Dependence of Nanofluid Viscosity on Nanoparticle Size and Material

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Abstract The viscosity of nanofluids is studied by molecular dynamics method. It is considered the model nanofluids based on liquid argon with aluminum and lithium nanoparticles. The nanoparticle size ranges from 1 to 4 nm. The volume concentration of nanoparticles is varied from 1% to 12%. It is shown that the viscosity of the nanofluid increases with decreasing nanoparticle size. Potential contribution to viscosity of nanofluid considerably exceeds the kinetic one. Therefore parameters of molecule-molecule and nanoparticle-molecule potentials make the considerable impact on viscosity of nanofluids which, thus, depends on material of nanoparticles.

Keywords: Nanofluids; Nanoparticles; Viscosity; Molecular Dynamics; Effect of Nanoparticles Size

1. Introduction

Since nearly all applications of nanofluids are related to channel flows, viscosity is a determining factor in their use. It has been well established that the viscosity of nanofluids is much higher than the viscosity of conventional dispersions at equal volume concentrations of dispersed particles and is not described by any classical theory of the viscosity of these fluids (Einstein, Batchelor, Mooney, Krieger, etc.) (see reviews [1–3]). It has been found that the effective viscosity of nanofluids depends not only on the concentration of nanoparticles, but also on their size. It is shown that the viscosity of the nanofluid increases with decreasing nanoparticle size. Evidence for this has been provided by molecular dynamics simulations for the hard-sphere potential [4, 5] as well as by experiments [3, 6–8]. However, opposite data have also been reported [9, 10]. In [3], it is noted that the viscosity of nanofluids may also depend on the nanoparticle material. This correlates with the data of the kinetic theory of gas nanosuspensions where this dependence has been well established [11, 12]. The first MD calculations have confirmed the existence of this dependence [13]. Obtaining systematic data that would give an unambiguous answer to the question of the dependence of the viscosity of nanofluids on the nanoparticle size

and their material is the objective of this paper. We studied the viscosity of model nanofluids in which the carrier fluid was argon of density $\rho = 0.707$ and temperature $T = 300$ K. The dispersed component was lithium and aluminum nanoparticles with a diameter from one to four nanometers. The volume concentration of nanoparticles was varied from 1% to 12%.

2. Simulation technique

The standard molecular dynamics method was used (see, e.g., [14–15]). A cubic cell and periodic boundary conditions were used. Interaction between the molecules of the carrier fluid was described by the Lennard-Jones potential

$$\Phi_{LJ}(r) = 4\varepsilon\left[(\sigma/r)^{12} - (\sigma/r)^6\right], \quad (1)$$

where σ is the effective diameter of the fluid molecules, ε is the depth of the potential well, and $r = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between molecules i and j.

Interaction between carrier fluid molecules and a nanoparticle was described by the Rudyak–Krasnolutskii (RK) potential [16, 17]

$$\Psi(r) = \Psi_9(r) - \Psi_3(r), \quad (2)$$

$$\Psi_i = C_i\left\{\left[\frac{1}{(r-R)^i} - \frac{1}{(r+R)^i}\right] - \right.$$

$$-\frac{a_i}{r}\left[\frac{1}{(r-R)^{i-1}}-\frac{1}{(r+R)^{i-1}}\right]\right\},$$

where

$$i=9,3,\quad a_9=9/8,\quad a_3=3/2,\quad V_p^{-1}=\rho_p/m_p,$$

$$C_3=(2\pi\varepsilon_{12}\sigma_{12}^6)/3V_p,\quad C_9=(4\pi\varepsilon_{12}\sigma_{12}^{12})/45V_p,$$

$V_p^{-1}=\rho_p/m_p$. Here ρ_p is the density of the nanoparticle material, m_p is the mass of the atom (molecule) of the nanoparticle, R is the radius of the nanoparticle, $\sigma_{ij},\varepsilon_{ij}$ are the parameters of the interaction potential (1) between a carrier fluid molecule and a molecule of the nanoparticle.

