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## Cluster-associate model of the viscosity of potassium carbonat

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### ABSTRACT

In the article, the temperature dependence of the viscosity of a complex inorganic substance - potassium carbonate was obtained and the proposed mathematical model was verified. Viscosity is considered as a chaosensitive property of a liquid inherent in it in motion and at rest. The mathematical model of viscosity was developed using the Boltzmann distribution and the concept of chaotic particles. On this basis, a hierarchical cluster-associate viscosity model is constructed, which takes into account not only the formation of primary clusters, but also secondary associates with respect to them, with the possibility of identifying the degree of cluster association. To adapt the cluster-associated model to experimental data, certain data processing techniques have been developed to identify unknown parameters of the model. The method of processing viscosity data using the entire set of three reference points allows you to determine the indicator of the degree of aggregation of associates. When processing the data on the viscosity of potassium carbonate, a high correlation coefficient was established calculated in comparison with reference values, which indicates the adequacy of the new relationship. This model makes it possible to predict the behavior of the viscosity of potassium carbonate in a higher temperature range. The degree of association of clusters with an increase in temperature decreases, corresponding to the dynamics of the destruction of associates and viscosity in general.

**Keywords:** concept of randomized particles, Boltzmann distribution, dynamic viscosity, potassium carbonate, cluster, associate.

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### Introduction

Viscosity is an important characteristic of a liquid substance. The nature of the viscous state is insufficiently studied, there is a disparity of temperature dependences of viscosity, fragmentarity and narrowness of experimental determination of this characteristic and the impossibility of displaying it in the full temperature range of the liquid state, especially for melts. This determines the relevance of these studies, in

particular, complex compounds [[1], [2], [3], [4], [5], [6], [7], [8], [9]].

In addition to its practical importance, the study of the viscosity of melts of inorganic compounds is also of great scientific interest, since viscosity is the most structurally sensitive characteristic of a substance that gives an idea of the forces of intermolecular interaction and the mechanism of molecular transfer processes in liquids. The accumulation of knowledge in this field allows us to solve many issues related to the theory of the liquid state [[10], [11], [12], [13], [14], [15], [16], [17]].

Based on the Boltzmann's distribution and the normalized dependence of particles on temperature, the authors [[18], [19], [20], [21], [22]] developed a semi-empirical cluster-associate model of viscous fluid flow, which allows us to evaluate the aggregation of clusters into associates.

This model for determining the regularity of viscosity by temperature based on the concept of chaotic particles does not contradict, but even complements the classical theory of viscosity [18-22]. According to the proposed concept, developers rely on the virtual presence of liquid and gaseous phases in the solid state of matter.

### The experimental part

The cluster-associate model of fluid viscosity makes it possible to estimate the degree of association of clusters or their number based on the temperature dependence of viscosity [[18], [19], [20], [21], [22]].

The viscosity equation according to the concept of chaotic particles is expressed by the formula:

$$\eta = \eta_1 (T_1/T)^a, \quad (1)$$

where  $\eta_1$  – reference point of dynamic viscosity at temperature  $T_1$  (K);  $a$  – degree of cluster association. The value of  $a$  is determined by:

$$a = a_2 \left(\frac{T_2}{T}\right)^b, \quad (2)$$

where  $b$  – the measure of lowering the degree of cluster association. Values  $a_2$  and  $b$ :

$$a_2 = \frac{\ln(\eta_2/\eta_1)}{\ln(T_1/T_2)}, \quad (3)$$

$$a_3 = \frac{\ln(\eta_3/\eta_1)}{\ln(T_1/T_3)}. \quad (4)$$

$$b = \frac{\ln(a_3/a_2)}{\ln(T_2/T_3)}. \quad (5)$$

Thus, the general form of a two-level hierarchical model will be presented as follows:

$$\eta = \eta_1 (T_1/T)^{a_2(T_2/T)^b}, \quad (6)$$

Reference points  $\eta_1$ ,  $T_1$ ,  $\eta_2$ ,  $T_2$ ,  $\eta_3$ , и  $T_3$  should be chosen at the beginning, middle and end of the entire experimental array, respectively [[21], [22], [23]]. In this case, we can limit ourselves to calculating  $a_2$ ,  $a_3$  and  $b$ , without processing the

entire experimental array, with further introduction of the necessary values into the model (6) and calculation of  $\eta$  for comparison with all experimental values by the correlation coefficient.

We will check the adequacy of the cluster-associate viscosity model on such an inorganic substance as potassium carbonate.

### Discussion of the results

Potassium carbonate is produced by carbonation of KOH solutions obtained by electrolytic means, or MgCO<sub>3</sub> suspensions in KCl solution, as well as a by-product during the processing of nepheline into alumina [24, pp. 189-190].

Potassium carbonate is used as a starting product for the production of various potassium compounds and as a potassium fertilizer [24, pp. 187-188].

