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Mathematical modeling of experimental data in the design of formulas for dairy products

Abstract

Main problem: the article is devoted to the issue of designing basic recipes for dairy products using mathematical modeling methods. The author analyzed the problems in the field of food technology and concluded that mathematical modeling is used in the following areas: clarification of technological process modes, designing recipes and assessing the quality of finished products, as well as predicting the shelf life of new products when they are put into production. The use of dihydroquercetin as a drug that prevents the oxidation of milk fat in the design of dairy products is substantiated. Mathematical modeling was carried out on the basis of experimental and analytical material obtained in laboratory and production conditions. Based on the maximum value of the objective functions, the optimal normalized mixtures and the maximum allowable concentration of dihydroquercetin were selected. The analysis of the received mathematical dependences and models is carried out, the system of linear equations is made.

Purpose: to study the effect of natural bioflavonoid antioxidant on the oxidative processes of milk fat and the viability of lactic acid cultures and their associations by mathematical modeling in order to use it in the technology of a new product; conduct an analysis of mathematical dependencies and models, compose a system of linear equations.

Methods: the article uses the method of mathematical analysis and the matrix method.

Results and their significance: a mathematical model was developed for the dependence of the viability of probiotic cultures on the mass fraction of dihydroquercetin when designing recipes for a creamy-protein curd product, a matrix of the chemical composition of dairy ingredients was presented, and a system of linear equations for basic recipes was compiled. In the course of the study, the spatial configurations of dihydroquercetin, as well as its effect on the oxidative processes of milk fat, were studied. Mathematical modeling of experimental data on the study of the effect of dihydroquercetin on the viability of microorganisms with probiotic properties was carried out. The normalization of the complex of obtained results on the study of the influence of the mass fraction of dihydroquercetin on the fermentation process was studied. Controlled factors characterizing the process of fermentation of model media with dihydroquercetin have been determined. A rationing of the dihydroquercetin complex of more than 0.50% was established; the target function decreases to its minimum value of 0.53 with a mass fraction of dihydroquercetin of 1.00%.

Keywords: mathematical modeling, dihydroquercetin, concentration, objective function, controlled factors, controlled factors.

Introduction

In the food industry, the use of mathematical methods has significantly expanded. This is due to the complication of technological processes, when any technically and economically unjustified solution leads to significant material losses. It is possible to avoid miscalculations in modern production conditions only by applying a strict quantitative assessment of technological processes based on mathematically described patterns of occurring phenomena. The translation of technological problems into a mathematical form allows not only to clarify the essential aspects of the problem itself, but also to significantly reduce the time and cost of solving it. Various mathematical methods are used both in the study and optimization of modes and parameters of various technological processes [1].

A large number of antioxidants of various activity and origin are known in the world. Dihydroquercetin, a biologically active flavonoid from Siberian larch, is known among them. Dihydroquercetin is currently the reference product, i.e. the product with the highest antioxidant activity.

Dihydroquercetin is presented as vitamin P and has the following characteristics: chemical formula - C15H12O7; molecular weight - 304.26; it contains 2,3 - dihydro - 3,5,7 - trihydroxy - 2- (3,4 - dihydroxyphenyl) - 4H - 1 - benzopyran - 4 - OH. The chemical formula of dihydroquercetin is shown in Figure 1.

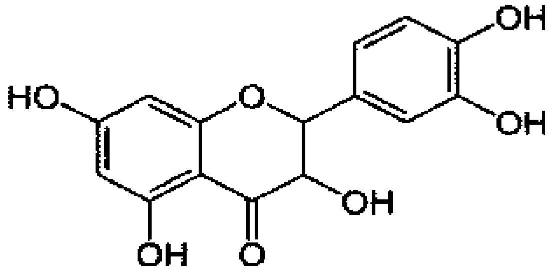

Figure 1 – Chemical formula of dihydroquercetin $C_{15}H_{12}0_7$

There are four spatial configurations of dihydroquercetin – R, R; R,S; S,S; S,R (Figure 2).

