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ЗАВИСИМОСТЬ МОЛЯРНОЙ ВЯЗКОСТИ ВОДЫ В ЖИДКОМ И ФЛЮИДНОМ СОСТОЯНИЯХ ОТ ДАВЛЕНИЯ

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Аномальное уменьшение вязкости воды с ростом давления известно уже более века. Считается, что этот эффект обусловлен, прежде всего, существованием тетраэдрической сетки водородных связей между молекулами воды. Для описания зависимости вязкости воды от давления пока существует лишь несколько моделей. Учитывая существование двух механизмов вязкого течения в жидкой и газовой фазах, мы предлагаем подход, который рассматривает воду в широком интервале температур и давлений как находящуюся в двух состояниях: жидкость и флюид. Показано, что в отличие от изученных ранее простых жидкостей и флюидов с универсальным типом межмолекулярных взаимодействий, для которых характерны линейные зависимости между молярными свойствами вязкости и объема при изменении давления, вода и спирты способны к образованию водородных связей, что приводит к нарушению линейных корреляций. В работе на основе использования метода рациональных параметров и концепции свободного объема представлены двухпараметрические уравнения для описания изотерм барической зависимости мольных характеристик вязкого течения (Fm и ηm) в области давлений от 0,1 до 100 МПа для жидкой воды (от 273 до 373 К) и для флюида (от 373 до 1023 К). Использование методов регрессионного анализа позволило определить статистически значимые коэффициенты уравнений. Показано, что изменение вязкости воды от давления можно описать через изменение молярного объема и плотности упаковки молекул в жидкости или флюиде. Для оценки адекватности описания барических зависимостей вязкого течения воды и спиртов проведено сравнение предложенного подхода с некоторыми моделями (Эйринга, Тэйта, теория трения и др.). Удовлетворительное согласие полученных в работе результатов с имеющимися в литературе экспериментальными данными показывает, что предложенные уравнения позволяют учитывать специфическую молекулярную структуру ассоциированных жидкостей и относительно просты по сравнению с другими соотношениями для описания изотерм вязкого течения в широком интервале давлений.

Ключевые слова: вода, вязкость, плотность, высокие давления, молярный объем, плотность упаковки, корреляции

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PRESSURE DEPENDENCE OF MOLAR VISCOSITY OF WATER IN LIQUID AND FLUID STATES

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The anomalous decrease in the viscosity of water with applied pressure has been known for over a century. It is primarily due to the existence of a tetrahedral network of hydrogen bonds between water molecules. To describe the dependence of water viscosity on pressure, there are still only a few models. Taking into account the existence of two mechanisms of viscous flow in the liquid and gas phases, we propose an approach that considers water in a wide range of temperatures and pressures as being in two states: liquid and fluid. It has been shown that, in comparison with previously studied simple liquids and fluids with a universal type of intermolecular interactions, which are characterized by linear dependences between the molar properties of viscosity and volume at change of pressure, the water and alcohols are capable of forming hydrogen bonds, which leads to a deviation from linear correlations. Based on the use of the method of rational parameters and the concept of free volume, the paper presents two-parameter equations for describing the isotherms of the baric dependence of the molar characteristics of viscous flow (Fm and ηm) in the pressure range from 0.1 to 100 MPa for liquid water (from 273 to 373 K) and for fluid (from 373 to 1023 K). The use of regression analysis methods allow to determine the statistically significant coefficients of the equations. It is shown that the change in the viscosity of water as a function of pressure can be described in terms of a change in the molar volume and packing density of molecules in a liquid or fluid. To assess the adequacy of the description of the pressure dependences of the viscous flow of water and alcohols, the proposed approach was compared with some models (Eyring, Taite, friction theory, etc.). Satisfactory agreement between the results obtained in this work and the experimental data available in the literature was obtained. Thus, the proposed equations make it possible to take into account the specific molecular structure of associated liquids and are relatively simple compared to other relations for describing viscous flow isotherms in a wide pressure range.

