¹;

OE – organoleptic evaluation, points;

CQI – complex quality index;

b₀ – constant;

C_{ts} – mass fraction table salt, %;

C_{gte} – mass fraction of green tea extract, %;

b₁, b₁₁, b₂, b₂₂, b₁₂ – coefficients for each element of the polynomial.

Central compositional rotatable plan was used in studies (Mancino et al. 2008). The choice of levels and intervals of variation of factors was performed according to the results of the preliminary experiments (Mardar et al. 2016; Mardar and Znacek 2014):

– mass fraction of table salt was varied within 0,5–1,5 %;

– mass fraction of green tea extract was varied within 0,25–0,75 %.

Mass fraction of spelt was determined in such a way that mixture of all raw material ingredients will be 100 %.

Planning matrix and experimental values of their response function are given in Table 1.

Pareto diagrams were built to verify the significance of regression coefficients (2), (3) and (4), which are

$$BM = 468.915 + 394.693 \cdot C_{gte} - 208.591 \cdot C_{gte}^2 \quad (6)$$

$$SD = 6.640 - 0.230 \cdot C_{ts} + 0.162 \cdot C_{ts}^2 - 0.748 \cdot C_{gte} \quad (7)$$

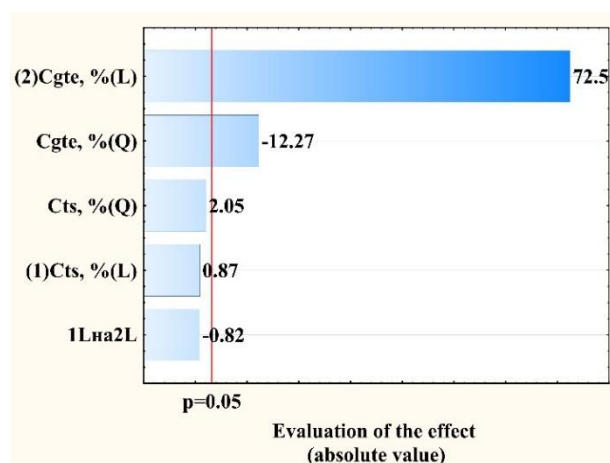
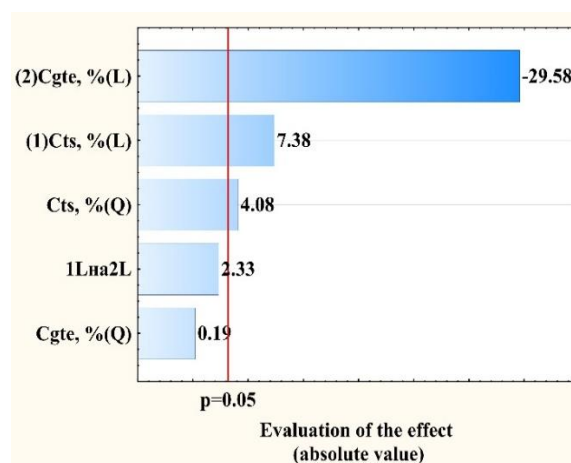
$$OE = -0.254 + 3.795 \cdot C_{ts} - 1.963 \cdot C_{ts}^2 + 11.592 \cdot C_{gte} - 11.835 \cdot C_{gte}^2 \quad (8)$$

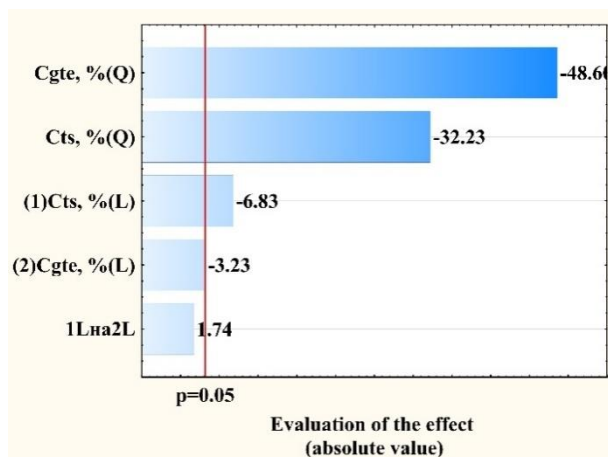
Table 1. Planning matrix and response functions