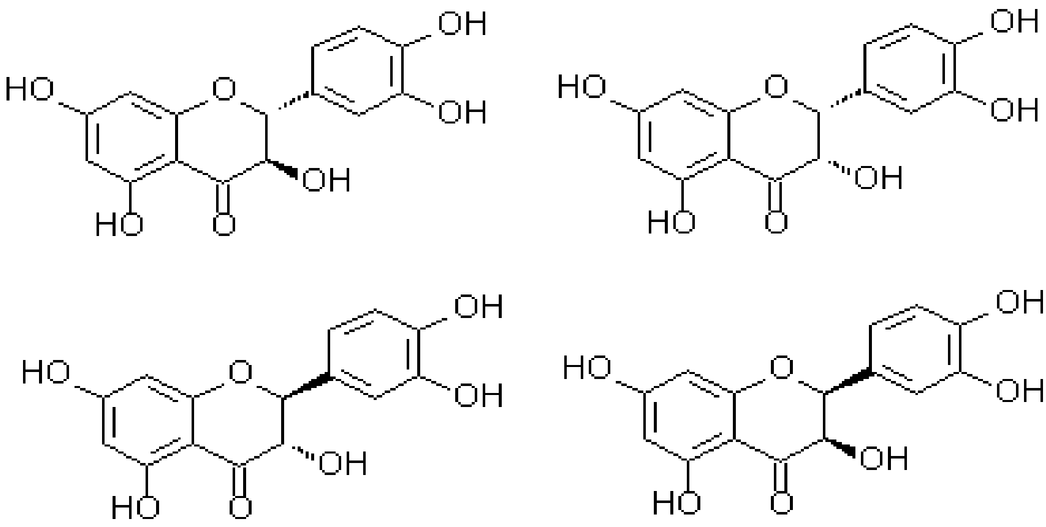

Figure 2 – Spatial configurations of dihydroquercetin

As a substance with a high degree of biological activity, dihydroquercetin, as a P-vitamin, enhances capillary permeability, has a whole range of positive effects on metabolic reactions and the dynamics of various pathological processes in the human body. The doses of dihydroquercetin recommended by doctors, physiologists and biologists as a prophylactic agent in the composition of dietary supplements or food products are 140-160 mg per day [2].

Dihydroquercetin is non-toxic, harmless to humans, has high activity at low concentrations. It does not add extraneous tastes and odors and does not change the color of products, it is resistant to thermal and mechanical influences used in the manufacture of products, that is, it meets all the requirements for all food additives in general and, in particular, for antioxidants. Dihydroquercetin is included in the list of food additives that do not have a harmful effect on human health when used for food preparation [3].

The use of dihydroquercetin as a drug that prevents the oxidation of milk fat must be studied for each dairy product individually, taking into account its chemical composition, the amount of fat component and the production process, since dihydroquercetin can affect their effectiveness. In the technology of curd products, milk fat during heat treatment and mixing comes into contact with atmospheric oxygen, equipment walls, which lead to a decrease in its quality due to the development of oxidative processes. Least of all, this process has been studied in milk cream and fermented products, as a result of which the task was to investigate the effect of a natural bioflavonoid antioxidant on the oxidative processes of milk fat and the viability of lactic acid cultures and their associations in order to use it in the technology of a new product.

Given the above, the topic of this scientific study is relevant and timely.

Materials and methods

Normalization of the complex of the obtained results on the study of the influence of the mass fraction of dihydroquercetin on the fermentation process was carried out according to the maximum value of a homogeneous indicator according to the formula:

$$Y = \frac{Y_i}{Y_{max}}, \quad (1)$$

The objective function was determined by the formula:

$$F_{1-3} = \sum_{n=3}^{n} Y, \quad (2)$$

Given that the duration of fermentation should be minimal, then the normalized value will enter the objective function with a minus sign [4]. Based on the maximum value of the objective functions, the normalized mixtures optimal for further research and the maximum allowable concentration of dihydroquercetin were selected, at which the optimal quality indicators and technological properties of the normalized mixtures are ensured.

Results

Mathematical modeling was carried out on the basis of experimental and analytical material obtained in laboratory and production conditions.