Key words: water, viscosity, density, high pressure, molar volume, density packing, correlations

INTRODUCTION

Investigations of transport properties of various substances at high pressures have vigorously developed in recent decades. The dynamic viscosity (η) is an important transport property in the design chemical processes and engineering problems dealing with heat-transfer, mass transfer operations, fluid-flow processes, etc. Experimental viscosity data were obtained for compounds and systems with different chemical structures, covering wide ranges of temperatures and pressures [1-6]. There is still a need to develop reliable and simple viscosity models applicable to both liquids and gases over wide ranges of temperature and pressure.

Every year new viscosity models or modifications of existing models are derived. Most of them are based on the corresponding state principle [6, 7], the kinetic theory of Enskog or Eyring`s theory [8], the free volume model [4, 9] and the friction theory [5]. All of them have advantages and disadvantages, and still none of them is able to estimate the viscosity of fluids in a fully predictive manner. There are fewer models to describe the dependence of viscosity on pressure in often limited range of state parameters for non-polar liquids and fluids [6]. The some viscosity models require knowledge of a series of hardly evaluated terms and adjustable parameters [4, 6]. Additionally, more investigations are necessary around free-volume approach. The study of viscosity is very important in the development of understanding of molecular motions and interactions in the liquids and fluids under various conditions (temperature, pressure).

The transport properties show a regular dependence on density. The pressure has a direct effect on the density and pressure can be indirectly effect on the viscosity through the density change. It should be noted that the viscosity of compound in the gaseous state is much lower than its viscosity in the liquid state. The reason is that the distance between the molecules in the gas phase is greater than in the liquid. In dilute gases, the main mechanism for transfer of momentum between layers of flowing fluid is the kinetic contribution by collisions of the freely migrating molecules. In the liquid case, the momentum transfer is mainly due to intermolecular interactions between the dense packed molecules, *i.e.* potential contribution [5, 6]. The most viscosity models have been tested on the non-polar hydrocarbon fluids. Recently [10], it was shown that for the supercritical fluids (Ar, Kr, Ne, He, N_2, NF_3, CH_4, N_2O, NF_3, CO_2) and non-associated liquids (n-butane, n-pentane, n-hexane, n-heptane, n-octane, n-nonane, n-undecane, toluene, benzene, cyclopentane, cyclohexane) with universal intermolecular interactions the molar characteristics of viscous flow ($\eta_m = \eta V_m$, $F_m = 1/\eta_m$) are the functions only of the molar volume in the wide pressures ranges. The effect of chemical structure on the viscosity of liquids under pressure was also observed. For more complex molecules, including liquids which contain functional groups such as alcohols (MeOH, EtOH, *n*-PrOH, *n*-BuOH), the changes in the molar fluidity under pressure are satisfactorily described by two-parameter regression equation over the range of pressures from 0.1 to 1200 MPa [10].

The anomalous decrease of the viscosity of water with applied pressure has been known for over a century [11, 12]. It occurs concurrently with major structural changes. It is well-known [11-14], that the water structure is the tetrahedral nearest ordering due to the hydrogen bonding between water molecules. Viscosity is a macroscopic witness of the existing of the tetrahedral hydrogen bond network that makes water so peculiar. For liquid water at temperatures below 323 K, the viscosity decreases with increasing pressure although the density increases. Similar viscosity behavior is observed for near supercritical water under pressure below the critical temperature ($T_c = 647.27$ K [13]). Because of the anomalous behavior of the pressure dependence of the water viscosity, almost no quantitative descriptions have been proposed to determine the pressure or density dependence of the viscosity [11, 12]. For the prediction of the pressure dependence of viscosity of water only few models exist so far [14]. Some viscosity equations were based on the assumption that the viscosity depends on the molecular free volume. In other cases, the viscosity of water had been presented by empirical equations for the temperature and density dependences which contain adjustable coefficients without physical meaning. It was found that the relative deviations between measured data and data extracted from various equations were (3 to 30)% as described by authors of works [6, 15].