	Mass fraction of table salt, (<i>Cts</i>)		Mass fraction of green tea extract, (<i>Cgte</i>)		Bulk mass (BM, kg/m ³)	Swelling degree (SD, cm ³ /g)	Organoleptic evaluation (OE, points)
	Coded level	%	Coded level	%			
1	−1	0.65	−1	0.32	574	6.35	3.74
2	−1	0.65	+1	0.67	630	6.02	3.80
3	+1	1.35	−1	0.32	578	6.41	3.67
4	+1	1.35	+1	0.67	632	6.14	3.8
5	−√2	0.50	0	0.5	620	6.20	4.09
6	+√2	1.50	0	0.5	618	6.26	3.88
7	0	1.00	−√2	0.25	550	6.35	3.9
8	0	1.00	+√2	0.75	658	6.03	3.58
9	0	1.00	0	0.5	614	6.20	4.4
10	0	1.00	0	0.5	612	6.18	4.42
11	0	1.00	0	0.5	615	6.21	4.44
12	0	1.00	0	0.5	613	6.20	4.40

Adequacy of the developed models (6), (7) and (8) was verified by analysis-of-variance method. The significance level of the loss of consistency for all three models is $p > 0.05$. The values of determination coefficients for all models are close to one: for model (6) $R^2 = 0.962$ and $R^2_{adj} = 0.953$; for model (7) $R^2 = 0.962$ and $R^2_{adj} = 0.947$; for model (8) $R^2 = 0.932$ and $R^2_{adj} = 0.894$. Consequently the results show that the models describe adequately the experiment. They are shown in Figure 2 (L – linear effect, Q – quadratic effect).

The specified Pareto diagrams (Fig.2) show standardized coefficients, which are sorted by absolute values. The results obtained show that the mass fraction of table salt is linear (C_{ts} , L) and quadratic (C_{ts} , Q), as well as the effect of the interaction of the studied parameters ($1L_{ha}2L$) for regression (2) are significant (columns of evaluation of these effects do not cross the vertical line, which is a 95% confidence probability). Taking into account this fact, the specified regression terms were eliminated from the model (2).

**a)****b)**



c)

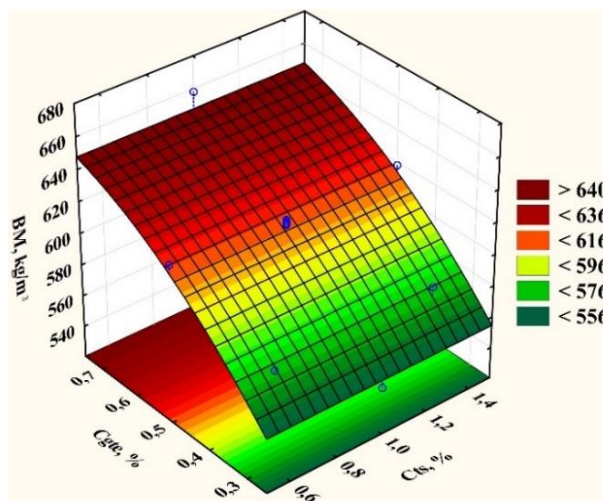
Figure 2. Pareto diagram for verification of significance of the coefficients:

a) – regression (2); b) – regression (3); c) – regression (4)

Mass fraction of green tea extract (C_{gte} , %) and the interaction effect of the studied parameters ($1L_{Ha}2L$) are insignificant for the regression (3) according to the data in Figure 2, b; that is why these regression terms have been eliminated from the model (3). As for the regression (4), one term was eliminated from it – effect of interaction of mass fractions of table salt and green tea extract ($1L_{Ha}2L$), because they are insignificant according to the data in Figure 2.