As the nanoparticle interaction potential we use a specially constructed potential [18], which for monodisperse nanoparticles has the form

$$U(r,R)=U_7(r,R)-U_1(r,R),\qquad(3)$$

where

$$U_7(r,R)=\frac{\pi^2}{315}\frac{\widetilde{\varepsilon}\,\widetilde{\sigma}^{12}}{V_p^2}\left\{\frac{R^2}{r}\left[\frac{1}{(r-2R)^7}+\right.\right.$$

$$+\frac{2}{r^7}+\frac{1}{(r+2R)^7}\right]-\frac{R}{3r}\left[\frac{1}{(r-2R)^6}-\frac{1}{(r+2R)^6}\right]-$$

$$-\frac{1}{30r}\left[\frac{1}{(r-2R)^5}-\frac{2}{r^5}+\frac{1}{(r+2R)^5}\right]\right\},$$

$$U_1(r,R)=\frac{2\pi^2}{3}\frac{\widetilde{\varepsilon}\,\widetilde{\sigma}^6}{V_p^2}\left[\ln\left(\frac{r^2-4R^2}{r^2}\right)+\right.$$

$$+2R^2\left(\frac{1}{r^2-4R^2}+\frac{1}{r^2}\right)\right].$$

Here R is the radius of the nanoparticles, $\widetilde{\varepsilon}$ and $\widetilde{\sigma}$ are the parameters of the Lennard-Jones (1) interaction potential of the nanoparticle atoms.

Potentials (2) and (3) were constructed under the assumption that the interaction between the carrier-fluid molecules and nanoparticle atoms and the interaction of the nanoparticle atoms are described by potential (1), respectively, with the parameters σ_{12}, ε_{12} and $\widetilde{\sigma}$, $\widetilde{\varepsilon}$. The simulation was performed as follows. Carrier-fluid molecules and nanoparticles were uniformly placed in the simulation cell according to the specified values of the density of the carrier fluid and the volume

concentration of nanoparticles. The density of the pure fluid was determined by the parameters: $\rho=N\sigma^3/V$ and $\alpha=V/V_0$, here V is the volume of the system (cell), $V_0=N\sigma^3/\sqrt{2}$ is the volume of close packing of N molecules. The volume of the simulation cell for the nanofluid was given by the relation $V=\alpha N_1\sigma^3/\sqrt{2}+4\pi k_V N_2 R^3/3$, where N_1 and N_2 are the number of molecules and nanoparticles, respectively. With the addition of nanoparticles, the coefficient k_V was chosen so that the nanofluid pressure was equal to the pressure of pure argon of the given density.

The initial velocities of molecules were specified according to the Maxwell distribution at the given temperature, and those of nanoparticles were set equal to zero. The calculation was started after an initial relaxation period, during which the whole system had come to equilibrium. The Newton's equations were integrated using Schofield's scheme [19].

Since the potentials used here have an infinite range, they should be truncated during the simulation. For potential (1), the truncation radius was 2.5σ, and for potential (2), it was $(R+b\sigma_{12})$. The value of b was chosen so that at the truncation radius for potential (2), the force exerted on a molecule by a nanoparticle was equal to the force of interaction between two molecules at the truncation radius for potential (1). The quantity b depends on the nanoparticle radius, material and the properties of the carrier-fluid molecules. In particular, for Li nanoparticles (for the diameter of the nanoparticles was 2 nm) in Ar, b was equal to 3.78, and for Al nanoparticles, it was 4.02. The nanoparticle interaction potential was truncated at a distance at which the interaction force between nanoparticles was zero, i.e., the so-called soft-sphere potential was used.

It should be noted that the simulation of the evolution of nanofluids imposes more severe restrictions on the size of the simulation cell as compared with homogeneous fluids. Since a nanoparticle should not interact with itself, the side length of the cubic cell L should be much greater than the range of the potential,

$L \gg \widetilde{R}$. In practice, the distance should be, at least, several times greater to avoid the corresponding correlations.

The parameters of the interaction potential of argon molecules were as follows: $\sigma = 3.405$ Å and $\varepsilon/k_B = 119.8$ K [20]. The parameters of potentials (2) and (3) were calculated using the following parameters of potential (1): for lithium, $\sigma = 3.95$ Å and $\varepsilon/k_B = 500$ K [21], and for aluminum, $\sigma = 2.551$ Å and $\varepsilon/k_B = 857.6$ K. The latter parameters were obtained from data on Young's modulus and the structure of the crystal lattice (face-centered cubic) using a method similar to that described in [22]. The parameters σ_{12} and ε_{12} were determined using the simple combinational relations: $\sigma_{12} = \sqrt{\sigma\widetilde{\sigma}}$ and $\varepsilon_{12} = \sqrt{\varepsilon\widetilde{\varepsilon}}$.