In this work, the effects of pressure and temperature on the viscosity and density of various compounds were described in the frame of the free-volume approach [4, 6] and the rational parameters method [10]. We propose an approach that treats water as occurring in two states (liquid and steam), and explains its viscosity properties. Aim of the study is the relationship between the molar viscosity and the volume parameters for the water in liquid and fluid states in wide range of pressures and temperatures using an available literature data [13].

THE CORRELATION APPROACH

There are many empirical models and methods available in the literature for the correlation and the estimation of the viscosity of a liquid and a fluid. The major effort is related to the variation of liquid viscosity with temperature. A few methods for the estimation of the effect of pressure on viscosity have also been known. It must be noted that the complete pressure – temperature dependence of the viscosity is very complex, and any single correlation is unlikely to be within the experimental accuracy over the entire measurable ranges of temperature and pressure. Some viscosity – pressure relationships have a similar form to the more successful viscosity – temperature equations. The free volume theory of viscous flow can provide a framework for a description of the temperature and pressure dependences of viscosity with the additional benefit that at least some of the parameters have physical meaning outside of the application to viscosity and may be independently measured.

As a known, the free volume is characteristic of the empty space, in which the molecules are free to move around. The free volume in a liquid increases and the viscosity decreases with increasing temperature. This is valid if dynamic viscosity and density vary with temperature far from the critical point. This is not suitable to represent viscous behavior of supercritical fluids under moderate and high pressures. The viscosity of a fluid in the gaseous state increases with increasing temperature, whereas the viscosity of a liquid decreases with increasing temperature [4]. The viscosity increases with rise pressure at a constant temperature. However, for dense supercritical fluids and water the viscosity decreases with increasing temperature down to a minimum and then increases with the temperature.

One of the main alternatives to experimental studying the viscosity on pressure is the use of a structure-property relationship, which quantitatively describe property in terms of molecular descriptors as function of pressure. The multiple linear regression method (MLR), as a most commonly used method, has been applied to the investigation. The main aim of the study is to establish an empirical function relating the structural descriptors of compounds under investigation to viscosities. There are a large number of molecular descriptors, including geometric, topological, quantum-chemical and other characteristics, which can be used. In this work, the geometric descriptors, such as the molar volume and the molecular packing density, are involved in the properties of viscosity of the compounds.

The multiple linear regression statistic technique was used to study the relation between the viscosity and the geometry descriptors. The accuracy of the model was mainly evaluated by the root mean square error (RMSE). Formula is given as follows:

$$\mathrm{RMSE} = [(1/n)\cdot\sum_{i=1}^{n}(y_{\mathrm{exp}}-y_{\mathrm{calc}})^2]^{1/2} \qquad (1)$$

where n is the number of experimental point, y_{exp} is the experimental value, y_{calc} is the predicted value and summation is of overall patterns in the analyzed data set. In addition, the value of the average absolute relative deviation (AAD) for viscosity was calculated by expression:

$$\mathrm{ADD} = (100/\mathrm{n})\cdot(y_{\mathrm{calc}}-y_{\mathrm{exp}})/y_{\mathrm{exp}}. \qquad (2)$$

The correlation coefficient (r_{corr}), standard deviation (SD) and coefficient of Fisher distribution ($F_{\mathrm{statistic}}$) have also been calculated.

Not so long ago, the regression method has been successfully employed by us to describe some properties of compounds (heat capacity [15], sublimation enthalpy [16], viscosity [17]). In this work, the simple equations have been obtained in the terms of the free volume concept and the rational parameter method which was earlier described in the literature [10, 17]. The so-called “molar” viscosity, $\eta_{\mathrm{m}} = \eta V_{\mathrm{m}}$, was proposed earlier [10, 17]. In the work [17], the molar viscosity has been used for representation of the temperature dependence of internal friction of the fluids with different intermolecular interactions. It was shown [10, 17] that the molar viscosity of various liquids over a wide range of temperatures could be represented by equation:

$$(F_{\mathrm{m}}-F_{\mathrm{o}})/F_{\mathrm{o}} = \mathrm{B}(V_{\mathrm{m}}-V_{\mathrm{o}})/V_{\mathrm{o}}, \qquad (3)$$

or by equation (4) derived from the equation (3):

