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APPLICATION OF GRADIENT METHOD FOR SOLVING CONSTRAINED OPTIMIZATION TASKS

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Abstract. The constrained optimization task of wool sheepskin tanning–greasing applying the gradient method is solved. The optimality criterion is formulated as a generalized additive objective function. The modified gradient method algorithm is based on software module. Mathematical description for a low-waste technology using dry chrome tanning agent is obtained and its constraints are determined.

Keywords: optimum task, objective function, algorithm, wool sheepskin, tanning.

1. Introduction

Formalization of the problem of chemical engineering and the selection of an optimization method is very challenging as far as most processes are characterized by a large number of physical, chemical, thermophysical and structural parameters, which significantly complicates the task. Difficulties occurring at this stage are, first of all, associated with obtaining the description of the process and the definition of the boundary conditions.

Vast experience in solving optimization problems allows receiving a solution for specific applications [1] as well as in a general form [1, 2]. However, a number of technological problems require special consideration. Quite often under the real conditions of production, the quality of optimization object service is estimated not by one, but by a set of criteria. At the same time, all these criteria are important. This leads to the necessity of finding optimal operating conditions based on a scheme of compromise. Therefore, when choosing a solution for the vector criterion, we can limit the search of the optimum area of compromise. This allows the use of conventional optimization methods for solving multi-objective optimization of chemical engineering for many feasible solutions to get the best ones [3, 4]. This paper deals with the efficiency of the gradient method for the development process of tanning–greasing of wool sheepskin, which is the main in terms of the structure and properties of the finished material. Optimization of tanning – greasing of semi-finished product will significantly reduce the cost of chemicals waste and their concentration in the exhaust solutions and to get wool sheepskin with a given set of physical and mechanical properties.

1.1. Analysis of Studies and Publications

The analysis of publications relating to the development of resource-saving and environmentally efficient technologies in the treatment of cattle hides has shown that the mathematical description of typical processing technologies is mainly obtained using the methods of experimental design [5, 13-15]. The optimization criterion is formed using desirability functions and for the finding of the extremum, the method of scanning is applied [5, 6]. Thus, the search for optimal solutions is based mainly on experimental and statistical approaches, and the general optimization criterion is formed using the Harrington's desirability function.

Such an approach to solving the optimization tasks is related to the complexity of formalizing criteria and requires significant amount of computation. In this case, the choice of the method depends on the experience of the researcher, and in some cases requires special mathematical training. The choice of optimization method and the method of forming the optimality criterion have a significant impact on the quality of the obtained decisions. Using the gradient method [3, 7] allows to achieve the optimum as soon as possible since the gradient vector points in the direction of the fastest growth of the objective function.

1.2. Formulation of the Problem

In this paper we solved the problem of multi-objective optimization process of wool sheepskin tanning–greasing using a dry chrome tanning agent (standards of Ulkraine) which takes into account technological constraints of the parameters and an application of the method of gradient. It involves the replacement of environmentally hazardous industrial oil I-12A as a plasticizer used together with non-ionic surfactants for its emulsification on the sulfonated dipropylene glycol ether (DPGE). The idea of this complex process is to process wool sheepskin with a structuring agent – basic chromium sulfate (BCS) and emulsion DPGE with a molecular weight of 705. Conduction of tanning–greasing process involves the preparation of wool sheepskin by previous acid- salt treatment (pickling) lasting 6–8 h at 313 K and the ratio of water/freshwater sheepskin dry weight of 7/1.