Rationing was carried out according to the following controllable factors presented in Table 1.

Table 1 – Controlled factors characterizing the process of fermentation of model media with dihydroquercetin

$У_i$	Name of factors	Units of measurement	Optimal meaning
$У_1$	Fermentation time	in hours	≤ 8,5
$У_2$	Organoleptic evaluation	in points	→ max (15)
$У_3$	Logarithm of the total number of microorganisms with probiotic properties	Colone-forming units/gram	Not < 8,0

The summary results of experimental studies to determine the main qualitative indicators characterizing the process of fermentation of model media in the presence of dihydroquercetin are shown in Table 2.

Table 2 – Summary of Experimental Data on Fermented Model Media

Experienced sample	Regulated factors	Controlled factors		
	X_1 (mass fraction of dihydroquercetin, %)	$У_1$	$У_2$	$У_3$
Experience 1	0,000	8,0	10,0	9,991
Experience 2	0,063	8,0	11,5	8,908
Experience 3	0,125	8,2	12,0	8,903
Experience 4	0,250	8,3	13,0	8,875
Experience 5	0,375	8,5	13,5	8,778
Experience 6	0,500	8,7	14,5	8,732
Experience 7	0,625	9,0	14,0	8,000
Experience 8	0,750	9,2	13,5	7,903
Experience 9	0,875	9,3	13,5	7,778
Experience 10	1,000	9,6	11,0	7,681

The calculation results of the objective function are presented in the form of Table 3.

Table 3 – Normalization of complex experimental data and calculation of the objective function

Position	Rationing of controlled factors			F_{1-3}
	$У_1$	$У_2$	$У_3$	
Experience 1	0,83	0,69	1,00	0,86
Experience 2	0,83	0,79	0,89	0,85
Experience 3	0,85	0,83	0,89	0,86
Experience 4	0,86	0,90	0,89	0,92
Experience 5	0,89	0,93	0,88	0,92
Experience 6	0,91	1,00	0,87	0,97
Experience 7	0,94	0,97	0,80	0,83
Experience 8	0,96	0,93	0,79	0,76
Experience 9	0,97	0,93	0,78	0,74
Experience 10	1,00	0,76	0,77	0,53

Analyzing the results obtained, the values of the objective function, we can conclude that the optimal concentration of dihydroquercetin is observed in experiment 6 and is 0.50 %. It can be noted that with a mass fraction of dihydroquercetin of more than 0.50 %, the objective function decreases to its minimum value of 0.53 with a mass fraction of dihydroquercetin of 1.00 % Thus, in a normalized mixture, the mass fraction of dihydroquercetin in an amount of 0.50 % is optimal and maximum allowable.

The subject of further analytical studies is to study the dependence of the influence of the mass fraction of dihydroquercetin on the activity and viability of lactic acid microorganisms (L. bulgaricus, S. thermophilus) and bifidobacteria (Bifidobacterium lactis).

Based on a set of experimental data on the process of fermentation of model media, a model of the effect of dihydroquercetin on the activity of cultures with probiotic properties has been developed.

The mathematical description of the established dependence has the form:

$f(x, y) = a + b \cdot x + c \cdot y + d \cdot x \cdot y + f \cdot x^2 + g \cdot y^2$,

Where x – mass fraction of dihydroquercetin, %;

y – fermentation time, hours;

f (x,y) – logarithm of the total amount of microflora;

a, b, c, d, f, g – coefficients.

At the next stage, the formulations of the dairy product were designed. A feature of the technology of the new product is the naturalness of its components: dairy and vegetable. The design of the basic recipe consisted of determining the quantitative ratio of dairy ingredients to ensure that the mass fraction of protein in the new product is at least 10%, the mass fraction of fat is from 5 % to 15 %. To solve this problem, ingredients were used, the chemical composition of which is given in Table 4.

