МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ`Я УКРАЇНИ
БУКОВИНСЬКИЙ ДЕРЖАВНИЙ МЕДИЧНИЙ УНІВЕРСИТЕТ

МАТЕРІАЛИ

ІІІ науково-практичної інтернет-конференції

РОЗВИТОК ПРИРОДНИЧИХ НАУК ЯК ОСНОВА НОВІТНІХ ДОСЯГНЕНЬ У МЕДИЦИНІ

м.Чернівці

21 червня 2023 року

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METHODS OF MATHEMATICAL ANALYSIS IN EXPERIMENT PLANNING

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Experiment planning is aimed at optimizing the conduct of research, choosing an experiment plan, methods of analysis to obtain the results of both theoretical and experimental research. The advantages of mathematical planning methods are statistical substantiation of the feasibility of using this research, reducing the number of conducted experiments and obtaining a general tendency to change the studied properties, along with which the costs of the research itself and its implementation are reduced. The use of mathematical planning methods makes it possible to improve the conditions of technological processes, as well as to obtain theoretically predicted results for research that cannot be performed experimentally.

There are a number of software packages that include experimental planning methods, in particular, Statistica, StatGrapfics, Stat-Sens and others, which can be used in modeling research in various directions.

Also, to generalize the results of the study of the additive effect of the synthesis conditions on the studied properties (characteristics), the method of mathematical planning of the experiment is used, namely the method of simplex Scheffe lattices [1-3]. The main premise of the simplex lattice method is the normalization of the sum of independent variables (the sum of the concentrations of all components must be equal to 1). Components can be both pure compounds and their mixtures [3]. Construction of composition-property dependence diagrams is an important part of physicochemical studies of mixture characteristics.

If we consider the Statistica program [4], it is worth highlighting that this program covers a large number of statistical analysis methods (more than 250 built-in functions), combined with specialized statistical modules that provide advanced interactive visualization tools. An important condition is the continuity of the function, which, depending on the number of experimental values covered by it, can be described by a linear, quadratic, cubic or higher order model. The choice of model determines the accuracy of the generalizing function (Fig. 1). For example, to build a mathematical model of the dependence "composition - property" of a three-component system, you can choose the option Ternary Plots, 3D (Mixture designs). The program provides a three-dimensional graphical interpretation of the function of three independent variables and its projection on the plane.

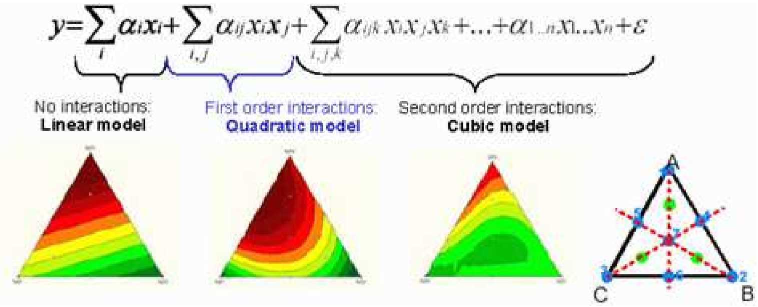

Fig. 1. An example of contour graphs describing the function y in the approximation of a linear, quadratic, and cubic model.

The user can enter the constraints of each factor and the program will automatically construct the corresponding plan on the subsimplex. As standard models use:

- linear: $y = b_1x_1 + b_2x_2 + b_3x_3$ (1.1.)

- quadratic: $y = b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3$ (1.2.)

- special: $y = b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{123}x_1x_2x_3$ (1.3.)

- full cubic models: $y = b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + d_{12}x_1x_2(x_1 - x_2) + d_{13}x_1x_3(x_1 - x_3) + d_{23}x_2x_3(x_2 - x_3) + b_{123}x_1x_2x_3$ (1.4.)

In contrast to the Statistaca program, to optimize the composition of the three-component system according to the Scheffe method, it is possible to use a polynomial of the higher, fourth degree [3] based on a database of 15 points evenly located in a triangle (Fig. 2). The empirical equation describing the dependence of the property on the composition of the three-component system with the approximation of the fourth power has the following form:

$\boldsymbol{y} = k_1\ x_1 + k_2\ x_2 + k_3\ x_3 + k_4\ x_1x_2 + k_5\ x_1x_3 + k_6\ x_2x_3 + k_7\ x_1x_2(x_1 - x_2) + k_8\ x_1x_3(x_1 - x_3) + k_9\ x_2x_3(x_2 - x_3) + k_{10}\ (x_1 - x_2)^2x_1x_2 + k_{11}\ (x_1 - x_3)^2x_1x_3 + k_{12}\ (x_2 - x_3)^2x_2x_3 + k_{13}x_1^2x_2x_3 + k_{14}x_1x_2^2x_3 + k_{15}x_1x_2x_3^2$, (1.5.)

where «y» is the desired property of the studied system.

To check the adequacy of the created model of functional dependence, the Student's test is used, evaluating the variance of the experiment.

So, a researcher who uses mathematical planning methods gets the maximum results with the minimum number of experiments, which will depend on the chosen mathematical model to describe the results of the additive effect of the conditions of the researched properties. The accuracy and visualization of the obtained results will also depend on the chosen model. This approach can be used in various fields of research.

Literature

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