3 Behavior of the correlation functions

Shear viscosity coefficient was calculated from the Green–Kubo formula [23]

$$\eta = \frac{V}{3k_B T}\int_0^\tau \left\langle J_{xy}(t)J_{xy}(t+t_1) + J_{yz}(t)J_{yz}(t+t_1) + \right.$$
$$\left. + J_{zx}(t)J_{zx}(t+t_1)\right\rangle dt_1, \qquad (4)$$

where the *xy* component of the stress tensor for a binary mixture has the form

$$J_{xy} = \frac{1}{V}\left[\sum_{\alpha=1}^{2}\sum_{i=1}^{N_\alpha}m_\alpha\dot{x}_i\dot{y}_i + \frac{1}{2}\sum_{\alpha=1,i\neq j}^{N_1}F_{x,ij}y_{ij} + \right.$$
$$\left. + \frac{1}{2}\sum_{\alpha=2,i\neq j}^{N_2}F_{x,ij}y_{ij} + \sum_{i=1}^{N_1}\sum_{j=1}^{N_2}F_{x,ij}y_{ij}\right]. \qquad (5)$$

Here subscript $\alpha=1$ refers to molecules, subscript 2 to nanoparticles, m_i is the mass of a particle (molecule or nanoparticle), V is the volume of the system, T is the temperature of the medium, τ is the time to reach a plateau value [24], F is the force acting on a molecule or nanoparticle, x and y are the coordinates of the molecule or nanoparticle, and N_1 and N_2 are the numbers of molecules and nanoparticles, respectively. The angular brackets in (4) demote an ensemble average.

Equations (4) were obtained in [23] for molecular systems, but in a book of one of the authors [25], it is shown that they have the same form for disperse systems, in particular, for nanofluids.

Fluctuation-dissipative theorem (4) gives the connection between the viscosity coefficient of the nanofluid and velocity correlation functions (the functions in the angular brackets). Therefore the value of the viscosity coefficient will be determined by the evolution of the appropriate correlation functions. According to (4), (5), the nanofluid viscosity coefficient contains several different contributions

$$\eta = \eta_k + \eta_p + \eta_{kp}, \qquad (6)$$

where the first term describes the kinetic contribution

$$\eta_k = \frac{1}{k_B TV}\sum_{\alpha,\beta=1,2}\int_0^\tau\left\langle\sum_{i=1}^{N_\alpha}m_\alpha\dot{x}_i\dot{y}_i(t)\sum_{j=1}^{N_\beta}m_\beta\dot{x}_j\dot{y}_j(t+t_1)\right\rangle dt_1, \quad (7)$$

the second term describes the potential contribution

$$\eta_p = \frac{1}{4k_B TV}\sum_{\alpha,\beta=1,2}\int_0^\tau\left\langle\sum_{i\neq j}^{N_\alpha}F_{x,ij}y_{ij}(t)\sum_{k\neq l}^{N_\beta}F_{x,kl}y_{kl}(t+t_1)\right\rangle dt_1 +$$
$$+ \frac{1}{k_B TV}\int_0^\tau\left\langle\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}F_{x,ij}y_{ij}(t)\sum_{k=1}^{N_1}\sum_{l=1}^{N_2}F_{x,kl}y_{kl}(t+t_1)\right\rangle dt_1 +$$
$$+ \frac{1}{2k_B TV}\sum_\alpha\int_0^\tau\left\langle\sum_{i\neq j}^{N_\alpha}F_{x,ij}y_{ij}(t)\sum_{k=1}^{N_1}\sum_{l=1}^{N_2}F_{x,kl}y_{kl}(t+t_1) + \right.$$
$$\left. + \sum_{k=1}^{N_1}\sum_{l=1}^{N_2}F_{x,kl}y_{kl}(t)\sum_{i\neq j}^{N_\alpha}F_{x,ij}y_{ij}(t+t_1)\right\rangle dt_1, \qquad (8)$$

and the third describes the cross effects

$$\eta_{kp} = \frac{1}{k_B TV}\left[\sum_{\alpha,\beta=1,2}\int_0^\tau\left\langle\sum_{i=1}^{N_\alpha}m_\alpha\dot{x}_i\dot{y}_i(t)\times\right.\right.$$
$$\left. \times\frac{1}{2}\sum_{k\neq l}^{N_\beta}F_{x,kl}y_{kl}(t+t_1)\right\rangle dt_1 +$$
$$+ \left.\sum_{\alpha=1,2}\int_0^\tau\left\langle\sum_{i=1}^{N_\alpha}m_\alpha\dot{x}_i\dot{y}_i(t)\sum_{k=1}^{N_1}\sum_{l=1}^{N_2}F_{x,kl}y_{kl}(t+t_1)\right\rangle dt_1\right], \quad (9)$$