$$F_{\mathrm{m}}(\mathrm{P}) = \mathrm{a} + \mathrm{b}\cdot V_{\mathrm{m}}(\mathrm{P}), \qquad (4)$$

where $F_{\mathrm{m}} = 1/\eta_{\mathrm{m}}$ is a molar fluidity, a = F_{o}(1-B) and b = B$F_{\mathrm{o}}/V_{\mathrm{o}}$; V_{m} is a molar volume, V_{o} is the molar volume for which the fluidity is close to zero; F_{o} is the molar fluidity of liquid when it acquires the free molar volume, V_{m}-V_{o}, equal to V_{o}. Value of V_{o} is excepted to be the close packing volume of liquid at fixed temperature. Values of B coefficient depend upon the capacity of molecules to absorb the momentum of viscous flow by reason of their mass, flexibility, softness, or inertia of rotation. The correlation method has been applied to the monatomic fluids and the polyatomic liquids for which viscosity and density data are available at high pressures.

RESULTS AND DISCUSSION

As it is known, the two different mechanisms need to be considered for the viscous flow in various phase states. The first one, occurring in liquid, is well known as momentum transfer by intermolecular interactions between the dense packed molecules. The second one, as the temperature increases very significantly, imply a momentum transfer by collision of the freely migrating molecules in the gaseous state. In the work, we presented two equations for the pressure viscosity behavior of liquid water in the temperature ranges (273 to 373) K and steam in the range (373 to 1023) K and pressures up to 100 MPa.

It was previously shown [10] that in the case of the liquids and fluids with universal intermolecular interactions the isotherms of $F_{\mathrm{m}} = f(V_{\mathrm{m}})$ and $\eta_{\mathrm{m}} = f(V_{\mathrm{m}})$ are close to linear, and this has been used as evidence of the role of the free volume in the viscous flow. Then, it was considered the liquids and dense gases that are able to form intermolecular hydrogen bonds. The most important problem was whether the change of the term “$\mathrm{V_m}$” (or “V_{m}-V_{o}”) reveals the correct change of interstitial space in the hydrogen bonding liquids with increasing a pressure. It was shown that the simple first-order approximations are not true for pressure dependence of viscosity of such polyatomic liquids, as alcohols and water. The molar fluidity – pressure relations are not linear and the models above used are less statistically significant for associated alcohols. The peculiar behavior of the liquids or fluids is related to the change of the void distributions and the degree of hydrogen bonding as a function of pressure or temperature [11, 12]. Some experimental and theoretical approaches revealed the fact that hydrogen bonding still exists in sub- and supercritical water and short chain alcohols [11, 18, 19].

In the work, we presented two equations for the pressure viscosity behavior of liquid water and steam in the range 273 to 1023 K and up to 100 MPa. The equation (5) have been used to describe the molar fluidity isotherms of liquid water in the range (273 to 373) K and pressure up to 100 MPa

$$F_{m}(P) = a' + b'_{1} \cdot V_{m}(P) + b'_{2} \cdot D_{w}(P), \qquad (5)$$

The dependence of the molar viscosity for fluid water in the range (373 to 1023) K and pressure up to 100 MPa can be given by the following expression

$$\eta_{m}(P) = q' + k'_{1} \cdot V_{m}(P) + k'_{2} \cdot D_{w}(P), \qquad (6)$$

where q′, k'_1 and k'_2 are constants. The geometric descriptor, $D_w = N_A V_w / V_m$ (where N_A is Avogadro number, V_w is van der Waals volume), is known as a molecular packing density in a liquid or a fluid. D_w may be taken as some function of molecular specific interactions which depend on the structure of the liquid. The change of molecules packing is also a function of the pressure and temperature. It is noted that D_w values increase with pressure for the associated liquids and fluid studied.