After completing pickling, a plasticizer is added to the system and BCS. In the developed technology the plasticizer I-12A is performed, which is caused by its considerable usage in the process – 10 g/dm^3 with 10 % of surfactant (nonionic surfactants) for its emulsification, while DPGE is a selfemulsifying matter, and as the previous studies have shown, its use can be reduced by more than half due to the high absorption structure of the sheepskin. It is also found that consumption of BCS together with DPGE ranges of 0.9–1.3 g/dm^3 to recalculate for Cr_2O_3, which corresponds to the reduction of costs of chrome tanning agents by 60 %. The effectiveness of the tanning process strongly depends on pH of the working solution, which directly affects its basicity[1] and therefore BCS chemical activity that requires controlled regulation of the technological process. As the acid-salt treatment forms the structure of wool sheepskin before tanning, fluffing it, which subsequently affects the basicity of chrome tanning agents reducing it, these parameters are fixed as technological requirements. This also applies to the concentration of sodium chloride and acid when pickling sheepskin [8]. The mechanism of tanning–greasing process of the intermediate product is in the diffusion of tanning chromium compounds in the structure of a semi-finished product to the active groups of collagen macromolecules with their subsequent reaction with carboxyl groups, the degree of ionization of which is determined by pH of the working solution and the formation of spatial chemical bonds of interacting components. Thus the given set of elastic- plastic properties of the finished wool sheepskin can be achieved only at optimal content of the plasticizer [5, 6]. When using hydrocarbon plasticizer and I-12A in the form of an emulsion, it does not provide a deep diffusion and uniform distribution in the fibrous structure of skin tissue, this requires excessive costs and is associated with high residual concentration in the exhaust solutions. Using hydrophilic DPGE is characterized by a high compatibility with collagen in skin tissue, allowing to achieve high plasticizing effect with its significantly lower costs. Finished wool sheepskin is obtained as a result of drying and moisturizing processes and finishing operations of skin tissue and fur by a model technology at the final stage.

Based on the analysis of the existing technologies the main factors that significantly affect the tanning–greasing process are the concentration of BCS with the specified initial basicity x_1, g/dm^3 Cr_2O_3, and electrolyte resistant sulfonated dipropylene glycol ether (DPGE) x_2, g/dm^3 of fat substances (FS), and pH of the environment at the final stages of tanning x_3 [5].

Since the efficiency of the technology depends not only on the waste of chemical materials at the appropriate manufacturing wool quality, but also on its environmental friendliness, the output variables are: temperature of semi-finished products welding y_1, K; concentration in the exhaust fluid under tannins and DPGE y_2, g/dm^3 Cr_2O_3 and y_3, g/dm^3 FS, the limit of tensile strength y_4, MPa and elongation at full strength of 4.9 MPa – y_5, %.

1.3. Solution for Multi-Objective Optimization Task

An important element in solving the problems of multi-objective optimization is the correct formation of the optimality criterion. In general, the multi-objective optimization task is formulated as follows. The quality of the optimization object is estimated by a vector function

$$f(\bar{x}) = (f_1(\bar{x}), f_2(\bar{x}), \mathbf{K}, f_k(\bar{x})) \qquad (1)$$

the components of which $f_i(\bar{x})$ $(i = 1, 2, \mathbf{K}, k)$ – specified functions of the vector $\bar{x} = (x_1, x_2, \mathbf{K} x_n)$. Linear or nonlinear constraints are usually imposed on the variables x_i $(i = \overline{1, n})$. Thus, the vector $\bar{x}$ belongs to the set X of its possible values. It is needed to find a point that will provide the optimal value of the functions $f_1(\bar{x}), f_2(\bar{x}), \mathbf{K}, f_k(\bar{x})$. Criteria $f_i(\bar{x})$ $(i = \overline{1, k})$ usually have different physical nature and, accordingly, different dimension. Therefore, when solving the problem of multi-purpose optimization, normalization of local criteria is used, with the help of which instead of $f_i(\bar{x})$ value, its relation to some regulatory value, which is measured in

[1] The degree of basicity is the relation of the number of associated with chromium OH groups to the oxidation degree of chromium.

the same units as the criterion itself, is considered [1, 3, 9]. As a result of this operation, all criteria $f_i(\overline{x})$ $(i=\overline{1,k})$ are the dimensionless quantities. In this paper, the dimensionless criteria $f_i(\overline{x})$ are determined by the formula:

$$f_i^*(\overline{x}) = \frac{f_i(\overline{x})}{f_{i\max}(\overline{x}) - f_{i\min}(\overline{x})} \tag{2}$$

where $f_i(\overline{x})$ – value of i criterion.