In the fig. 1 the typical example of correlation functions χ_i, entering into expressions (7)-(9) and defining coefficient of viscosity of the nanofluid Ar-Al with particles of diameter 2 nm is given. Volume concentration of nanoparticles equals 10% in this example. Pressure of the nanofluid equals to pressure of

pure Ar at density $\rho = 0.707$ and temperature $T = 300$ K. Correlation functions χ_i are normalized on $(N_1 + N_2)k_B T/V$, time is normalized on $\sigma/v_{T,1}$, where $v_{T,1}$ – thermal velocity of molecules of carrying media. Function χ_1 on the fig. 1 (dotted line) corresponds to the kinetic contribution to coefficient of viscosity (see (7)), function χ_2 (dash-dotted line) corresponds to the potential one (the formula (8)), function χ_3 (dashed line) corresponds to the potential-kinetic one (the formula (9)). At last the solid line corresponds to the total correlation function $\chi = \chi_1 + \chi_2 + \chi_3$.
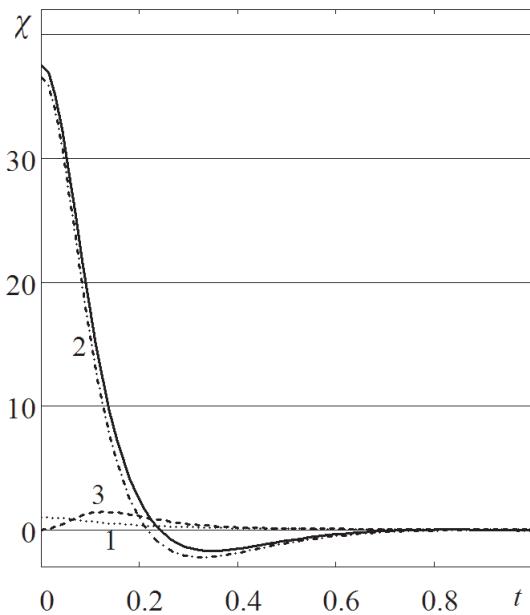

Fig. 1. The normalized kinetic, potential, potential-kinetic and total correlation functions for coefficient of viscosity of nanofluid

Analysis of the fig. 1 shows that function χ is mainly determined by the function χ_2 defining the potential contribution to transport of impulse. It considerably exceeds the kinetic χ_1 and potential-kinetic χ_3 functions. The consequence of this is that parameters of potentials (1), (2) make the considerable impact on value of coefficient of shift viscosity of nanofluids. Therefore it should depend on material of nanoparticles. This point of view is confirmed with the data of

modeling too.

Table. Contributions of different components to the viscosity of nanofluids (µPa·s)

	Ar	Al-Ar	Li-Ar
η	117.4	169.8	182.9
η_k	13.4	11.6	11.0
η_p	88.0	138.5	153.0
η_{kp}	16.1	19.7	18.9
$\eta_{p1,1}$	88.0	81.7	83.0
η_{p12}		34.7	44.0
$(\eta_{p1,p12} + \eta_{p12,p1})$		22.1	25.9

This table shows a comparison of each of the contributions for argon and the two nanofluids considered. In both cases, the concentration of nanoparticles was equal to $\varphi = 0.097$, and the diameter of the nanoparticles was 2 nm. The pressure of all three fluids was the same and equal to the pressure of pure Ar at a density $\rho = 0.707$ and a temperature $T = 300$ K. The sixth row of the table shows the potential contribution to the viscosity due to the interaction of argon molecules, the seventh row shows the potential contribution due to the correlation between the intermolecular forces and the interaction forces of the molecules with the particle (the third term in formula (8)). Finally, the last row shows the contribution due to the last term in (8). From an analysis of the Table's data, it appears that, first, although the overall viscosity of nanofluids is significantly higher than the viscosity of the carrier fluid, the kinetic contributions η_k are lower. This decrease is due to a reduction in the number density of molecules in the nanofluid compared to the carrier fluid. On the other hand, the kinetic contribution of nanoparticles is small since the volume (and mass) of a nanoparticle is much higher than the volume (mass) of the molecule, with the conservation of the average kinetic energy of the molecules and nanoparticles. It should also be emphasized that since the fluid is dense, the contribution of the kinetic processes to the transfer of the momentum (viscosity) is small: for argon, it is about 11%, and for the nanofluids, 6–7%.