Standard multiparameter regression analysis was used to obtain the coefficients of the equations (5) and (6). The equations (5) and (6) are validated by the values of correlation coefficient (r_{corr}), root mean square deviation (RMSD) for regression and F-distribution coefficient ($F_{statictic}$). It is interesting to note that D_w term become important for determining the molar fluidity of the associated liquids (alcohols, water). The correlation significantly improves to $r_{corr} > 0.99$ after the inclusion of the effect of packing of molecules. A successful evaluation of the water viscosity was carried out over the range of pressure from 0.1 to 100 MPa and in the above temperature ranges. The results obtained are given in Tabls 1, 2. The correlations between experimental viscosity and calculated one based on these models are quite significant as indicated by statistical values in Tables 1, 2.

Table 1

Coefficients and statistical parameters of the equation (5) for isotherms of liquid water [13] at pressure range (0.10 – 100) MPa

***Таблица 1.* Коэффициенты и статистические параметры уравнения (5) для изотерм воды в жидкой фазе [13] в диапазоне давлений (0,10 - 100) МПа**

Coefficients	At temperature: T, K				
	273	298	323	348	373
a′	1.202±0.062	1.872±0.021	2.260±0.112	1.776±0.157	1.623±0.095
$10^2 \cdot b'_1$	-3.581±0.191	-5.285±0.054	-6.010±0.332	-4.222±0.463	-3.339±0.267
b'_2	-0.982±0.062	-1.601±0.019	-2.010±0.110	-1.633±0.146	-1.572±0.094
r_{corr}	0.9997	0.9999	0.9878	0.9994	0.9999
$F_{statistic}$	29253	174264	752.2	6282.5	77666
10^2·RMSD	0.0022	0.0005	0.0029	0.0046	0.0026

Table 2

Coefficients and statistical parameters of the equation (6) for isotherms of fluid water [13] at pressure range (0.10 – 100) MPa

***Таблица 2.* Коэффициенты и статистические параметры уравнения (6) для изотерм воды в газообразном состоянии [13] в диапазоне давлений (0,10 - 100) МПа**

Coefficients	At temperature: T, K			
	423	523	623	658
q′	-23.32±1.56	-7.386±0.52	-0.115±0.036	-0.0043±0.031
k'_1	0.5712±0.040	0.1724±0.012	0.0222±0.001	0.0232±0.0001
k'_2	31.941±1.54	13.767±0.583	4.589±0.108	4.323±0.102
r_{corr}	0.9999	0.9999	0.9999	0.9999
$F_{statistic}$	124134	77740	491638	465526
10^2·RMSD	0.0617	0.0660	0.0439	0.0458
Coefficients	At temperature: T, K			
	723	823	923	1023
q′	0.1670±0.031	0.3003±0.023	0.3868±0.017	0.4401±0.014
k'_1	0.0264±0.001	0.0305±0.001	0.03455±0.001	0.0384±0.001
k'_2	3.956±0.127	3.8152±0.158	3.822±0.152	3.922±0.159
r_{corr}	0.9999	0.9999	0.9999	0.9999
$F_{statistic}$	594844	$2.133 \cdot 10^6$	$7.16 \cdot 10^6$	$1.69 \cdot 10^7$
10^2·RMSD	0.0743	0.0541	0.0392	0.0324

The equations (5) and (6) hold over the above regions with a very high precision. In the case of the liquid and fluid, the AAD does not exceed 1.16%, which is comparable to the accuracy of the viscosity experimental data.

Thus, it was found that the coefficients of Eqs. (5) and (6) are functions of temperatures and independent of pressure. It is noted that for the water steam the values of coefficient k'_1 in Eq. (6) increase linearly with increasing temperature from 373 to 1023 K. At the same time, the values of coefficient k'_2 decrease with increasing temperature down to a minimum at near ~T_c, but in the temperature range from 700 to 1023 K the slight growth of coefficient k'_2 is observed for the water fluid (Fig.).