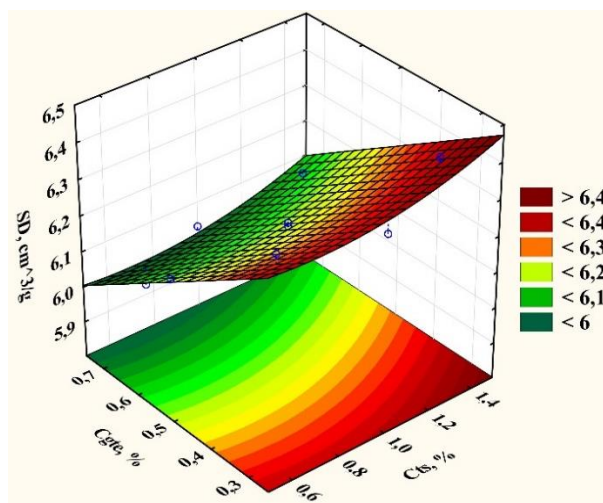
The obtained equations with the calculated coefficients are as follows:

Described by polynomials (6), (7) and (8) the combined effect of the mass fraction of table salt (C_{ts} , %) and green tea extract (C_{gte} , %) to the bulk mass (BM, kg/m^3), swelling degree (SD, $cm^3 \cdot g^{-1}$) and organoleptic evaluation (OE, points) of crisp bread in graphical form is shown in Figure 3 - a, b, c respectively. Increase in the formulation of crisp bread of mass fraction of green tea extract (C_{gte} , %) contributes to a significant increase in a bulk mass (17.1 %). In turn, the increase in the mass fraction of table salt does not almost affect this indicator (Fig. 3 a).



a)

The maximum value of the bulk mass (658 kg/m^3) has crisp bread containing 0.75 % of green tea extract concentrate and 1.0 % of table salt. As for the indicator – swelling degree (SD, $cm^3 \cdot g^{-1}$), there is a decrease in the value of this indicator with increase in the mass fraction of green tea extract (C_{gte} , %) (Fig. 3 b). This is probably due to the decrease in the formulation of crisp bread component (spelt), namely, we note the maximum values of the indicator (SD, cm^3/g) for products containing a minimum mass fraction of green tea



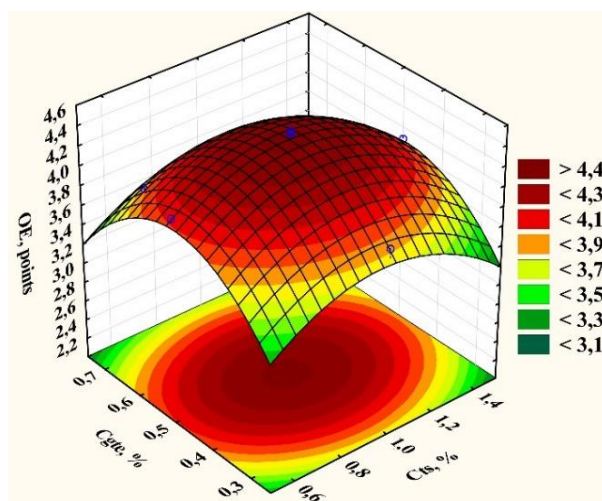
b)

extract. Thus, when the minimum percentage of green tea extract (C_{gte} , %) – 0, 25%, swelling degree is $6.35 \text{ cm}^3 \cdot \text{g}^{-1}$, with a maximum mass fraction of green tea extract (C_{gte} , %) – 0,75%, swelling degree is $6.03 \text{ cm}^3 \cdot \text{g}^{-1}$. With respect to the mass fraction of table salt, there is a slight decrease of swelling degree of crisp bread with increase of its content in the formulation (C_{ts} , %) from 0.5 to 1.0%, which is also explained by decrease in the content of crisp bread component in the initial mixture. Further increase in the mass fraction of table salt from 1.0 to 1.5 % causes a slight increase in the investigated index (SD, $\text{cm}^3 \cdot \text{g}^{-1}$), due to the hygroscopic properties of the salt. Samples of crisp bread have the highest swelling degree, where the mass fraction of green tea extract is 2.5%, and salt – 1.5%.