The potential contribution of the

molecules $\eta_{p1,1}$ (sixth row of in the Table) in the nanofluids is also slightly reduced. The role of the cross terms η_{kp} (fifth row in the table) is small and is about ten percent. In all our calculations, the potential contribution of the particle interaction was almost equal to zero. Thus, the increase in the viscosity is due mainly to nanoparticle–molecule interactions and the correlations between molecule–molecule and molecule–nanoparticle interactions. Dependence of value of these contributions on a size of the dispersed particles is easy for qualitative estimating. Let there are particles with radiuses R_1 and R_2, for definiteness we will consider that $R_2 > R_1$. At the given volume concentration numbers of those and other particles in a unit volume are in inverse proportion to cubes of their radiuses: $N_2 / N_1 = R_1^3 / R_2^3$. On the other hand, total cross-sections of scattering of molecules of a carrying fluid with those and with other particles are accordingly equal $S_1 = N_1 \pi R_1^2$ and $S_2 = N_2 \pi R_2^2$. Therefore the ratio of these cross-sections which determine value of considered potential contributions, appears to be inversely proportional to their radiuses: $S_2 / S_1 = R_1 / R_2$. These simple estimations show that with growth of particle sizes the relative value of these contributions will decrease.

4 Simulation results

Since all the nanofluids studied had a relatively low concentration of nanoparticles, it might be expected that the resulting viscosity would be described by a quadratic dependence on the volume concentration of nanoparticles φ

$$\eta / \eta_0 = \eta_r = 1 + a_1 \varphi + a_2 \varphi^2 . \qquad (9)$$

where η_0 is the viscosity of pure argon. Our calculations have shown that it is indeed so. The dependence of the dimensionless viscosity η_r on the volume concentration of nanoparticles is shown in Fig. 2. Here the density of the carrier fluid was $\rho = 0.707$, and the temperature $T = 300$ K; circles represent

data for the nanofluid with Li particles, and triangles represent data for the nanofluid with Al particles. In all cases, the diameter of the nanoparticles was 2 nm. As a result, for the nanofluid with lithium nanoparticles, in formula (9) we obtained $a_1 = 3.20$ and $a_2 = 25.38$ (dash-dot line number 1 in Fig. 2), and for the nanofluid with aluminum nanoparticles, $a_1 = 3.25$ and $a_2 = 13.06$ (dotted line number 2 in Fig. 2.) In all cases, the viscosity of two considered nanofluids is substantially higher than that for conventional dispersions. Thus, even at low particle concentrations, the effective viscosity of nanofluids is not described by Einstein's theory, which gives $a_1 = 2.5$. The dashed line number 3 in Fig. 2 shows the dependence obtained by Batchelor [26] taking into account the hydrodynamic interaction of dispersed particles and their Brownian motion. The Batchelor formula provides a good fit to various experimental data for conventional disperse systems, but the values given by this formula are significantly smaller than those for nanofluids (see Fig.2).
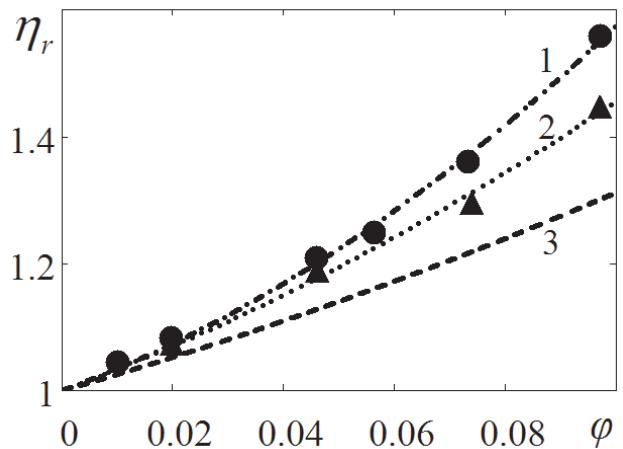

Fig. 2. Dependence of the dimensionless viscosity of a nanofluid on a volume concentration of nanoparticles which are made of different materials

The second important point is that the viscosities of the nanofluids with aluminum and lithium nanoparticles are significantly different. Thus, the viscosity of nanofluids indeed depends on the nanoparticle material. To answer the question of how nanofluid

viscosity depends on the nanoparticle size, we performed calculations for nanofluids with lithium nanoparticles of diameter 1, 2, and 4 nm at volume concentrations of nanoparticles φ = 2% and 4%. The results can be approximated, e.g., by the following exponential dependence on the nanoparticle diameter with precision about 5%

$$\eta_r = \eta_B + \left(5.25\varphi + 40.94\varphi^2\right)\exp\left(-0.208D/d\right), (10)$$

where D is the diameter of the nanoparticles and d is the diameter of the molecules. In the limit $D/d \gg 1$ the formula (10) coincides with Batchelor formula.