To solve the problem of multi-objective optimization of the process of tanning–greasing wool sheepskin in the given formulation, the following method for constructing generalized optimality criterion was used:

$$f(\overline{x}) = \sum_{i=1}^{k} a_i f_i^*(\overline{x}) \tag{3}$$

where a_i – weight coefficients, $\sum_{i=1}^{k} a_i = 1$. As a rule, a_i is determined on the basis of expert estimates [2, 3, 5].

To solve the problem of multi-objective conditional optimization (1)–(3) the gradient method was used [2, 7]. The algorithm of the method is shown in Fig. 1. The selected method was applied successfully for solving various problems of nonlinear programming as the extreme value search is performed in the direction of the fastest change in the objective function. The method uses information about the objective function and constraints of the task at every stage.

The formulation of the optimization problem is as follows. Suppose you want to maximize the function

$$f(\overline{x}) = f(x_1, x_2, \mathbf{K}, x_n) \tag{4}$$

where $\overline{x} = (x_1, x_2, \mathbf{K}\, x_n)$ is determined by the explicit constraints:

$$l_j \le x_j \le u_j \;\; (j = 1, 2, \mathbf{K}, n) \tag{5}$$

and implicit constraints:

$$q_i(\overline{x}) \le b_i \;\; (i = 1, 2, \mathbf{K}, m) \tag{6}$$

The method of gradient indicates the direction of the fastest growth of the objective function. In this paper, the method was modified taking into account technological constraints (5) and (6).

The first stage involves finding acceptable initial point. The point that satisfies the conditions (5) and (6) is allowable.

The initial allowable point $\overline{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \mathbf{K}, x_n^{(0)})$, if possible, can be specified, or the following formula can be used:

$$x_j = l_j + r_j(u_j - l_j), \; (j = 1, 2, \mathbf{K}, n) \tag{7}$$

where r_j – random numbers uniformly distributed in the interval (0; 1).

