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COTTONSEED OIL DEODORIZATION PROCESS IN MATHEMATICAL MODELING

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ABSTRACT

Planning and modeling is a progressive method of studying chemical and technological processes, which makes it possible to optimize existing technological processes and improve the quality of products [1-4]. The use of these methods in experimental studies significantly reduces the number of studies and provides more reliable results. Not enough research has been done in the direction of planning and modeling of cottonseed oil deodorization processes. Therefore, the study of these issues is of scientific and practical interest.

The relative numbers of repeated observations, or weights as they were called, are rational numbers and satisfy the normalization condition:

$$\sum_{\nu=1}^{n} p_\nu = 1,\ p_\nu \geq 0$$

We would like to emphasize one important circumstance: only those variables whose values can be varied when choosing a plan can act as coordinates of plan points. If the levels of a variable are chosen a priori, then such a variable cannot serve as a coordinate of a plan point. An extremely important role in the design of the experiment is played by the Fisher information matrix, [6,7] or the information matrix of the expression plan M, which for some types of models has been indicated above. Along with this, the standardized (for one dimension) information matrix of the plan is widely used:

$$M(\varepsilon_N) = N^{-1} M$$

The normalized information matrix of the plan is equal to:

$$M(\varepsilon_N) = \sum_{\nu=1}^{n} f(t_\nu)\sigma^{-2}(t_\nu)p_\nu f^T(t_\nu)$$

A similar expression for a multi-response linear model is:

$$M(\varepsilon_N) = \sum_{\nu=1}^{n} F(t_\nu)D^{-1}(t_\nu)p_\nu F^T(t_\nu)$$

And another important concept is the information matrix of single observations at the point of the plan M (t).

For Single-Response Linear Model

$$M(t) = f(t)\sigma^{-2}(t)f^T(t)$$

In the case of a multi-response model

$$M(t) = F(t)D^{-1}(t)F^{T}(t)$$

The information (normalized information) matrix of the plan for uncorrelated observations is a weighted sum of the information matrices of single observations

$$M = \sum_{v=1}^{n} r_v M(t_v), M(\varepsilon_N) = \sum_{v=1}^{n} p_v M(t_v),$$

To characterize the accuracy of parameter estimates of a model built according to the plan, a normalized variance matrix of parameter estimates is used along with the variance matrix of parameter estimates. It is understood as a variance matrix of parameter estimates multiplied by the number of experiments:

$$D\{\varepsilon_N, \hat{\theta}\} = ND\{\hat{\theta}\}$$

The normalized dispersion matrix of parameter estimates is related to the normalized plan information matrix by the ratio

$$D\{\varepsilon_N, \hat{\theta}\} = M^{-1}\{\varepsilon_N\}$$

In the theory of experimental design, the following concepts are also used: normalized variance of estimating the predicted response value in the case of a single-response model

$$d(t, \varepsilon_N) = Nd(t) = f^{T}(t)D\{\varepsilon_N, \hat{\theta}\}f(t)$$

And the normalized dispersion matrix for estimating the predicted vector response in the case of a multi-response model

$$d(t, \varepsilon_N) = Nd(t) = F^{T}(t)D\{\varepsilon_N, \hat{\theta}\}F(t)$$

The plan information matrix and the variance matrix of parameter estimates will depend on parameter estimates. To reflect this circumstance, the plan information matrix, the normalized plan information matrix, and the information matrix of single observations were recorded at the plan point, with the vector of parameter estimates θ additionally indicated in parentheses.

The generalized plans were drawn up as follows. A continuous normalized plan is given by a closed field of action Ωt and a certain probabilistic measure P(t) defined in this area and satisfying the normalization conditions

$$\int_{\Omega_t} dP(t) = 1, P(t) \geq 0, t \in \Omega_t$$

A measure can also be concentrated in a finite number of points, i.e., a normalized plan can be discrete. In this case, the function P(t) can be expressed in terms of the Dirac delta function: [1,3,9]

$$P(t) = \sum p_v \delta(t - t_v)$$

Discrete Normalized Plan E can be written in the same way as εN, but unlike the usual exact plan, it removes the requirement for the rationality of the numbers pv. They only have to meet

the existing conditions of rationing. Continuous and discrete normalized plans were called generalized plans.

Thus, the planning and modeling of the cottonseed oil deodorization technology made it possible to assess the impact of the technological parameters of the process on the quality, physical and chemical characteristics of the resulting product. This property is of great practical value. It means that it is always possible to replace a continuous normalized plan, which has certain extreme indicators of the information matrix, with an equally efficient discrete plan, the spectrum of which contains no more than n0 points.

At present, the method of statistical modeling is widely used to assess the impact of technological parameters of the process on the quality of the resulting product [53, pp.215-345; 54, pp.215-285].

A statistical model is an empirical description of a complex technological process based on the "black box" principle

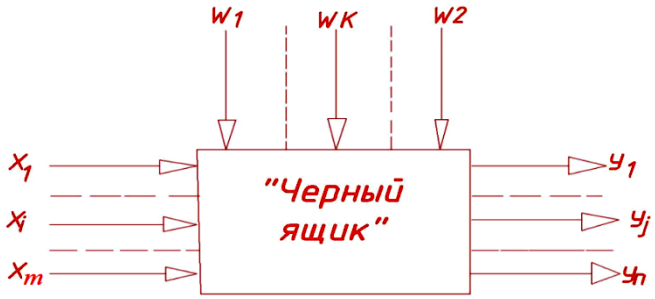

Fig.1. Schematic representation of the modeling object:

xi – input parameters (factors), 1≤x≤m: y – output parameters (Response functions), 1 ≤ i ≤n; Wk – uncontrolled parameters (noise),1≤k≤l

By varying the input parameters and recording the changes in the output (i.e., by conducting an experiment), it is possible to organize these data into equations that relate changes in inputs to changes in outputs.

