

PERSONALIZED NUTRITION AND “DIGITAL TWINS” OF FOOD

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ABSTRACT

Mathematization of research is one of the most effective methods of virtual substantiation of foodstuff recipe and technology. This approach allows creating a product that meets consumer's individual needs, i.e. personalized foodstuff (ethnicity, cultural preferences, regional and environmental characteristics, lifestyle), and at the same time reducing the time and cost of decision-making. The article discusses the hypothesis that the “digital twin” of a food product is a virtual model of the product, namely its mathematical model (simulation model). A simulation model is a logical and mathematical description of a food product that is used to conduct a computerized experiment in order to design desired characteristics and properties. The “digital twin” combines all variety of factors from chemical composition, functional and technological properties to organoleptic indicators. The application of the “digital twin” model of the foodstuff will allow: (1) reacting quickly to changes in the composition, properties and types of raw ingredients, (2) adjusting the product recipe in response to changes in consumer preferences, (3) designing products with a given chemical composition, nutritional value and functional orientation, (4) creating functional, specialized products taking into account the metabolism of nutrients (ethnicity, cultural preferences, health status and clinical factors). Products adapted to the needs of small categories of people will help reducing the risks for those who already have diseases, and will meet the needs of those who would like to make their diet more appropriate to individual needs. The proposed approach to creating a model of the “digital twin” of the foodstuff includes several stages. The first stage involves optimization of the nutritional and biological value of the designed product. The second stage is related to designing the food product's structural forms. But even if the recipe of a food product is optimally selected in the first stage, it does not guarantee its transformation during processing into a stable system with the required structural, mechanical, functional and technological parameters. Evaluation of the developed food product's efficiency is possible only by analysing numerous and various parameters and indicators. It is convenient to generalize (convolute) many parameters and indicators into a single quantitative dimensionless indicator. To assess the quality and adequacy of the food product, it is suggested to use an integral indicator in the form of additive convolution – the ‘functional’ of the food product quality.

Keywords: simulation model; personalized nutrition; digital twin; food product; integral indicator

INTRODUCTION

Personalized nutrition pursues the idea of individualization (Ordovas et al., 2018), thus, recommendations and nutritional advice should not be based on the average norms of nutritional intake applied to gender and age groups of population differentiated by the level of physical activity.

Personalized nutrition, as other scientific fields at an early stage, applies many concepts and descriptors, for example, accurate nutrition, multi-layer nutrition, and individual nutrition.

As we move from the stratified to personalized and high-accuracy nutrition, it becomes necessary to apply more and more indicators or characteristics to achieve the desired goal. For example, stratification can be performed using

one or more parameters, such as age, gender, or health status. Personalized nutrition needs to take into account the complexity of relations between the individual diet and phenotype, thus, a wide range of indicators will need to be used to achieve the goal of accurate nutrition, possibly including “big data” approaches.

At this stage of research, the authors adhere to the concept of creating products for the “individually selected diet”.

In 2016, Japan introduced the concept of ‘Society 5.0’, which offers more comprehensive and more advanced application of digital technology in all areas of human life. According to this strategy, advanced technologies, after having been introduced into all spheres of life, should lead to the emergence of new forms and types of business.

One of the Sustainable Development Goals for Society 5.0. is to improve nutrition through the use of 'smart products' produced by advanced biotechnological methods.

To develop "smart" foodstuff that have a functional effect on the human body, levelling the risks of disease, it is necessary to take into account many different factors (physical and chemical, structural and mechanical, functional and technological, etc.). "Playing" with (imitating) all possible structural relations and restrictions is possible only with the use of a virtual product model.

Grievess (2014) in his work notes that the term 'digital twin' appeared in 2003 as part of reading for the discipline 'Product Lifecycle Management' at the Florida Institute of Technology (<https://www.fit.edu/>).

The term digital twin has numerous definitions (Bolton et al., 2018; Claessgen and Stargel, 2012; El Saddik, 2018; Lee, Bagheri and Kao, 2015; Söderberg et al., 2017; Tao et al., 2018).

For a digital twin food product, the definition of Söderberg et al. (2017) is relevant, objective and realistic – 'using a digital copy of a physical system for real-time optimization'.