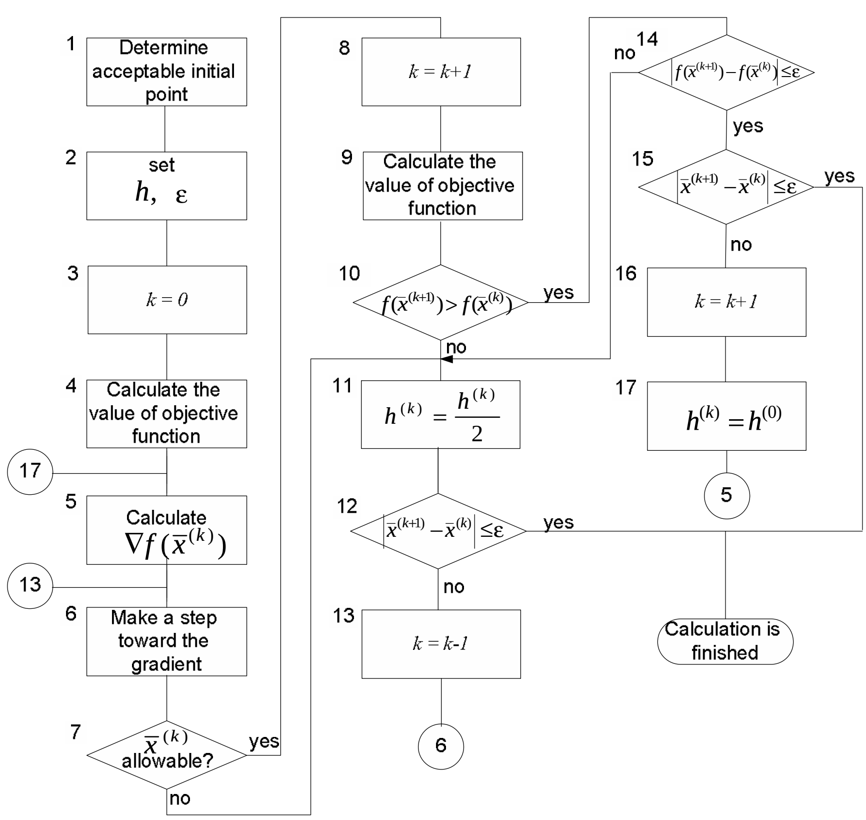

Fig. 1. Algorithm of the gradient method

Thus, the point obtained is checked for permissibility by calculating the function $q_i(\bar{x})$, ($i = 1, 2, \mathbf{K}, m$) within the limits (6). The process continues until the point is found that satisfies all the constraints of the task. At this stage, as well, the precision of optimization e, the magnitude of the stage in the direction of the gradient $h^{(0)}$ and the number of optimization stages, $k = 0$, are set.

At the second stage, the value of the objective function $f(\bar{x}^{(k)})$ and partial derivatives value $\nabla f(\bar{x}^{(k)})$ of all variables at the point $\bar{x}^{(k)}$ are calculated:

$$\frac{\partial f(\bar{x}^{(k)})}{\partial x_1}, \frac{\partial f(\bar{x}^{(k)})}{\partial x_2}, \ldots, \frac{\partial f(\bar{x}^{(k)})}{\partial x_n} \qquad (8)$$

At the third step, the direction of movement toward the gradient is changed. The coordinates of the new point are calculated by the formula:

$$x_j^{(k+1)} = x_j^{(k)} + h^{(k)} \frac{\partial f(\bar{x}^{(k)})}{\partial x_j} \; (j = 1, 2, \mathbf{K}, n) \qquad (9)$$

and calculate the value of the function $f(\bar{x}^{(k+1)})$.

At the fourth stage $f(\bar{x}^{(k)})$ and $f(\bar{x}^{(k+1)})$ are compared:

– if $f(\bar{x}^{(k+1)}) < f(\bar{x}^{(k)})$, then the initial value of the stage is reduced by half $h^{(k)} = \frac{h^{(k)}}{2}$ and the calculations are repeated, starting from the third stage;

– if $f(\bar{x}^{(k+1)}) > f(\bar{x}^{(k)})$, then the stage toward the gradient is successful, and the conditions of the end are checked: $|\bar{x}^{(k+1)} - \bar{x}^{(k)}| \le e$.

If the inequality is performed, the calculation is stopped, otherwise the iteration number is increased by one: $k = k + 1$, $h^{(k)} = h^{(0)}$ and the calculations of the second stage are repeated.

2. Experimental

The described algorithm was the basis for the software module that is implemented using object-oriented programming language "Visual Basic for Application". The developed software module is used to find the optimal values of the generalized objective function.

Table 1

Experiments plan

Factor	Experimental point																			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
x_1	+	–	+	–	+	–	+	–	+α	–α	0	0	0	0	0	0	0	0	0	0
x_2	+	+	–	–	+	+	–	–	0	0	+α	–α	0	0	0	0	0	0	0	0
x_3		+	+	+	–	–	–	–	0	0	0	0	+α	–α	0	0	0	0	0	0

Note: the correspondent levels +1 i –1 are marked by the signs "+" and "–", and the value of an axial distance is α = 1.682.