The quantitative value of organoleptic parameters (OE, points) changes mainly with increase in the formulation of the mass fraction of green tea extract (C_{gte} , %). Increase in green tea extract from 0.25 to 0.75% helps to improve the organoleptic characteristics of the developed products.

Crisp bread was characterized by the correct form, a rough surface, without deformations and tears, of light cream color, with pleasant, clear taste and a smell. Further increase in the mass fraction of green tea extract to 0.75% affects adversely the organoleptic characteristics of crisp bread.

Products were slightly deformed, with minor cracks and fractures at the edges, there were dark spots on the surface, there was too strongly pronounced smell and taste of green tea extract. As for table salt (C_{ts} , %), the changes of the its mass fraction in the formulation slightly affects organoleptic characteristics of rice. The highest organoleptic evaluation – 4.44 points (Fig. 3 c) have samples of crisp bread containing 1.01% of table salt and 0.47% of green tea extract.



c)

Figure 3. Dependence of: a) – bulkmass(BM); b) – swelling degree (SD); c) – organoleptic evaluation (OE) on mass fraction of green tea extract (C_{gte} , %) and mass fraction of table salt (C_{ts} , %)

The obtained results do not allow to determine the optimal mass fractions of raw ingredients. To optimize the formulation of crispbread, a complex quality index (CQI) is used. It is defined as a function of evaluation of single quality indices – bulk mass, swelling degree and organoleptic evaluation (Table 2), converted into a scaled value, taking into account the weight coefficients of individual indicators (M_i) (Tkachenko et al. 2016; Tkachenko et al. 2017):

$$CQI = M_1 \cdot BM_s + M_2 \cdot SD_s + M_3 \cdot OE_s \quad (9)$$

where BMs, SDs, OEs – bulk mass, swelling degree, organoleptic evaluation of crispbread, respectively, converted into scaled values; M_1 , M_2 , M_3 – the weight coefficients of unit indicators-bulk mass, swelling degree and organoleptic evaluation of the products, respectively. In this case (Tkachenko et al. 2016; Tkachenko et al. 2017):

$$\sum_{i=1}^n M_i = 1,0 \quad (10)$$

Table 2. The scaled values of the single indicators and the values of the complex quality index

Number of experiment	Scaled bulk mass (BMs)	Scaled swelling degree (SDs)	Scaled organoleptic evaluation (OEs)	Complex quality index (CQI)
1	3.00	8.62	7.17	6.97
2	7.67	1.00	7.30	6.39
3	3.33	10.00	7.01	7.09
4	7.83	3.77	7.30	6.82
5	6.83	5.15	7.95	7.42
6	6.67	6.54	7.48	7.26
7	1.00	8.62	7.53	7.04
8	10.00	1.23	6.81	6.29
9	6.33	5.15	8.65	7.89
10	6.17	4.69	8.70	7.85
11	6.42	5.38	8.74	8.00
12	6.25	5.15	8.65	7.89

To convert single indicators into the range (1...10), the initial data given in Table 1, are scaled by expression (11) (Tkachenko et al. 2016; Tkachenko et al. 2017):