Solving the problems of an individual (personalized nutrition) taking into account many parameters, such as health status, lifestyle, clinical factors, ethnicity, cultural preferences, etc., may be associated with the development of specialized foods.

The authors of the article propose an approach to building a digital twin food product, using the example of an *anti-sclerotic meat product*.

Scientific hypothesis

This article discusses the hypothesis that the "digital twin" of a food product is a virtual model of this product, namely its mathematical model (simulation model), which combines the whole variety of factors from the chemical composition, functional and technological properties to organoleptic indicators. A simulation model is a logical and mathematical description of an object that can be used for digital experiments on a computer in order to design, analyse and evaluate the functioning of this object (Mukha, 2010).

Using the digital twin of a food product before its launch into mass production, technological engineers can analyse the nutritional, biological and energy value and other characteristics of the product.

The virtual simulation model will allow technologists reacting to changes in the physical and chemical composition of raw materials used or replacement of main or auxiliary raw materials in a real time mode, and accordingly adjusting the recipe to obtain a product with the specified chemical composition and guaranteed quality.

The "digital twin" will allow scientists obtaining interpolation and extrapolation data without conducting additional laboratory studies with a 95% confidence level (or $p < 0.05$)

MATERIAL AND METHODOLOGY

As an example of applying the virtual modelling approach, the task was set to create a digital twin of a meat product for the functional nutrition from the hearts and aortas of pigs, intended for dietary nutrition, in order to reduce the risk of developing and preventing hyperlipidemia and atherosclerosis. Step-by-step scientific experiment and laboratory research have been described (Kotenkova and Chernukha, 2019; Chernukha, Fedulova and Kotenkova, 2018).

Another object was a meat food product enriched with iodine for school-age children.

When designing these products, we are interested in the best solution to the problem, taking into account the metabolism of nutrients (ethnicity, cultural preferences, health status, lifestyle, and clinical factors). The indicator that characterizes the quality of the task is called the objective function or criterion of optimality. The general optimization problem is formulated as follows: to select for variables x_1, x_2, \dots, x_n the appropriate values that provide the extremum of the objective function (Mastyeva, Goremykina and Semenikhina, 2016).

If the objective function and the constraint system are non-linear, the optimization problem is called a non-linear programming problem.

To solve non-linear programming problems, various iterative procedures are used to find the optimum: the gradient method, the coordinate descent method and the steepest descent method.

The software implementation of the models is possible in the universal simulation systems Simplex3, AnyLogic, etc. (Schmidt, 2001; Ivashkin, 2016; Karpov, 2005).

RESULTS AND DISCUSSION

We will consider the mechanism for creating a "digital twin" of a food product, using the example of modelling the recipe and technology of a meat product for elderly nutrition (option 1) and baby food (option 2).

One of the main purposes while creating a functional and/or specialized diet is to provide the nutrients missing in the diet, as well as to reduce the risk of developing and preventing a particular disease.

Formulation of the problem's structural optimization, at different levels of the technology description of the digital twin food product, is reduced to minimizing the deviation of the actual parameters from the specified normative (reference, desired) values by finding a balance for the selected indicators between the input and output flows of the material.

The digital twin of the food product will allow employees of food industry enterprises to respond quickly to changes in the properties and types of raw ingredients, to respond to changes in consumer preferences and to create products with a predetermined chemical composition, nutritional value and functional orientation to a particular category of consumers. The optimal solutions to these problems in the design of food products can be achieved using formalized mathematical descriptions – mathematical models that reflect in an analytical way the set of functional relations between the technological, economic and other parameters inherent to the raw ingredients, the required characteristics of the finished product (objective function or optimization

criterion) and a number of restrictions arising from regulatory documentation requirements.

The first stage is related to the analysis of raw materials.

Option 1 is used to level out pathological processes and reduce the risk of hyperlipidaemia and atherosclerosis.

Based on the initial conditions for the raw meat – protein content at least 18%; fat content not more than 15%; the presence of tissue-specific peptides with molecular weights 809.4 ±1.0, 776.5 ±1.0, 162.1 ±1.0, 156.0 ±1.0, 148.1 ±1.0, 140.2 ±1.0 and 133.1 ±1.0 kDa; the presence of Apo 1 (which participates in the formation of high-density lipoproteins) or the presence of pre-Apo A-1 (which participates in the suppression of oxidative stress) – pork aorta and pork heart were chosen as the main raw material samples.