The division of parameters into input xi-factors, output ui-response functions, and uncontrolled W-k-noise is conditional.

The main task is to improve the quality of products while reducing waste and losses.

Factors: in deodorization – process temperature, pressure; – duration, state of acute steam.

Response functions: in deodorization, the mass fraction of tocopherols in the deodorized oil, the color and yield of the deodorized oil.

Usually, a statistical model is a functional dependence between factors and response functions in the form of power series (Taylor series) or, if the dependence is periodic, trigonometric (Fourier series) [53, pp.215-345].

In technological research, periodic dependence is rarely observed, so we will consider the Taylor power series, which has the form

$$y(x) = y(a) + y'(a)(x-a) + y''(a)\frac{(x-a)^2}{2!} + \cdots + y^n(a)\frac{(x-a)^n}{n!} + \cdots,$$

Taking a *= 0 and denoting* $y^n(a)$=bn, we have a polynomial

$$y(x) = b_0 + b_1x + b_2x^2 + \cdots + b_nx^n + \cdots$$

If the response function of the dependence of two factors is x1 and x2, then an analogous polynomial is of the form

$$y(x_1, x_2) = b_0 + b_1x_1 + b_2x_2 + b_{12}x_1x_2 + b_{11}{x_1}^2 + b_{22}{x_2}^2 + \cdots$$

As the order of the polynomial increases, the accuracy of the description increases, but it becomes more difficult to determine the coefficients (bn), because the more coefficients there are, the more experiments need to be performed. The accuracy of the model is severely constrained by uncontrolled parameters that do not allow for accurate determination of the values of the coefficients (bn). Therefore, it is generally common to use polynomials of no higher than the third order when creating statistical models. Let us consider the relationship between the yield of deodorized oil (factor) and the content of concomitant substances (response function), shown in Figure 2.

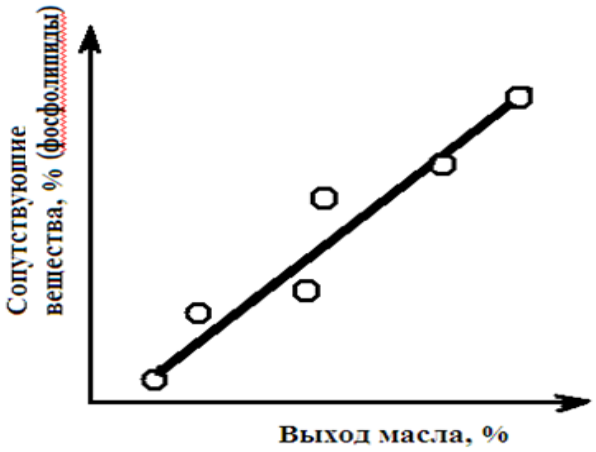

Fig.2. Dependence between the concentration and yield of deodorized oil and the content of co-substances in the oil

The data of the figure indicate that the hanging oil yield is accompanied by an increase in the content of phospholipids in it.

Analyzing the chart, we see that this relationship can be represented by a direct line and, therefore, has the form

$$\hat{y} = b_0 + b_1 x$$

The coefficients b0 *and* b1 *must be selected in such a way that the line described by equation (34) is as close as possible to the experimental points. To find* the coefficients bi, we use the method of least squares, in which these coefficients are chosen in such a way that the sum of the squares of the deviations of the calculated values y from the experiments would be the smallest.

In our case, the sum of squares *s(b0, b1)* will be of the form

$$s(b_0, b_1) = \sum_{i=1}^{N} [y_i - (b_0 + b_i x_i)]^2$$

where I is the experimental value of the response function at point i; xi is the experimental value of the factor at point i; N is the number of experimental points; b0, b1 are the coefficients in equation 34.

To find the minimum of the function (35), we need to equal its partial derivatives of the arguments b0 and b1 to zero.

$$\left.\begin{aligned}\frac{\partial s}{\partial b_0} &= \sum_{i=1}^{N} 2[y_i - (b_0 + b_1 x_i)] = 0 \\ \frac{\partial s}{\partial b_1} &= \sum_{i=1}^{N} 2[y_i - (b_0 + b_1 x_i)] x_i = 0\end{aligned}\right]$$

By revealing the sign of the sum, and transferring the terms that do not contain the coefficients b0, b1, behind the sign of equality, we get a system of linear equations with two unknowns:

$$\left.\begin{aligned} b_0 N + b_1 \sum_{i=1}^{N} x_i &= \sum_{i=1}^{N} y_i\,, \\ b_0 \sum_{i=1}^{N} x_i + b_1 \sum_{i=1}^{N} {x_i}^2 &= \sum_{i=1}^{N} x_i y_i\,,\end{aligned}\right]$$

The advantages of the statistical model include simplicity, which is especially important when studying complex multifactorial technological processes, and high reliability of interpolation (i.e., description of the process within the framework of an experiment).

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