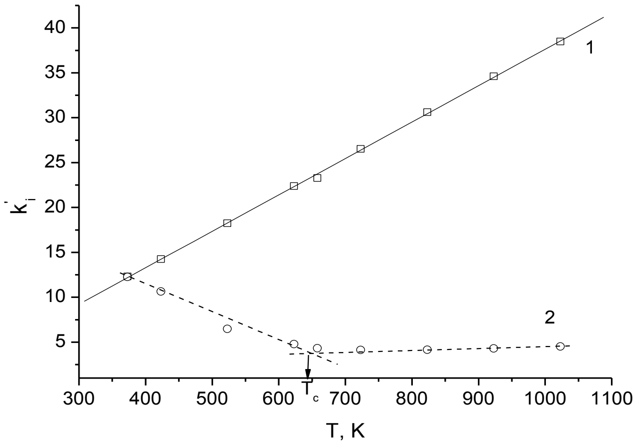

Fig. Temperature dependences of coefficients k'_i of equation (6): $1 - 10^{-3}\ k'_1$, $2 - k'_2$

Рис. Температурные зависимости коэффициентов k'_i уравнения (6): $1 - 10^{-3}\ k'_1$, $2 - k'_2$

In order to evaluate the performance of the present approach, a comparison of the equations of this work with the models of the famous theories [15, 18-22] was carried out. The average absolute relative deviation (AAD) and the maximum absolute relative deviation (MxD) between the experimental data from literatures and the results calculated from our and other models are shown in Table 3 for water and two alcohols (methanol, ethanol).

As it can be seen from the Table 3, on the average, our approach have better results respect to friction theory and Tait-like equation for liquid water. For the viscosity of the alcohols at pressures up to 71 MPa, the literature values of AAD was determined to be (0.54 to 3.40)% by Tait-like equation, free volume and friction theory. The present equation (5) has the similar accuracy at pressures up to 1200 MPa indicating that the approach is suit for modeling the viscosities of polar liquids over wide range of pressure. Thus, in analysis of results of the evaluation and comparison, the above proposed approach has been demonstrated the satisfactory agreement with the experimental data from literature, the ability to take into account the specific molecular structure of liquids and the simplicity in comparison with other considered models.

Table 3

Comparison of the calculated values of ADD and MxD for some models of the viscosity of water and alcohols

***Таблица 3.* Сравнение рассчитанных значений ADD и MxD для некоторых моделей вязкости воды и спиртов**

	Error	H_2O (liquid)	MeOH	EtOH
This work	AAD, %	0.06	1.54	3.08
	MxD, %	0.11	3.15	7.29
Free volume theory	AAD, %	-	3.46 [19]	1.18 [19]
	MxD, %	-	-	-
Friction theory	AAD, %	35.2 [20]	1.32 [5]	0.72 [5]
	MxD, %	137 [20]	8.99 [5]	2.35 [5]
Eyring`s theory	AAD, %	-	7.16[19] 0.81[21]	1.12[19] 1.24[21]
	MxD, %	-	5.24[21]	6.7[21]
Tait-like equation	AAD, %	3.0[22]	0.84[3]	0.57[3] 1.6[18]
	MxD, %	20[22]	5.1[18]	-

CONCLUSIONS

In case of water, using the rational parameter method and the free-volume concept, the pressure dependences of the molar characteristics of viscous flow (F_m and η_m) have been represented in the two-parameter regression forms (equations (5) and (6)) over the range of pressure from 0.1 to 100 MPa and in the temperatures ranges (273 to 373) K for liquid water and (373 to 1023) K for steam. This demonstrates the important point of view that the magnitude of the viscosity coefficient depends upon pressure through the molar volume and the molecular packing density in a liquid or a fluid.

The coefficients of the equations proposed have been tabulated to facilitate direct and quick estimation of the liquids and fluids viscosity. A comparison of key statistical terms (ADD, MxD) of these equations obtained with the models of the famous theories was carried out. It was shown that our approach is suit for describing the viscosity of liquid water and fluid water over wide ranges of pressure and temperature. The accuracies of the viscosity calculation by equations (5) and (6) are comparable with the experimental uncertainties of its measurements. If the dynamic viscosity will be used instead of molar one, the error of viscosity prediction by the above equations increases more than twice. The equations could be used for estimation of the unknown values of viscosity of liquid and fluid under high density conditions from the data obtained near to zero-density (P_o~0.101 MPa) at the same temperature.

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The authors declare the absence a conflict of interest warranting disclosure in this article.

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