Option 2 is used to eliminate deficient conditions – hypovitaminosis, lack of trace elements (in particular iodine), leading to the development of a number of diseases. The amino acid methionine (binds 56 – 60% of iodine) must be present for the absorption of iodine from the fatty acid-iodine complex in the human body.

Restrictive parameters for the development of the product formulation for the raw meat are protein content of not less than 16% and fat content of not more than 16%; for vegetable oils – vitamin E of not less than 10 mg; for vegetable raw materials – content of β-carotene of not less than 5 mg; for iodine-containing raw materials – iodine content of not less than 0.1%.

As a result of the operator's work with the database, a list of raw materials of animal and plant origin that can be used in the formulation of an iodine-enriched product under the above boundary conditions was obtained.

For baby food, it is possible to use raw meat such as the first-category beef and pig meat (the choice is related to the main criterion – the presence of amino acids: tyrosine, phenylalanine, proline and histidine; PUFA).

For vegetable oils - soy oil, corn oil, which contains a sufficient amount of linoleic and linolenic acids along with a high content of vitamin E, as well as sunflower oil and peanut oil due to the high content of vitamin E and PUFA.

When choosing a plant component – a source of β-carotene, the choice of red carrots is obvious because of the high content of β-carotene in its composition. Along with this, the amino acid and vitamin composition of carrots contains histidine, phenylalanine, tyrosine and proline, which are necessary for a young body and contribute to better absorption of iodine.

As an iodine-containing raw material, fucus extract is used – a product of brown fucus seaweed processing, obtained by water extraction of brown fucus seaweed (*Fucus vesiculosus* L.), followed by the distillation of the extractant and obtaining a dry extract by spray drying.

Varying the structural ratio of the recipe components within the present restrictions, we see a way of changing the nutritional and biological values of the product, the ratio between protein and fat, etc.

When designing functional products, for example a meat gerodietic product, one of the main restrictions in optimization problems arises from the amino acid conformity criterion of protein that determines the ratio of mass fractions of amino acids such as methionine, cysteine, tryptophan and lysine, taking into account the roles of

isoleucine, leucine, phenylalanine and tyrosine as gerontological competitors of tryptophan (Ivashkin and Nikitina, 2016).

The mathematical record of the criterion is as follows:

$$K = \frac{a_{(Met+Cys)}}{a_{Lys} \cdot C_{Trp}} \cdot \frac{\sum_{j=1}^4 a_{jn}}{\sum_{j=1}^4 a_{j\beta}} = 1$$

Where: K is the coefficient of amino acid conformity, fractional units; $a_{(Met+Cys)}$ and a_{Lys} are the mass fraction of the amino acids methionine + cystine and lysine, g/100 g protein; C_{Trp} is the score of the amino acid tryptophan in the protein of the gerodietic product in relation to the FAO/WHO standard, fractional units; a_{jn} , $a_{j\beta}$ are the mass fractions of the j^{th} amino acids in the protein and the FAO/WHO standard, respectively, g/100 g of protein; and index j identifies, respectively, the amino acids: 1 – isoleucine, 2 – leucine, 3 – phenylalanine and 4 – tyrosine.

Using this criterion (ideally $K = 1$), it is possible to quantify the protein composition of the designed gerodietic products.

The biomedical requirement for gerodietic products in terms of the mass fraction of saturated (SFA), monounsaturated (MUFA) and polyunsaturated (PUFA) fatty acids is that they should correspond to a ratio of 3:6:1. In a mathematical arrangement, the task looks as follows:

$$\sum_{k=1}^7 \sum_{j=1}^m q_{kj} l_j x_j + \sum_{k=8}^{10} \sum_{j=1}^m q_{kj} l_j x_j < 9 \sum_{k=11}^{13} \sum_{j=1}^m q_{kj} l_j x_j$$

Where:

q_{kj} is the mass fraction of the k^{th} fatty acid in the fat of the j^{th} recipe component, %; l_j is the mass fraction of fat in the j^{th} component of the recipe, %; x_j is the mass fraction of the j^{th} fat-containing component of the recipe, %; and the coefficient k is 1 – 7 for SFA, 8 – 10 for MUFA and 11 – 13 for PUFA accordingly.