Table 2

Experimental results

Output variable	Experimental point									
	1	2	3	4	5	6	7	8	9	10
y_1	82.0	67.0	80.0	66.0	73.0	62.0	74.0	63.0	84.0	53.0
y_2	0.23	0.07	0.18	0.05	0.32	0.10	0.39	0.07	0.38	0.01
y_3	0.31	0.39	0.07	0.11	0.22	0.34	0.06	0.09	0.13	0.38
y_4	13.3	15.0	13.9	14.1	14.4	14.6	13.0	12.4	12.1	11.0
y_5	32.0	28.0	25.0	23.0	42.0	29.0	34.0	26.0	24.0	18.0
y_i	11	12	13	14	15	16	17	18	19	20
y_1	76.0	74.0	78.0	65.0	75.0	76.0	76.0	75.0	76.0	74.0
y_2	0.07	0.09	0.04	0.26	0.08	0.06	0.07	0.08	0.06	0.05
y_3	0.47	0.02	0.10	0.02	0.06	0.04	0.05	0.05	0.04	0.06
y_4	15.0	13.1	14.0	11.7	14.5	14.7	14.8	14.6	13.9	14.3
y_5	49.0	27.0	40.0	47.0	45.0	44.0	43.0	43.0	45.0	42.0

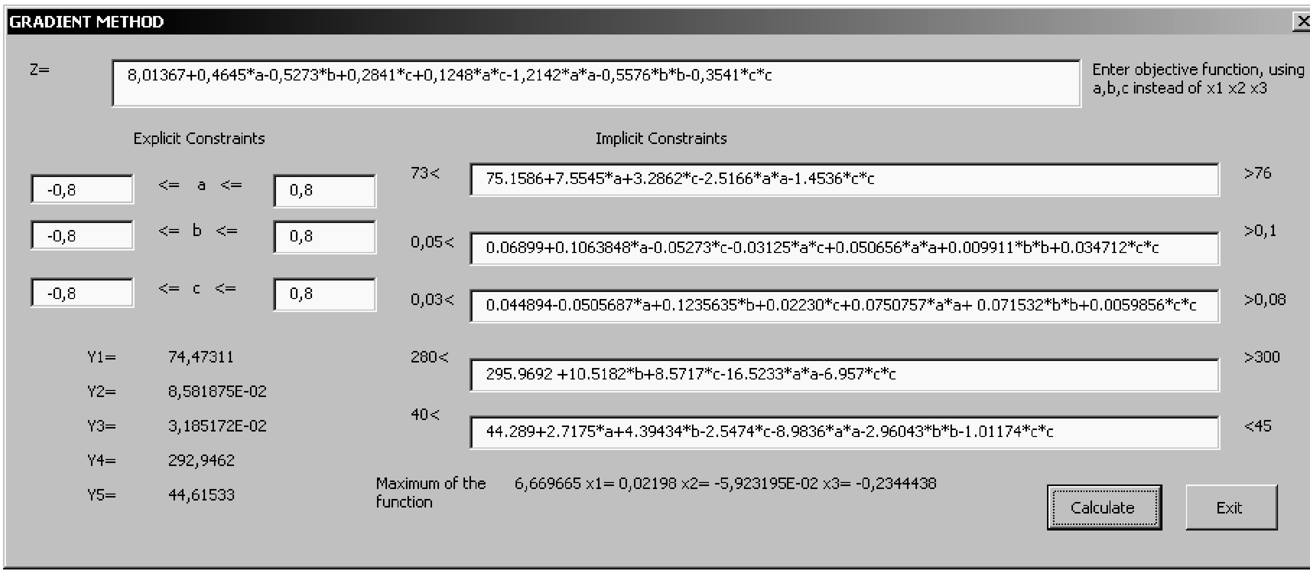

Fig. 2. Main window of software module

The task of determining the optimal composition of the ternary mixture that is used in tanning-greasing of wool sheepskin was considered as the task of nonlinear programming. The meaning of the factors X_1, X_2, X_3 varied at two levels with the correspondent interval: 0.5, 1.0, 0.25, and a plan center is situated in a factor space with the point: 1.0, 4.0, 3.5.