It easily reacts with sulfur carbon monoxide, upon completion of which crystallohydrates are formed. This interaction is possible only in saline solution.

When the substance is heated to 1200 °C and above, it decomposes into two components - potassium oxide and carbon dioxide. The substance reacts perfectly with non-oxidizing acids, bases, carbon (under high temperature conditions) and with sulfur oxide.

Potassium carbonate is actively used in various industries in calcined and 1.5-in one form, 1st, 2nd and 3rd grades. The chemical industry, glass production, agricultural complex, fire fighting, light industry, photo production and other industrial areas cannot do without it.

The presented data array and melting point  $T_m = 1169$  K of potassium carbonate were taken from the reference [25]. There is no boiling point in this handbook. In the source [26] indicated that at a temperature above the melting point, potassium carbonate decomposes. From the presented values [25], the following were selected as reference values:  $T_1 = 1190$  K,  $\eta_1 = 3,03$  mPa·s,  $T_2 = 1220$  K,  $\eta_2 = 2,23$  mPa·s,  $T_3 = 1250$  K,  $\eta_3 = 1,66$  mPa·s. The data is given only up to 1250 K.

The necessary values were calculated using formulas (3)-(5):  $a_2 = 12,3129$ ;  $a_3 = 12,2330$ ;  $b = 0,2679$ . Then  $a_2$  and  $b$  were substituted into expression (6)

$$\eta = 3,03 \left(\frac{1190}{T}\right)^{12,3129 (1220/T)^{0,2679}}, \quad (7)$$

In addition to this, the exponential equation is given in the reference book [25]

$$\eta = 1,161 \cdot 10^{-5} \exp(29487/RT), \quad (8)$$

derived from data [27] (5 points in the temperature range 1186,2-1257,2 K; torsional vibration method [17] of a hollow cylinder). The accuracy corresponds to the standard deviation  $s = 0,0272$  (1,23%). The uncertainty is estimated at  $\sim 3,0\%$ . The authors [25] additionally give the viscosity value at one temperature (1173,2 K), obtained by S.V. Karpachev and collaborators [28] using the method of torsional vibrations of the ball. This value is lower than the corresponding value in [27], so it was not used when comparing reference and calculated data.

The calculation results for all viscosity values, reference [25] and calculated by (7) and (8), together with the calculations of the temperature dependence of the degree of association (2) are shown in Table 1 and Figure 1.

**Table 1** - Reference [25] and calculated by formulas (7) and (8) data on dynamic viscosity for potassium carbonate

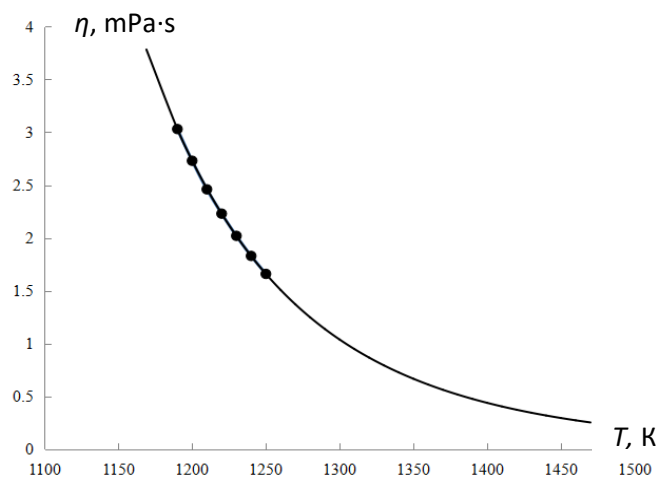
T, K	$\eta$ [25], mPa·s	$\eta$ (7), mPa·s	$\eta$ (8), mPa·s	$a$
$T_m = 1169$	-	3,78	0,000241	12,46
1190	3,03	3,03	0,000229	12,40
1200	2,73	2,73	0,000223	12,37
1210	2,46	2,47	0,000218	12,34
1220	2,23	2,23	0,000213	12,31
1230	2,02	2,02	0,000208	12,29
1240	1,83	1,83	0,000203	12,26
1250	1,66	1,66	0,000198	12,23
1300	-	1,04	-	12,11
1350	-	0,67	-	11,98
1400	-	0,44	-	11,87
1450	-	0,30	-	11,76
1460	-	0,28	-	11,73
1470	-	0,26	-	11,71
1473	-	0,25	-	11,71

It should be noted that the values obtained from equation (8) are very different from the reference values [25] and calculated from equation (7). Apparently, there is a typo in the first coefficient of equation (7), so these values were not taken for comparison with experimental data.

The correlation coefficient when comparing the reference data [25] with the proposed cluster-associate model (7) of viscosity is quite high  $R =$

0,999979 with its significance  $t_R = 52091 \gg 2$ , which indicates the adequacy of the new dependence.