Meat raw materials are multicomponent and variable in composition and properties. This can lead to significant fluctuations in the quality of the finished product. In this regard, it is very important to know the functional and technological properties (FTP) of various types of basic raw materials and their components, to understand the role of auxiliary materials and the essence of FTP changes under the influence of external factors.

Thus the second stage is related to designing the structural forms of a food product. The optimal formulation of a food product recipe at the first stage does not guarantee its conversion into a stable system with the required structural-mechanical and functional-technological parameters during technological processing.

Foods have individual structural forms (consistency, appearance, binding coherence, texture, etc.) due to peculiarities in the occurrence of protein–protein, protein–water, protein–fat and water protein–fat types of colloidal chemical processes.

Table 1 Major functional and technological properties of some raw meats (Zharinov, 1994).

Type of raw meat	Before thermic processing							
	Moisture-binding capacity, % of the total moisture		Plasticity, $\times 10^{-1} \text{ m}^2/\text{kg}$		Water absorption, % of the initial mass		Fat absorption, % of the initial mass	
	3 mm	Mince cutter	3 mm	Mince cutter	3 mm	Mince cutter	3 mm	Mince cutter
Beef, 2 nd grade	78.0 ±2.8	87.0 ±5.0	9.74 ±0.4	11.76 ±0.8	56.2 ±4.4	55.3 ±3.8	28.4 ±3.0	30.9 ±1.6
Semi-fat pork	73.8 ±6.0	74.6 ±3.8	9.46 ±0.3	11.5 ±0.5	34.9 ±2.3	64.2 ±4.2	22.5 ±1.2	28.6 ±2.1
Fat pork	-	-	10.52 ±0.2	12.31 ±0.3	29.2 ±2.4	32.2 ±2.6	19.8 ±2.0	23.4 ±1.7
Beef honeycomb	49.8 ±3.7	65.4 ±4.2	5.8 ±0.6	7.7 ±0.4	53.2 ±4.4	58.3 ±3.8	26.1 ±2.2	37.8 ±2.5
Beef lungs	94.3 ±1.6	96.0 ±1.2	11.3 ±0.9	11.5 ±0.8	30.6 ±2.8	35.0 ±4.0	25.2 ±2.2	32.8 ±3.1
Beef spleen	66.6 ±3.4	64.2 ±4.0	18.1 ±0.4	18.8 ±0.3	26.0 ±2.0	29.3 ±2.7	16.6 ±1.1	18.2 ±0.8
Beef oesophagus meat	78.2 ±3.3	80.2 ±2.8	8.1 ±0.6	8.7 ±0.4	15.1 ±1.1	16.5 ±1.4	9.8 ±0.9	12.2 ±1.3
Cattle snout	100 ±0.0	100 ±0.0	4.2 ±0.5	4.8 ±0.5	5.1 ±0.6	6.1 ±0.6	9.34 ±0.8	9.8 ±0.4

The protein component of the recipe usually acts as the main structure-forming agent in meat systems (even with its high quantitative content and balanced amino acid composition). Protein can manifest its native properties to various degrees depending on its origin (muscle, connective tissue, vegetable, milk, etc.), structure (fibrillar, globular), environmental conditions (pH, temperature, ionic strength) and many other indicators (degree of raw material mincing, depth of autolytic changes, etc.) (Zharinov, 1994).

To implement the second stage, it is necessary to have information about the actual FTP values of the main raw materials (Červenka, Frühbauerová and Velichová, 2019), auxiliary ingredients, the kinetics of biochemical and colloid-chemical processes (structuring – first of all) in multicomponent food systems, and the analytical and

Along with the introduction of increasingly convenient tools for big data processing and storage, it becomes possible to increase the frequency of use and number of alternatives for creating a digital twin food product, which in its turn increases the reasonableness and feasibility of decisions.

The following mathematical formulas are used to calculate the FTP of multicomponent products:

1) model of the water-binding capacity (WBC):

$$WBC = \sum_{i=1}^N w_i x_i$$

where w_i is the WBC of the i^{th} prescription component;

2) model of the fat-binding capacity (FBC):

$$FBC = \sum_{i=1}^N l_i x_i$$

where l_i is the FBC of the i^{th} recipe component;

3) model of the water-holding capacity (WHC):

$$WHC = \sum_{i=1}^N v_i x_i$$

where v_i is the WHC of the i^{th} recipe component;

4) model of the critical shear stress (CSS):

$$CSS = \sum_{i=1}^N q_i x_i$$

empirical dependencies that characterize the basic laws of heterogeneous dispersed systems with varying physico-chemical factors.