3. Results and Discussion

Experimental results of the technological parameters research of wool sheepskin treatment influencing the physical and chemical properties of the finished wool sheepskin are given in Table 2.

The developed software module is applied in the study of low-waste technology of semi-finished leather tanning [10]. The main window of nonlinear programming software is presented in Fig. 2 and makes it possible to visualize the initial data and the obtained results of calculation. When developing a software module, the ability to work with explicit and implicit constraints and calculation unit of statistical indicators to assess the adequacy of the model is provided.

The mathematical description of the process of tanning was obtained from the composite Box-Hunter central rotatable plan of the second order of 6 experimental points in the center of the plan and presented by the following regression equation [11]:

$$y_1 = 75{,}1587 + 7{,}5545x_1 + 3{,}2862x_2 - 2{,}5166x_3 - 2{,}5166x_1^2 - 1{,}4537x_3^2$$

$$y_2 = 6{,}8995\cdot10^{-2} + 0{,}1064x_1 - 5{,}27382\cdot10^{-2}x_3 - 0{,}03125x_1x_3 + 5{,}0657\cdot10^{-2}x_1^2 + 9{,}9113\cdot10^{-3}x_2^2 + 3{,}4713\cdot10^{-2}x_3^2$$

$$y_3 = 4{,}4894\cdot10^{-2} - 5{,}0568\cdot10^{-2}x_1 + 0{,}1236x_2 + 2{,}2309\cdot10^{-2}x_3 + 7{,}5076\cdot10^{-2}x_1^2 + 7{,}1533\cdot10^{-2}x_2^2 + 5{,}9857\cdot10^{-3}x_3^2$$

$$y_4 = 295{,}97 + 10{,}5183x_2 + 8{,}5718x_3 - 16{,}5234x_1^2 - 6{,}957x_3^2$$

$$y_5 = 44{,}289 + 2{,}7175x_1 + 4{,}3943x_2 - 2{,}5475x_3 - 8{,}9837x_1^2 - 2{,}9604x_2^2 - 1{,}0117x_3^2$$

Checking the adequacy of the obtained equations was performed by the Fisher's criterion. The calculation results show that the resulting equation describes the abovementioned experimental data rather precisely, that is the calculated Fisher criterion value does not exceed the ones given in the Table.

The restriction of the optimization task is selected according to technological reasons:

$$\begin{array}{lll} & & 73 < y_1 < 76 \\ 0.9 < x_1 < 1.3 & & 0.05 < y_2 < 0.1 \\ 3.7 < x_2 < 4.2 & & 0.03 < y_3 < 0.08 \\ 3.6 < x_3 < 3.8 & & 280 < y_4 < 300 \\ & & 40 < y_5 < 45 \end{array}$$

Based on the requirements of the process, both technological and economic, the output values y_1, y_4, y_5 are maximized and y_2, y_3 are minimized.

To calculate the weighting coefficients the method of peer review is used, namely ranking method [12], which is based on assigning by experts the individual factors that affect the process with a sequence number of their importance. In this case, the most important criterion is assigned with number one, then the second one, *etc*. These ranks are converted as follows: rank 1 receives an estimate m (the number of partial criteria), rank 2 – assessment of $m-1$, *etc*. denoting the estimates r_{tk} (where i – number of i-th expert, k – number of k-th criterion). The results of the expert survey were entered into a spreadsheet and the total score for each criterion was counted:

$r_i = \sum_{j=1}^{L} r_{ji}$, $(i = 1, 2, \mathbf{K}, m)$, where L – the number of experts.

The weights for each criterion are defined as follows: $a_i = \frac{r_i}{\sum_{i=1}^{m} r_i}$ $(i = 1, 2, \mathbf{K}, m)$.

