(0.323e for H and 0.646e for O). Comparing the family of Morse curves corresponding to different values of n with the curve obtained by averaging the electrostatic interactions, the authors showed that satisfactory agreement is obtained at n = 5.

This value will also be used here in subsequent calculations. In these calculations, we used the cophasal frequencies of water molecules in different groups: ν_0 for D_2O, in accordance with [2], was assigned a value of 2671 cm^{-1}; ν_0 was determined from the solution of Eq. (3), and the force constant K_{O-D_2} was found from curve 1 (Fig. 3) at $K_{O-Me} = 0.22\cdot10^6$ cm^{-2}; K_{O-D_2} corresponds to a value of $12\cdot10^6$ cm^{-2}; $K_{O-D_1} = 12.40\cdot10^6$ cm^{-2}.

Thus, we determined all of the values needed to calculate r from Eq. (6) (this is the D_2-O_2 spacing in Fig. 4).

The results of the calculations are shown in curve 1 in Fig. 4 in the form of the total projection of the lengths of the chemical bonds (A−B) to the oxygen atom O_2 of the second molecule. Curve 2 shows the density of the substance distributed within the volume of dimers of water molecules coordinated close to active centers on the surface of the mineral.

The density of adsorbed water in such groups turns out to be 1.06 g/cm^3 for the natural form of montmorillonite and 1.15 g/cm^3 for the Fe-form. Here, it is necessary to note that for the measurements made for the natural form of Glukhov kaolinite using nitrobenzene and toluene with allowance for lattice deformation, the density of the combined water (with surface coverage from 0.4 to 2% of the moisture content, i.e., to complete blockage of the active centers) was determined in the form of a monotonic function with the maximum 1.22 g/cm^3.

Thus, calculations for model structures of two types of groups have confirmed that there exists a density of adsorbed water which differs appreciably from the density of water in the liquid state.

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MASS-TRANSFER CHARACTERISTICS OF BULK ORGANIC MATERIALS BY MASS-SPECTROMETRIC ANALYSIS

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UDC 621.384.8+630.53

The mass-spectrometric method was used to analyze the mass transfer characteristics of bulk materials, using seed being subjected to heat treatment as an example. The resulting data are used to propose temperature limits for the safe heating of seed while preserving its sowing qualities.

Complex, multicomponent gaseous systems are analyzed by the mass-spectrometric method, which makes it possible to investigate all classes of organic compounds. A small amount of the substance is needed

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All-Union Correspondence Institute of the Food Industry. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 40, No. 3, pp. 455-459, March, 1981. Original article submitted January 29, 1980.

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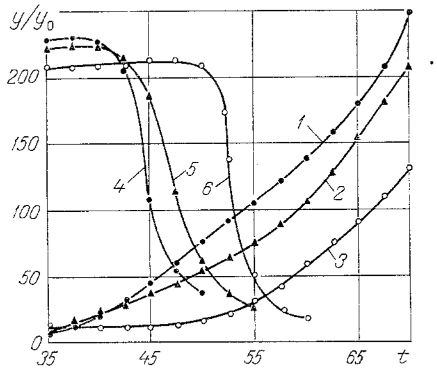

Fig. 1

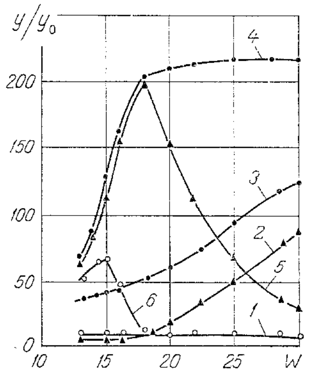

Fig. 2

Fig. 1. Dependence of content of components (rel. units) in the gas phase of a seed mass on its heating temperature (°C) at different initial moisture contents (%): 1) at 30%; 2) at 25%; 3) at 18% (for oxygen); 4) at 30%; 5) at 25%; 6) at 18% (for carbon dioxide).

Fig. 2. Dependence of content of components (rel. units) in the gas phase of a seed mass on moisture content (%) at different heating temperatures (°C): 1) at 40°C; 2) at 50; 3) at 60°C (for oxygen); 4) at 40°C; 5) at 50; 6) at 60°C (for carbon dioxide).

in both structural and quantitative studies in order to achieve this purpose, while the threshold sensitivity of the quantitative determination is higher for the mass-spectrometric method than for other physicochemical methods of analysis. This method is presently used in the metallurgical, chemical, and other sectors of industry to control and determine the composition of complex multicomponent mixtures [1].

The study of the effect of high temperatures on the sowing properties of seed by physicochemical methods of analysis is of great theoretical and practical interest, since the treatment of seed with heat is the basis of many processing operations. The gas phase of the seed mass is a medium which sensibly reacts to any change in the condition of the seed during its heating [2].

The mass spectrometric method that we propose to use here to investigate mass-transfer characteristics makes it possible to study the gas phase of a seed mass during heat treatment and storage of the seed [3]. The investigation was conducted on a laboratory unit of a design which took into account the requirements for maintaining constant temperatures within fixed intervals. The change in the gas phase of seed masses with different initial moisture contents was studied under specified temperature conditions. The seed was heat-treated by the convective method in closed vessels supplied with heat. The gas phase was subjected to mass-spectrometric analysis in accordance with a procedure developed in the physics department of the All-Union Correspondence Institute of the Food Industry [4]. Both standard spectra and data from chromatographic and chemical analyses were used to quantitatively interpret the mass spectra. Study of the results makes it possible to confirm the presence of water vapor, oxygen, carbon dioxide, etc., in the gas phase under the influence of heat. Figures 1 and 2 show the intensities of the components of the mass spectra of the gas phase of a seed mass in relation to temperature and initial moisture content. The seed heat-treatment time was fixed and was about 60 min.