Food product databases now should contain information not only on the main parameters – moisture, protein, fat content, energy value, and amino acid, fatty acid, vitamin and mineral composition, but also on the FTP of raw materials of animal and vegetable origin.

As an example, we give the main characteristics of the FTP of some kinds of protein-containing raw materials (Table 1). They can be used to determine the compatibility conditions of the components in a formulation and optimize the choice of ingredient ratios, taking into account the probability of mutual regulation of the properties both of individual components and of the whole system obtained as a result. where q_i is the value of the CSS of the i^{th} recipe component;

5) model of the dynamic viscosity (η):

$$\eta = \sum_{i=1}^N \frac{V_i x_i}{\eta_i}$$

where η_i is the η of the i^{th} recipe component; and V_i is the volume fraction of the recipe component;

6) model of density (ρ):

$$\rho = \left(\sum_{i=1}^N \frac{x_i}{\rho_i} \right)^{-1}$$

where ρ_i is the ρ of the i^{th} recipe component;

7) model of the active acidity indicator (pH):

$$pH = -\lg \left(\sum_{i=1}^N x_i 10^{-pH_i} \right)$$

where pH_i is the pH of the i^{th} recipe component; and x_i is the mass fraction of the i^{th} recipe component in the formulations presented here under numbers (1) to (7).

The employees of the Russian Research Institute of the Meat Processing Industry (VNIIMP) (<http://www.vniimp.ru>) have developed a method to define WHC, fat holding capacity (FHC) and minced meat stability (MMS):

$$WHC = (Wm_1 M_1 - Mm_2) \cdot 100;$$

$$FHC = (Fm_1 M_1 - Mm_3) \cdot 100;$$

$$MMS = \left[\frac{(m - M)}{m_1} \right] \cdot 100;$$

where W is the moisture content in minced meat, %; F is the fat content in minced meat, %; M is the mass of all separated broth with fat, g; M_1 is the mass of the tested broth with fat, g; m_1 is the weight of minced meat suspension, g; m_2 is the mass of water in the tested broth, g; and m_3 is the mass of fat in the tested broth, g.

The most crucial step in obtaining guaranteed quality in the production of meat products is the heat treatment stage.

To calculate thermograms of heat treatment of meat products, a mathematical model is used that describes a non-stationary field of temperatures containing the product. The mathematical model is a parabolic Fourier's thermal conductivity equation, in cylindrical coordinates with variable coefficients, with specified initial conditions (the initial temperature field in the product before the next stage of processing):

$$\frac{dU(r,t)}{dt} = a \frac{d^2U(r,t)}{dr^2} + \frac{1}{r} \cdot \frac{dU(r,t)}{dr} \quad 0 < r < R, \quad 0 < t < t_k$$

Initial conditions (product temperature before the heat treatment):

$$U(r,t) = U_0 = const, \quad t = 0 \quad 0 < r < R$$

Boundary conditions (on the side surface of the product):

$$\frac{dU(r,t)}{dr} = SU_{cp}(t) - U(R,t), \quad S = \frac{\alpha}{\lambda}, \quad r = R, \quad 0 < t < t_k$$

Conditions for the symmetry of geometry and heating in the center of the loaf

$$\frac{dU(0,t)}{dr} = 0, \quad U(0,t), \quad r = 0, \quad 0 < t < t_k$$

Where: U – current product temperature; U_0 – initial product temperature; U_{cp} – temperature of heating medium; U_k – final product temperature; R – outer product radius; r – radial coordinate; α – heat transfer coefficient; λ – coefficient of thermal conductivity.