Table 4 – Dairy Ingredients Chemistry Matrix

Ingredients	Mass fraction, %				X_i
	dry substances	including			
		fat	protein	carbohydrates	
Milk protein concentrate	20,0	3,11	10,0	4,3	X_1
Cream with a mass fraction of fat 25 %	32,0	25,00	3,0	4,0	X_2
Cream with a mass fraction of fat 35 %	42,0	35,00	3,0	4,0	X_3
Skimmed milk powder	94,0	1,00	36,0	53,0	X_4

Based on the data given in Table 4, a system of linear equations was compiled for the first basic product recipe (using milk cream with a fat mass fraction of 25%):- by fat ($У_1$): $0,311X_1 + 0,25X_2 + 0,01X_4$;

– for proteins ($У_2$): $0,10X_1 + 0,03X_2 + 0,36X_4$;

– by carbohydrates ($У_3$): $0,043X_1 + 0,040X_2 + 0,53X_4$;

– on dry matter ($У_0$): $0,20X_1 + 0,32X_2 + 0,94X_4$.

The following conditions are accepted in the basic recipe.

For a product with a mass fraction of fat 5 %:
$У_1$ = 5 %;
$У_2$ = 10 %;
$У_3$ – not standardized, that is, in fact;
$У_0$ = 32-33 %.
For a product with a mass fraction of fat 10 %:
$У_1$ = 10 %;
$У_2$ = 10 %;
$У_3$ – not standardized, that is, in fact;
$У_0$ = 38-39 %.
For a product with a mass fraction of fat 15 %:
$У_1$ = 15 %;
$У_2$ = 10 %;
$У_3$ – не not standardized, that is, in fact;
$У_0$ = 45-47 %.

The composition of the recipe in kg/ton is determined by the weight participation of the components and can be represented by the following equation:

$Z_0 = X_1 + X_2 + X_4 = 1000$ (kilogram)

For the second version of the basic recipe for a new product in the equations, instead of cream with a mass fraction of fat 25 %, used cream with a mass fraction of fat 35 %:

– by fat ($У_1$): $0{,}311X_1 + 0{,}35X_3 + 0{,}01X_4$;
– for proteins ($У_2$): $0{,}10X_1 + 0{,}03X_3 + 0{,}36X_4$;
– by carbohydrates ($У_3$): $0{,}043X_1 + 0{,}040X_3 + 0{,}53X_4$;
– on dry matter ($У_{0)}$: $0{,}20X_1 + 0{,}42X_3 + 0{,}94X_4$.

After determining the main recipe, the composition of the recipes will be determined in the assortment with the introduction of functional and flavoring additives.

Discussion

The effect of natural bioflavonoid antioxidant on the oxidative processes of milk fat and the viability of lactic acid cultures and their associations was studied by mathematical modeling in order to use it in the technology of a new product. Mathematical relationships have been established that characterize the viability of cells of probiotic microorganisms on the amount of dihydroquercetin in model media. The analysis of mathematical dependencies and models was carried out, a system of linear equations was compiled.

Conclusion

Analysis of the obtained mathematical dependencies and models allows us to draw the following conclusions:

1. For lactic acid microorganisms (L. bulgaricus, S. thermophilus), the optimal number of cells is observed in areas of response surfaces corresponding to the mass fraction of dihydroquercetin in the fermentation medium of 0.2-0.6 %.

2. The optimal amount of bifidobacteria (Bifidobacterium lactis) in the fermented medium is observed in areas of the response surfaces corresponding to the mass fraction of dihydroquercetin in the fermented medium in the range of 0.2-0.5 % during fermentation for 7.5-8.0 hours.

Based on the results of normalization of experimental data and analysis of mathematical models, the optimal mass fraction of dihydroquercetin (0.5 %) was established, which does not reduce the viability of microorganisms involved in the fermentation of the protein base (L. bulgaricus, S. thermophilus, Bifidobacterium lactis). Therefore, the level of dihydroquercetin in the composition of the product should not exceed the prescribed amount, which will ensure its quality and functional properties.

Thus, on the basis of the ingredients established experimentally, recipes will be drawn up that meet the regulatory requirements for a new product.