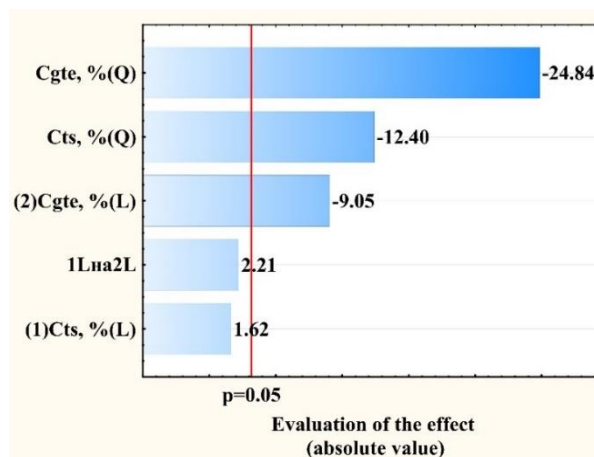
$$y = \frac{(y_{\max} - y_{\min}) \cdot (x - x_{\min})}{x_{\max} - x_{\min}} + y_{\min} \quad (11)$$

where y – the scaled data; x – output data given in Table 1; $x_{\min}$ and $x_{\max}$ – the minimum and maximum values of the output data (for the bulk mass $x_{\min}$ and $x_{\max}$ are calculated according to the model (6).

For swelling degree – according to the model (7). For an organoleptic evaluation $x_{\min}=1$ point, $x_{\max}=5$ points (according to 5-point evaluation). $y_{\min}$ and $y_{\max}$ – the minimum and maximum values of the new range (1 and 10, respectively).

The scaled values of the single indicators and the values of the complex quality index (CQI) calculated according to the expression (9) are given in Table 2 (the following values of the weight coefficients are adopted for the calculation of the CQI: according to the recommendations of the

expert commission: M 1 = 0.10; M 2 = 0.15; M 3 = 0.75). To test the significance of the regression coefficients (5), the Pareto chart is constructed, which is shown in Figure 4 (L –linear effect, Q – quadratic effect).

**Figure 4.** Pareto diagram for verification of significance of regression coefficients (5)

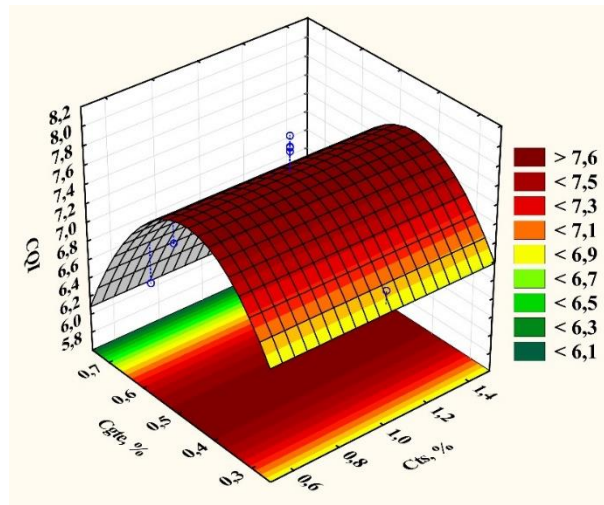
Mass fraction of table salt linear (C_{ts} , L) and the effect of interaction of the studied parameters (1Lon2L) for regression (5) are insignificant (Fig.

4). Taking into account this fact the specified regression terms were eliminated from the specified model. The resulting equation with the calculated regression coefficients is as follows:

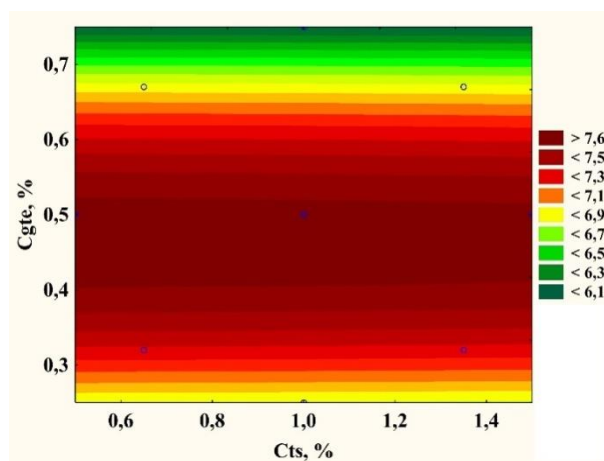
$$CQI = 3,551 - 0,010C_{ts} + 17,817 \cdot C_{gte} - 19,247 \cdot C_{gte}^2 \quad (12)$$