Analysis of the results makes it possible to examine the dynamics of the change in these gas-phase components. It follows from Figs. 1 and 2 that there is a substantial change in the intensities of the spectral lines within the temperature range 50-70°C and in relation to the initial moisture content of the seed. This is evidence of an intensification of transfer processes, both within the seed and in the seed—environment system. In the course of its normal activity as a living biological organism, the seed is the site of respiratory transfer processes. Here, the seed requires oxygen from the air, giving off equivalent amounts of carbon dioxide to the environment. A disturbance in this equilibrium indicates changes in the biological structure of the object. For example, an increase in the carbon dioxide content of the gas phase with heating indicates the beginning of activity within the grain, while a decrease in the carbon dioxide content signals a slackening of respiration processes, a lessening of activity, and the occurrence of destructive processes in the biological structure of the seed. The inverse relation is seen for the gas-phase component which determines the oxygen content.

TABLE 1. Data from Correlation Analysis to Determine Equations Describing Relationship between Correlation Indicators

W, %	t, °C	x	y	y_x	$\overline{y}_x$	R
30	50	30	43,0	46,74	75,25	0,973
	45	95	65,0	61,35		
	40	220	84,0	89,44		
	35	220	95,0	89,44		
25	55	20	42,0	44,94	74,79	0,983
	50	56	59,0	54,14		
	45	180	80,0	85,83		
	40	216	96,0	95,04		
	35	212	97,0	94,01		
20	55	12	65,5	64,36	86,80	0,978
	50	140	81,0	84,30		
	45	210	92,5	95,21		
	40	208	98,0	94,90		
	35	210	97,0	95,21		
18	60	10	60,0	67,53	85,61	0,902
	55	38	79,0	71,36		
	50	201	86,0	93,66		
	45	204	94,0	94,08		
	40	202	98,0	93,80		
	35	198	97,0	93,25		

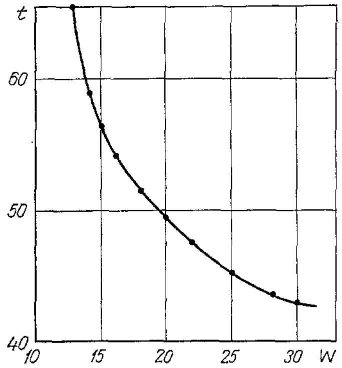

Fig. 3. Dependence of limiting tolerable temperature (°C) of seed-mass heating on initial moisture content (%) according to analysis of mass spectra.

Examining the change in gas-phase components under different conditions, we may conclude that the rate of the transfer processes occurring in the seed during heat treatment is a function of the initial moisture content. Analysis of the mass spectra allows us to propose temperature limits for safe heat treatment of seed. Between these limits, both the processing properties and sowing qualities of the grain are preserved. The data obtained are shown in Fig. 3. If the above conclusions are valid, then a comparison with the traditional parameter for determining seed quality – germinating power – should yield positive results. To this end, parallel with the analysis of the gas phase by mass spectrometry, in all of the tests involving seed heating under different conditions we determined the germinating power in accordance with GOST 10839-64. The two sets of data were compared by the method of correlation analysis. As signs of a correlation, we chose the content of carbon dioxide in the gas phase of the seed mass and the germinating power of the seed. Table 1 shows the experimental data used to form the equations describing the correlation between these two characteristics within prescribed temperature intervals. The correlation index, characterizing the closeness of the connection between the carbon dioxide content of the gas phase of the seed mass and the germinating power of the seed, has values of 0.973, 0.983, 0.986, and 0.902. This shows the closeness of the relationship between these two characteristics. The theoretical equations for the relationship between the characteristics, obtained on the basis of analysis, describe the process with a high degree of accuracy. Shown below are theoretical equations for the relationship obtained on the basis of the empirical data by the method of correlation analysis for different moisture contents:

for a moisture content of 30% $y_x = 40 + 0.22\,x$;
for a moisture content of 25% $y_x = 40 + 0.26\,x$;
for a moisture content of 20% $y_x = 62.5 + 0.16\,x$;
for a moisture content of 18% $y_x = 66 + 0.14\,x$.

TABLE 2. Comparative Data on Limiting Tolerable Seed-Heating Temperatures Obtained on the Basis of Mass-Spectrometric Analysis of the Gas Phase (I) and Analysis of Seed Germinating Power (II)

Moisture content of seed mass, %	Limiting tolerable heating temperature t, °C	
	I	II
13	64,0	64,2
15	56,5	57,3
18	52,0	51,5
20	49,3	47,3
25	45,2	43,1
30	42,5	42,2

Table 2 shows comparative data on the maximum permissible temperatures for heating the seed while preserving its sowing qualities at the class I level. The data were obtained using various methods of analysis. Comparing the limiting-temperature data obtained from analyzing seed germinating power under different conditions and the data obtained on the basis of mass spectra analysis, we can see that the results are in agreement. The difference between the results here does not exceed 1°C. Thus, the results obtained from mass-spectrometric analysis agree well with the standard characteristics of seed activity and mean that such analysis can make an additional contribution to the solution of problems concerning changes in the biological state of seed during heat treatment.

NOTATION

W, seed moisture content; t, seed-heating temperature; x, content of carbon dioxide in gas phase, rel. units; y, germinating power of seed under the same conditions; y_x, seed germinating power determined theoretically on the basis of correlation equation; $\bar{y}_x$, mean value of seed germinating power for a given moisture content; R, correlation index.

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