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Сүт өнімдерінің формулаларын жобалау кезінде эксперименттік деректерді математикалық модельдеу

Мақала математикалық модельдеу әдістерін қолдана отырып, сүт өнімдерінің негізгі формулаларын жобалау мәселесіне арналған. Автор тамақ технологиялары саласындағы мәселелерді талдап, математикалық модельдеу келесі бағыттарда қолданылады деген қорытындыға келді: технологиялық үрдістердің режимдерін нақтылау, формулаларды жобалау және дайын өнімдердің сапасын бағалау, сондай-ақ оларды өндіріске қою кезінде жаңа өнімдердің жарамдылық мерзімдерін болжау. Мақсатты функциялардың максималды мәніне сүйене отырып, оңтайлы қалыпқа келтірілген қоспалар және дигидрокверцетиннің шекті рұқсат етілген концентрациясы таңдалады. Алынған математикалық тәуелділіктер мен модельдерге талдау жасалды, сызықтық теңдеулер жүйесі жасалды.

Пробиотикалық дақылдардың өміршеңдігінің дигидрокверцетиннің массалық үлесіне тәуелділігінің математикалық моделі кремді ақуызды сүзбе өнімінің формулаларын жобалау кезінде жасалды, сүт ингредиенттерінің химиялық құрамы матрицасы ұсынылды, негізгі формулалардың сызықтық теңдеулер жүйесі жасалды. Зерттеу дигидрокверцетиннің кеңістіктік конфигурацияларын, сондай-ақ оның сүт майының тотығу үрдістеріне әсерін зерттеді. Дигидрокверцетиннің пробиотикалық қасиеттері бар микроорганизмдердің өміршеңдігіне әсерін зерттеу бойынша эксперименттік деректерді математикалық модельдеу жүргізілді. Дигидрокверцетиннің массалық үлесінің ашыту үрдісіне әсерін зерттеу бойынша алынған нәтижелер кешенінің қалыпқа келуі зерттелді. Дигидрокверцетинмен модельдік ортаны ашыту үрдісін сипаттайтын басқарылатын факторлар анықталды. Дигидрокверцетин кешені 0,50% - дан жоғары нормалау белгіленді, мақсатты функция оның ең төменгі мәні 0,53-ке дейін төмендейді.

Түйін сөздер: математикалық модельдеу, дигидрокверцетин, концентрация, мақсатты функция, басқарылатын факторлар, бақыланатын факторлар.

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Математическое моделирование экспериментальных данных при проектировании рецептур молочных продуктов

Статья посвящена вопросу проектирования базовых рецептур молочных продуктов с применением методов математического моделирования. Автором проанализированы проблемы в области пищевых технологий и сделан вывод, что математическое моделирование применяется в следующих направлениях: уточнение режимов технологических процессов, конструирование рецептур и оценка качества готовых продуктов, а также прогнозирование сроков годности новых продуктов при постановке их на производство. На основании максимального значения целевых функций выбраны оптимальные нормализованные смеси и предельно допустимая концентрация дигидрокверцетина. Проведен анализ полученных математических зависимостей и моделей, составлена система линейных уравнений.

Разработана математическая модель зависимости жизнеспособности пробиотических культур от массовой доли дигидрокверцетина при проектировании рецептур сливочно-белкового творожного продукта, представлена матрица химического состава молочных ингредиентов, составлена система линейных уравнений базовых рецептур. В ходе исследования изучены пространственные конфигурации дигидрокверцетина, а также его влияние на окислительные процессы молочного жира. Проведено математическое моделирование экспериментальных данных по исследованию влияния дигидрокверцетина на жизнеспособность микроорганизмов с пробиотическими свойствами. Исследовано нормирование комплекса полученных результатов по изучению влияния массовой доли дигидрокверцетина на процесс ферментации. Определены управляемые факторы, характеризующие процесс ферментации модельных сред с дигидрокверцетином. Установлено нормирование комплекс дигидрокверцетина более 0,50 % происходит снижение целевой функции до ее минимального значения 0,53 при массовой доле дигидрокверцетина 1,00 %.

Ключевые слова: математическое моделирование, дигидрокверцетин, концентрация, целевая функция, управляемые факторы, контролируемые факторы.

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