According to this method the processed results of the survey of seven experts in this field were used. The weight coefficients of the function a_i are derived from expert ratings a_1 = 0.2; a_2 = 0.2; a_3 = 0.3; a_4 = 0.15, a_5 = 0.15. The generalized objective function is obtained by the formula (3), where $f_i^*(\overline{x}) = y_i^*$, and $y_i^* = \frac{y_i}{y_{i\max} - y_{i\min}}$:

$$f(\overline{x}) = 8.0137 + 0.4645x_1 - 0.5273x_2 + 0.2841x_3 + \\ + 0.1248x_1x_3 - 1.2142x_1^2 - 0.5576x_2^2 - 0.3541x_3^2.$$

According to the formulated optimization task, the derived generalized objective function is maximized.

As a result, the optimum values of the factors and output variables that meet these criteria are found: x_1 = 1.20; x_2 = 3.46; x_3 = 3.71; y_1 = 75.912; y_2 = 6.86·10^{-2}; y_3 = 3.83·10^{-2}; y_4 = 296,24; y_5 = 43,82.

Thus, as a result of the conducted calculations, the optimal values of the parameters of the process of wool sheepskin tanning–greasing and corresponding values of the objective function are found.

In this way, the extremum of the objective function found with regard to the conditions (5) and (6). Thus, the gradient method can be effectively used to solve the tasks of conventional optimization.

The disadvantages of this method include the need to find partial derivatives of the objective function, which complicates the programming and requires appropriate mathematical manual training. In some cases, the objective function is not given analytically, which is quite typical for the problems of chemical technology, then the partial derivatives that define the gradient can be calculated in the desired points with approximation by replacing them with respective difference relations:

$$\frac{\partial f}{\partial x_i} \approx \frac{f(x_1, \mathbf{K}, x_i + \Delta x_i, \mathbf{K}, x_n) - f(x_1, \mathbf{K}, x_i, \mathbf{K}, x_n)}{\Delta x_i}$$

Thus Δx_i is not recommended to be too small, and the value of the function should be calculated with a sufficiently high precision exponent, otherwise when calculating the difference $\Delta f = f(x_1, \mathbf{K}, x_i + \Delta x_i, \mathbf{K}, x_n) - f(x_1, \mathbf{K}, x_i, \mathbf{K}, x_n)$, a significant error may appear.

4. Conclusions

The problem of multi-objective optimization of conventional wool sheepskin tanning greasing process using the method of gradient is solved and the parameters of the process to ensure the maximum output of semi-finished product by area are set.

The optimality criterion for chrome tanning process of semi-finished product represented as a generalized objective function for which the calculation with the values of weight coefficients, provided by experts, is made. According to the chosen criterion the optimum values of the process of wool sheepskin tanning are determined.

The proposed algorithm of a modified method of gradients, which is in the basis of the developed software module can significantly reduce the time of searching an optimal solution and can be used without a fundamental change to determine the optimal parameters of similar technological processes.

The developed technology allowed to replace environmentally hazardous industrial oil plasticizer I-12A at substantially reduced costs of hydrophilic plasticizer – the sulfonated dipropylene glycol ether without a surfactant and gives a wool sheepskin high plasticity. In this case, almost complete absorption of chromium tannins and greasy substances from the working solution are achieved, which increases the sustainability of the developed technology of the wool sheepskin processing.

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ЗАСТОСУВАННЯ МЕТОДУ ГРАДІЕНТА ДЛЯ ВИРІШЕННЯ ЗАДАЧІ ОПТИМІЗАЦІЇ

Анотація. *Розв'язано задачу багатокритеріальної умовної оптимізації дублення-жирування хутрової овчини із застосуванням методу градієнта. Критерій оптимальності сформульований у вигляді узагальненої адитивної цільової функції. Алгоритм модифікованого методу градієнта покладений в основу програмного модуля. Отримано математичний опис для маловідхідної технології з використанням хромового дубителя і пластифікатора з визначенням обмежень на технологічні параметри процесу.*

Ключові слова: *задача оптимізації, цільова функція, алгоритм, хутрова овчина, дублення.*