Bakery dough is also a complex system where yeast cells produce carbon dioxide during the loosening process. **Stanke, Zettel and Hitzmann, 2014** proposed a model that describes the loosening process by introducing the specific rate of CO_2 production as a variable and biomass as a parameter. Using different amounts of yeast at different temperatures, they modeled the process with an average percentage error of less than 0.5%

$$F(q_{co_2}, \eta, N_b) = \sum_{i=1}^n (V_{rel,i} - \hat{V}_{rel,i})^2 + (P_n - \hat{P}_n)^2 = min$$

where q_{co_2} - CO_2 specific capacity; η - viscosity; N_b – amount of bubbles per volume; $V_{rel,i}, \hat{V}_{rel,i}$ - relative volume of bakery dough; P_n, \hat{P}_n - porosity.

When producing dairy products, functional and structural characteristics must also be taken into account. The research (**Musina et al., 2018**) substantiates the reason for the swelling of whey protein extract in combination with

various berry purees in the recipe of whipped frozen milk dessert at different temperatures.

The third stage is organoleptic assessment of the designed product by expert assessment methods with consistency testing.

Thus, the optimality of various structural options is analysed and verified on the basis of a comprehensive simulation model of a food product, i.e. on the digital twin.

Evaluation of the developed food product's efficiency is possible only by analysing the numerous heterogeneous indicators.

It is convenient to generalize (reduce) a set of indicators into a single quantitative dimensionless indicator. To do this, you have to enter a dimensionless scale for each of them, which must be the same for all the combined indicators. This technique makes them comparable.

One of the most common generalized indicators is the generalized Harrington function (**Harrington, 1965**).

To assess the quality and adequacy of a food product, **Nikitina, Chernukha and Nurmukhanbetova (2019)** used the 'functional' – an integral indicator in the form of an additive convolution.

First of all, the functional determines the compliance with the set requirements for the chemical composition, FTP and organoleptic parameters. The functional reflects the weighted average total deviation of the actual values of the state parameters from the normative values. Taking into consideration the weighting indicators and the allocation of certain groups of indicators, this functional has the following form:

$$F(x) = 1 - \sqrt{\frac{1}{n} \sum_{i=1}^n a_i \sum_{j=1}^{n_i} b_{ij} \left(\frac{x_{ij} - x_{ij}^0}{\Delta x_{ij}^k} \right)} \rightarrow max$$

Where n is the number of joined indicators; x_{ij}, x_{ij}^0 are the actual and desired values; Δx_{ij}^k is the limit deviation from the desired value for the k^{th} level of quality; b_{ij} is the weight coefficient of the j^{th} parameter in the i^{th} group; and a_i is an indicator of the group significance.

The value of the quality indicator changes from 1 (when the obtained values completely coincide with the recommended ones, i.e. best quality) to 0 when the lowest level of quality is reached (limit value), so that in the case of negative values of the functional, the product does not correspond to the specified quality level.

If all the considered indicators n are equal, then weight coefficients are determined by the formula:

$$b_{ij} = \frac{1}{n}$$

When determining weight coefficients at the inequality of weight coefficients one may use the method of expert estimates or the method of full factorial experiment, when columns of the response function (output parameter) y_{kr} of the r -th parallel repetition in the k -th experiment contain values: 1-0.7 – when the product features a very good quality level; 0.7-0.3 – good quality level; 0.3-0 – satisfactory quality level; 0-(-0.2) – poor quality level; less (-0.2) – very poor quality level.

CONCLUSION

When developing products for personalized nutrition, taking into account the metabolism of nutrients, it is necessary to take into account the whole variety of different variables and factors. This is almost impossible in a laboratory scientific experiment, and/or involves a lot of labor. It is possible to choose the optimal version of the recipe when “playing out” various situations in virtual space using a digital (computer, mathematical) model of the foodstuff.

The generalized mathematical model should include not only physical and chemical parameters (fat, protein, etc.), but also knowledge of dependencies of functional, technological, structural and mechanical characteristics that determine the conversion of the optimal formulation in the process of technological processing into a stable system.

Thanks to the use of mathematical modeling methods and a simulation model of the designed product, it is possible to obtain a “digital twin” of the foodstuff. ‘New’ technologies with the help of a digital twin make it possible to take into account the whole range of qualitative and quantitative indicators of meat products to develop recipes for new food products with a complex composition and characteristics, which allow non-drug prevention of diseases. Testing in the virtual world saves time, money and resources for physical scientific experiments.

Using an example of selected meat products, we showed the possibility of creating a digital model of the personalized foodstuff meeting all requirements.

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