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Review

Application of modern computer algebra systems in food formulations and development: A case study

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ABSTRACT

Background: Nutritional security determines the level of public health within a population while inadequate nutrition is one of the major factors in development of various health problems. This can be alleviated with sufficient and affordable access to currently available or newly designed nutritious foods.
Scope and approach: Formulation of new foods can be very costly, so methods able to lower design expanses are of utmost importance to the industry. Hence, the purpose of this work was to rationalize utilization of modern computerized algebraic systems (CAS) in solving traditional problems for formulating food mixtures by food combinatoric principles (FCP).
Key findings and conclusions: Practical aspect of FCP approach was shown in a case of formulating new food with predefined nutritional features (targeting amino acids content) from 14 components (curd and 13 varieties of grains and beans). The application of FCP in CAS saves time and provides mathematically perfect solutions. Such solutions should be tested for supplementary production parameters (sensory, feasibility, etc.) prior to industrial production of large scale quantities.

1. Introduction

Nutritional security is one of the most important indicators in determining the level of public health within a certain population. Inadequate nutrition is regarded as one of the major factors for direct and indirect development of various diseases and morbidities with corresponding mortalities. One of the requirements for nutritional security is the sufficient access to macro- and micronutrients at affordable price. Along with foodborne diseases, micronutrient (e.g., iron, zinc, folate, calcium, magnesium, iodine, and vitamins) deficiencies pose serious problems in all countries irrespective of their developmental level (Alibabić et al., 2014; Kim et al., 2011; Lean, 2015; Shaw, 2016; Tulchinsky & Varavikova, 2014). Hence, various public health interventions are needed that could improve the health status in the general population. Widespread nutritional deficiencies in populations can be prevented or eliminated with regular consumption of essential nutrients (Mannar & Khan, 2016). Enrichment and fortification of foods are useful processing approaches able to deliver necessary nutrients to people. Food fortification is commonly used in developed and developing countries to improve the public nutritional status.

In order to assure the health of their people, national

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governments have the responsibility and principal authority for providing nutritional security through public health policies. For example, the US government revises and reissues "Dietary Guidelines for Americans" every five years for about 322 million people (DeSalvo, Olson, & Casavale, 2016; Flock & Kris-Etherton, 2011; Pérez-Escamilla & Putnik, 2007). In Russia, with its 146 million people, the federal laws define such policy and public health topics for the period until 2020 (The Russian Government issued Resolution No 559R, which approved the Strategy for Development of the Russian Food Industry until 2020). Besides influencing the public health policies, Russian Government issued strategy for the processing industries for the same period of time in order to provide development and implementation of new technologies that are able to produce new generation of products with specific nutritional characteristics (Country Commercial Guide: Russian Federation, 2000).

2. Formulation of food products by food combinatoric principles

Currently, nutritional sciences sufficiently identified the major recommended daily requirements for macro- and micro-nutrients and other relevant principles for obtaining a balanced and healthy diet in population (Lara et al., 2014; Mcclements, Decker, Park, & Weiss, 2009; Montagnese et al., 2015; Péter et al., 2014; Story, Kaphingst, Robinson-O'Brien, & Glanz, 2008). Hence, the next logical step in tackling nutritional scarcity consists of designing affordable foods based on such principles. That is neither a simple nor an affordable task to achieve in food industry, as commonly entirety of the R&D budget is allocated for the new product development. R&D budget is commonly burdened by high failure rate of pilot-food products on the market (Arteaga, Li-Chan, Vazquez-Arteaga, & Nakai, 1994; Filippetti & Archibugi, 2011; Makkonen, 2013; Mulyanto, 2016; Winger & Wall, 2006). New product development depends on the market demands, production price, legislation, and production environment (Granato & de Araújo Calado, 2014). With all such requirements in sight, it is important to optimize formulation of the product(s) prior to manufacturing, aiming at saving the industrial resources as much as possible.

There are various approaches to the food formulations and design (Table 1). In most of the cases, they have a multifactorial character (Bower, 2013) and can be derived from various types of raw materials, additives, etc. Therefore, it is important to note that "food design" in this manuscript primary refers to the process of creating formulations/mixtures that will have tendency to provide desired quantity of certain nutrients in engineered foods. Full factorial, response surface method, Taguchi's orthogonal arrays, mixture designs, etc. are some of the numerous experimental designs used for optimizing formulation of new and existing composite food products (Arteaga et al., 1994; Granato & de Araújo Calado, 2014).

In Russia, one of the main research directions for food design employs food combinatoric principles (FCP) (Kiselev, 2008; Lisitsyn, 2010; Oreshchenko, 1999). The FCP leans to the concepts for balanced composite product design (Lipatov, 1990), where the term "composite products" reflects less to the features of formulations, but more to the optimal and proportionate combination of ingredients in the food mixture (Donskova, 2013). Hence, FCP gives framework for designing food products with required set of nutritional characteristics (Lipatov & Rogov, 1987; Lipatov, Lisitsyn, & Yudina, 1996). For instance, from the set of protein-containing ingredients, it is possible to calculate the optimal food formulations, where the ratio of such ingredients provides a balanced content of amino acids in the product. Amino acid content for ingredients could be easily obtained from nutrient database for a standard reference (Lipatov, 1990).

In order to obtain the desired nutritive features of food mixtures, FCP employs the set(s) of mathematical equations that provide solutions for altering composition of such mixtures, usually by manipulating the weights of the raw materials. Sets of mathematical equations can be expanded according to the production needs. Hence, modern food design methods based on FCP are flexible enough to incorporate new technical approaches for solving complex problems and increase general usefulness for food production (Donskova, 2013).

Manual calculation of new product formulas is time-consuming and daunting task. On the other hand, there are numerous useful programs available for mix/recipe calculations and for composite products design (Datta & Nakai, 1992; Giese, 2003; Goff & Hartel, 2013; Lisin, 2007; Muratova, Tolstyh, Dvoreckij, Zjuzina, & Leonov, 2011; Powers & Hoover, 1989; Reinivuo & Laitinen, 2007). Although the available software can greatly help with food products formulation, it is still only a useful tool that needs to be supplemented with other food technology parameters. This is somewhat expected as mathematical equations do not always produce the most practical solutions. Consequently, final formulations should be carefully evaluated on various parameters, including strongly recommended sensory evaluation. Thus, the main objective of this study is to methodically review and justify the utilization of modern computerized algebraic systems in solving traditional problems in formulating food mixtures by FCP. To achieve this, it was intended to give an overview of: (i) currently available software for food design, (ii) to list the main advantages and disadvantages of the FCP, and (iii) to argument that application of FCP is not warranted without the use of the specialized software.

Table 1
Approaches to food design.

	Design method	Results	References
Optimizing formulation of new and existing composite food products	Full factorial method	Designed mixture	Arteaga et al. (1994); Granato and de Araújo Calado (2014)
	Response surface method	Optimized formula	
	Taguchi's orthogonal arrays	Optimized formula	
Balanced composite product design/food products with required set of nutritional characteristics	Food combinatoric principles	Balanced food mixture with the optimal combination of ingredients	Kiselev (2008); Lisitsyn (2010); Oreshchenko (1999); Lipatov (1990); Donskova (2013); Lipatov et al. (1996); Lipatov and Rogov (1987)
Mix/recipe calculations	Software (programs)	Designed composite product	Datta and Nakai (1992); Giese (2003); Goff & Hartel, 2013; Lisin (2007); Muratova et al. (2011); Powers and Hoover (1989); Reinivuo and Laitinen (2007)