The degree of association of clusters decreases with increasing temperature, amounting to the value  $a_m = 12,46$ , at the melting point, corresponding to the general dynamics of the destruction of associates and the behavior of viscosity as a whole.



**Figure 1** - Dependence of the dynamic viscosity of potassium carbonate on temperature

### Conclusions

The cluster-associate viscosity model made it possible to construct a model for potassium carbonate. Comparison of the reference data with the newly developed model establishes the high adequacy of the presented cluster-associate model of dynamic viscosity of a complex inorganic substance.

The correlation coefficient of potassium carbonate is high, which indicates the possible application of the developed viscosity models in the future.

In addition, an exponential equation was given, the value of which was significantly lower than the corresponding value, so it was not used when comparing reference and calculated data.

One of the most important characteristics of the cluster-associate model – the degree of cluster association – naturally decreases with increasing temperature, corresponding to the dynamics of the destruction of associates.

The proposed viscosity model adequately describes the entire range of the liquid state of a substance, and thus allows predicting behavior at higher temperatures up to the boiling point.

### Conflict of interest

On behalf of all the authors, the correspondent author declares that there is no conflict of interest.

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## Калий карбонаты тұтқырлығының кластерлі-ассоциаттық моделі

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### ТҮЙІНДЕМЕ

Мақалада күрделі бейорганикалық заттың - калий карбонатының тұтқырлығының температуралық тәуелділігі алынды және ұсынылған математикалық модель тексерілді. Тұтқырлық сұйықтықтың қозғалыста және тыныштықта өзіне тән хаосқа сезімтал қасиеті ретінде қарастырылады. Тұтқырлықтың математикалық моделі Больцманның таралуын және хаотикалық бөлшектер тұжырымдамасын қолдана отырып жасалды. Осы негізде тұтқырлықтың иерархиялық кластерлі-ассоциаттық моделі құрылған, ол тек бастапқы кластерлердің құрылуын ғана емес, сонымен қатар кластерлер қауымдастығының дәрежесін анықтау мүмкіндігімен оларға қатысты қайталама ассоциацияларды да ескереді. Кластерлі-ассоциаттық модельді эксперименттік деректерге бейімдеу үшін белгісіз модель параметрлерін анықтау үшін деректерді өңдеудің белгілі әдістері жасалды. Тұтқырлық туралы мәліметтерді үш нүктенің жиынтығын қолдана отырып өңдеу әдісі ассоциаттардың агрегация дәрежесін анықтауға мүмкіндік береді. Калий карбонатының тұтқырлығы туралы мәліметтерді өңдеу кезінде анықтамалық мәндермен салыстырғанда есептелген жоғары корреляция коэффициенті анықталды, бұл жаңа тәуелділіктің жеткіліктілігін көрсетеді. Бұл модель калий карбонатының тұтқырлығын жоғары температура диапазонына дейін болжауға мүмкіндік береді. Кластерлердің қауымдастық дәрежесі температураның жоғарылауымен төмендейді, ассоциаттардың бұзылу динамикасына және тұтастай тұтқырлыққа сәйкес келеді.

**Түйін сөздер:** ретсіз бөлшектер туралы түсінік, Больцманның таралуы, динамикалық тұтқырлық, калий карбонаты, кластер, ассоциат.

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## Кластерно-ассоциатная модель вязкости карбоната калия

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### АННОТАЦИЯ

В статье авторами была получена температурная зависимость вязкости сложного неорганического вещества - карбоната калия и проведена проверка предложенной математической модели. Вязкость рассматривается как хаосочувствительное свойство жидкости, присущее ей в движении и в покое. Математическая модель вязкости была разработана с использованием распределения Больцмана и концепции хаотизированных частиц. На этой основе построена иерархическая кластерно-ассоциатная модель вязкости, которая учитывает не только образование первичных кластеров, но и вторичных по

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отношению к ним ассоциатов с возможностью выявления степени ассоциации кластеров. Для адаптации кластерно-ассоциатной модели к экспериментальным данным разработаны определенные приемы обработки данных для идентификации неизвестных параметров модели. Метод обработки данных по вязкости с использованием из всего множества трех реперных точек позволяет определить показатель степени агрегации ассоциатов. При обработке данных по вязкости карбоната калия был установлен высокий коэффициент корреляции рассчитанных по сравнению со справочными величинами, что указывает на адекватность новой зависимости. Данная модель позволяет прогнозировать поведение вязкости карбоната калия в более высокий температурный диапазон. Степень ассоциации кластеров с повышением температуры понижается, соответствуя динамике разрушения ассоциатов и вязкости в целом.

**Ключевые слова:** концепция хаотизированных частиц, распределение Больцмана, динамическая вязкость, карбонат калия, кластер, ассоциат.

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