The adequacy of the developed model (12) was tested by analysis-of-variance method. The obtained data, in particular, the absence of consistency loss (significance level $p=0.052$) and the values of determination coefficients ($R^2=0,943$ i $R^2_{adj}=0,921$) close to one, allow us to conclude that the obtained model (12) adequately describes the response. The combined effect of the mass fraction of green tea extract ($C_{gte}, \%$) and table salt ($C_{ts}, \%$) on the complex quality index (CQI) of crisp bread described by polynomial is represented in graphical form in Figure 5. The increase in the formulation of crisp bread of mass fraction of green tea extract ($C_{gte}, \%$) from 0.25 to 0.47% results in increase of CQI. With a further increase in the content of this raw ingredient in the formulation of crisp bread, CQI value decreases (Fig. 5). With an increase in the mass fraction of table salt from 0.5 to 1.5% we note minor changes in CQI (Fig. 5). A more significant effect on the change in CQI is the change in the mass fraction of green tea extract, which is due to the significant influence of this optimization criterion on all the studied response functions (Fig. 3 a, b, c).

Processing of polynomial (12) in Statistica 10 environment allowed to determine the optimum values of mass fractions of green tea extract and table salt – 0.47 and 1.01 %, at which the maximum value of CQI (7,663) is achieved. Organoleptic and physico-chemical criteria of new crisp bread obtained on the basis of a pre-calculated



a)



b)

Figure 5. Dependence of complex quality index (CQI) on mass fraction of table salt ($C_{ts}, \%$) and mass fraction of green tea extract ($C_{gte}, \%$):

a) – response surface; b) – counter plot

formulation are given in Table 3. On the basis of the performed experimental studies it has been established that the developed crisp bread is characterized by improved organoleptic properties, pleasant physical and chemical properties, high nutritional and biological value.

Table 3. Organoleptic and physico-chemical criteria of new crisp bread (n=3, p≤0,05)

Criterion	Criterion characteristic
<i>Organoleptic criteria</i>	
Colour	Even, light cream with slight inclusions of the additives used
Odour	Attractive, strongly pronounced odour of plant components
Appearance	Regular shape, rough surface, without deformations and tears, articles have the respective sizes, characterized by attractive appearance
Taste	Attractive, strongly pronounced taste of the additives used
Structure	Enough crunch, with a developed porosity, without signs of a thorough stirring
<i>Physico-chemical criteria</i>	
Bulk mass, kg/dm ³	613.0±1.0
Swelling degree, cm ³ /g	6.19±0.01
<i>Nutritional value</i>	
Mass fraction of protein, %	15.46±0.23
Mass fraction of starch, %	62.3±0.57
Mass fraction of fiber, %	2.35±0.21
Mass fraction of fat, %	1.8±0.07
Kalium (K)	350±0.21
Calcium (Ca)	43±0.20
Magnesium (Mg)	131±0.19
Phosphorus (P)	405±0.18
Ferrum (Fe)	5.35±0.23

Conclusions

1) The optimum mass fractions of green tea extract and table salt have been substantiated as components of crisp bread – 0.47 and 1.01% respectively.

2) On the basis of experimental studies it has been established that crisp bread produced on the basis of a pre-calculated formulation is characterized by:

- the improved organoleptic properties (have a pleasant, pronounced odour and taste of the additives used, light cream color, regular shape and crunchy, porous structure),
- have normalized physical and chemical parameters – bulk mass of products is 613.0±1.0 kg/dm³ and swelling degree is 6.19±1.0 cm³.g⁻¹ – characterized by high protein content –

15.46±0.23%, fiber 2.35±0.21% and complex of micro-and macroelements.

Prospects for further research are: product-line expansion and scientific and practical substantiation of formulations of new functional crisp bread; manufacture of these products and their comprehensive assessment of quality indicators; development of a set of measures for the effective introduction of new functional grain products into the consumer market.

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