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Mathematical modeling of a three-component system to investigate the formation and characteristics of glass

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Abstract. The article investigates glass formation and its properties in a three-component system using mathematical modeling. The authors have applied the method of mathematical planning to increase the efficiency of research and to establish the dependences of glass properties on the composition. The authors propose a mathematical model of structure relaxation and two-dimensional stress field in grade glass products, considering the temperature dependencies of glass viscosity of a given chemical composition.

1 Introduction

Modern industries pay more and more attention to the use of automated data processing systems. Modern technological processes require considerable material and time expenditures. Many productions cannot be without the prior creation of process models. An example of such products can be glass melting. This area has a lot of competition and other problems of unsatisfactory design of production technology.

The choice of insufficient parameters of technological process, such as charge composition, temperature, and pressure of glass melting, caused tons of glass not satisfying the output parameters to be melted down. This leads to equipment downtime and huge losses.

Theoretical-experimental methods are an assumed structure or development of a theory with subsequent verification by experiment, refinement, and determination of necessary parameters.

Conducting experiments often requires considerable financial expenses and a long time. To prepare for experiments, it is necessary to use a mathematical approach aimed at minimizing the number of experiments without loss of quality and reliability of the results [1, 2].

The solution to this problem is the mathematical planning of experiments and the application of specific practical tasks.

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2 Methodology

This work optimizes the initial raw material components to determine the optimal composition of glass, with a minimum amount of research, and installation of physical and chemical properties of glasses depending on the composition of the initial components. To solve the problems, we use methods of control systems analysis, heat exchange theory, temperature stress theory, mathematical modeling, software development, algorithm theory, and numerical optimization.

We have developed a mathematical model of structure relaxation and two-dimensional stress field in grade glass products that considers temperature dependences of viscosity and elongation for a glass of certain chemical composition.

3 Results

We investigated the area of glass formation in the three-component system loess loam - ash-slag-flotation waste of the fluorite concentrator [3, 4, 5]. Table 1 presents the chemical composition of the initial raw materials.

Table 1. The chemical composition of the initial raw materials.

Components	Mass content, %									
	SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	Na_2O	K_2O	SO_3	CaF_2	p.p.p
Loess	52,37	11,46	3,92	12,34	2,72	2,17	1,96	-	-	13,06
Ash-and-slag	45,10	19,84	17,25	6,52	0,97	0,70	1,15	1,27	-	7,20
Flotation waste of the fluorite concentrator	76,62	5,46	1,14	4,15	0,54	0,38	1,97	0,10	5,0	3,40

The complicated theoretical and practical question of research of glass technology (for effective solution of a concrete technical problem) is the development of composition with the set properties.

Such cases require consideration of the influence of each component on the physicochemical properties of the system under study. Such an approach, however, requires many melting of glass samples.

To reduce the number of experiments in the search for optimal compositions, it is advisable to apply the method of mathematical planning of the experiment [6, 7].

Scientists most often use the simplex-lattice planning method (Scheffe Test).

Glass melting takes place at 1300-14000 C^0 for 1 hour.

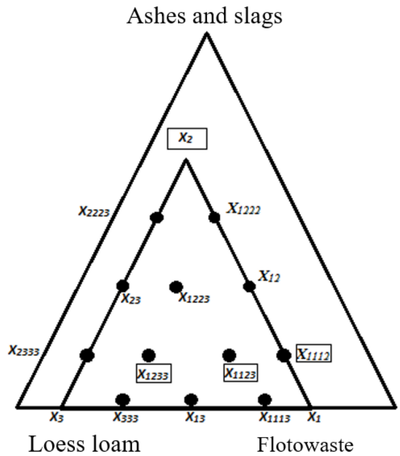

Fig. 1. Indexing of fourth-order experimental points for glasses of a three-component system.

Glass melt had a dark brown, black color depending on the composition of the glass. The mathematical modeling regulated the properties depending on the content of components. The resulting models allow us to say about the properties of glasses limited by experiments in the composition of loess loam - ash-slag - flotation waste of the fluorite concentrator. We investigated the local area of the diagram as a triangle (Fig.1.). $X_1 = 90$, $X_2 = 0$, $X_3 = 10$, $X_1 = 30$, $X_2 = 30$, $X_3 = 40$ и $X_1 = 30$, $X_2 = 0$, $X_3 = 70$.

Regression equations of the second and incomplete third orders proved to be inadequate. We chose a fourth-order polynomial, considering the compositional nature of the simplex lattice plans. The regression equation for the study of the properties

$\hat{Y} = \beta_1 z_1 + \beta_2 z_2 + \beta_3 z_3 + \beta_{12} z_1 z_2 + \beta_{13} z_1 z_3 + \beta_{23} z_2 z_3 + \nu_{12} z_1 z_2 (z_1 - z_2) + \nu_{13} z_1 z_3 (z_1 - z_3) + + \nu_{23} z_2 z_3 (z_2 - z_3) + \delta_{12} z_1 z_2 (z_1 - z_2)^2 + \delta_{13} z_1 z_3 (z_1 - z_3)^2 + \delta_{23} z_2 z_3 (z_2 - z_3)^2 + \beta_{1123} z_1^2 z_2 z_3 + + \beta_{1223} z_1 z_2^2 z_3, \beta_{1233} z_1 z_2 z_3^2$

where $\hat{Y}$ - calculated property;

β, ν, δ – the coefficients of the regression equation.

Based on the experimental data, we calculated the coefficients of the regression equations to test their adequacy using the following ratios (% hereafter, mass content):

1. 40 loess loam × 40 ash-and-slag × 20 flotation waste of the fluorite concentrator.
2. 30 loess loam × 40 ash-and-slag × 30 flotation waste of the fluorite concentrator.
3. 30 loess loam × 30 ash-and-slag × 30 flotation waste of the fluorite concentrator.

The adequacy of the regression equations was checked for each test point by Student's test. Then we compared the values got with the table value of the similar criterion at a significance level of 0.05. We considered the equation to be adequate if the calculated value of the Student's t-test was less than its tabulated value.

Table 2 contains coefficients of the regression equations of the glass properties. According to the regression values, we set the properties of glasses.

4 Discussion

The analysis of the data "Composition - properties" showed regular changes in the properties of glasses depending on the composition (Table 2). The glasses containing more flotation waste from the fluorite concentrator have lower chemical stability (from 0.76 to 1.61mg/dm) when treated with 6n. HCl) and a high coefficient of linear thermal expansion (55.42 - 76.25 10 deg -1).

Table 2. Regular changes in the properties of glasses depend on the composition.

Coefficients	Density, kg/m³	Microhardness, kg/m²	Chemical resistance	
			acid resistance, mg/dm²	alkalinity, mg/dm²
β_1	2650,6	661,0	1,70	171
β_2	2670,3	681,0	1,30	150
β_3	2683,4	678,0	1,41	165
β_{12}	2661,2	673,0	1,60	171
β_{13}	2657,9	669,0	1,60	163
β_{23}	2675,3	687,0	1,55	165
ν_{12}	2658,3	673,-0	1,70	169
ν_{13}	2614,2	656,5	1,10	95
ν_{23}	2659,3	671,0	1,45	156
δ_{12}	2653,1	665,0	1,70	167
δ_{13}	2671,7	712,0	1,23	89
δ_{23}	2663,2	678,0	1,35	167
β_{1123}	2661,1	675,0	1,51	158
β_{1223}	2643,1	657,0	1,60	164
β_{1233}	2651,6	663,0	1,70	169

5 Conclusion

Increasing the proportion of ash and slag leads to a decrease in density and microhardness, while the chemical stability increases.

The results using mathematical modeling correlate with the experimental data.

The application of the simplex lattice planning method allows us to calculate without error the most optimal compositions with predetermined properties and, as a result, to reduce the number of experimental studies.

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