5 Discussion of Results

The data presented in the previous section suggest that the effective viscosity of nanofluids increases with increasing concentration of nanoparticles. At moderate volume concentrations of particles, the dependence of the viscosity on the concentration of nanoparticles can be described by the quadratic function (9), as for conventional dispersed fluids. At the same time, the viscosity of nanofluids at a given particle concentration is substantially higher than that for conventional dispersed fluids. This is consistent with virtually all existing experimental data (see [1–3]). In addition, the viscosity of a nanofluid cannot be described by existing classical theories because it depends not only on the concentration of nanoparticles, but also on their size. For the model nanofluids considered in this paper, this dependence is given by relation (10), which is in qualitative agreement with the data of [3, 6–8]. The viscosity of nanofluids decreases with increasing particle size. Physically, this is a reasonable result since as the particle size tends to the size of conventional macroscopic particles, relation (10) should reduce to the classical formulas for the viscosity of nanofluids, e.g., in Batchelor formula.

Another important feature that distinguishes the viscosity of nanofluids from that of conventional dispersions is its dependence on the nanoparticle material. This dependence should disappear with increasing nanoparticle size. However, if the particles are sufficiently small, accounting for this dependence is important and one cannot hope to obtain a universal formula for the viscosity. It can be expected that this dependence can be neglected even for nanofluids with a characteristic particle size of more than ten nanometers. Indirect evidence for this is provided by kinetic theory [11, 12] and molecular dynamics simulations of the diffusion of nanoparticles [27]. It should also be noted that the appearance of the dependence on the nanoparticle material is not due to the choice of a particular interaction potential; it has also been recorded for the hard-sphere potential [4, 5]. The appearance of this dependence is due to taking into account the individual characteristics of nanoparticles (in particular, their masses and interaction potential parameters) in their interaction with carrier fluid molecules and with each other, as is the case in conventional molecular fluids,. To see this, it is necessary to analyze the simulation process of nanofluids from a molecular-kinetic point of view.

The last interesting question is following, why do the viscosity coefficients of nanofluid and course dispersed fluid with low particle concentration differ?

A simple explanation of this may be found in the following consideration. In a suspension with macroscopic particles at volume concentrations less than or of the order of $\varphi \sim 10^{-3}$, the distances between the particles are large enough, so that their interaction can be neglected. Indeed, suppose that the dispersed particle size is $D \sim 10^{-4}$ cm. Then, at the specified volume concentration of these particles, the average distance between them is $l_m^p \sim n_p^{-3}$, where $n_p = 6\varphi/(\pi D^3)$ is the number density of the particles. For these data, $n_p \sim 2 \cdot 10^9$ and $l_m^p \sim 10^{-3}$ cm. In this case the mutual influence of particles on the perturbations induced by these particles in the carrier fluid velocity field can be neglected. Therefore the viscosity coefficient of the suspension can be described by Einstein's formula $\eta_B = 1 + 2.5\varphi$.

In nanofluids, the particle size is of the order

of $\beta \cdot 10^{-7}$ cm, where the parameter β takes values of 1 to 10^2. At the same volume concentration ($\varphi \sim 10^{-3}$), the average distance between nanoparticles in the fluid is $l_m^{np} \sim n_{np}^{-3}$. The number density of nanoparticles in this case is of the order of $n_{np} \sim 10^{19} \beta^{-3}$ and varies from $2 \cdot 10^{19}$ to $2 \cdot 10^{13}$, depending on the size of the particles. Accordingly, the distance between the particles varies from $4 \cdot 10^{-7}$ to $4 \cdot 10^{-5}$ cm. In all cases the distance between the nanoparticles are of the order of their size. Therefore we need to take into account the hydrodynamic interaction of the particles even at these low concentrations.

6 Conclusion

In conclusion, two things must be pointed out. In this paper, we considered nanofluids based on a very dense gas. Argon becomes a liquid at much lower temperatures and then the relative viscosity is even much higher. This, in particular, is due to the fact that in liquids, the role of the potential contributions is even greater. In particular, in nanofluid Ar-Al at carrying media density ρ = 0.707, volume concentration φ = 9.91% of aluminum particles of diameter 2 nm, at temperature T = 140 K the relative coefficient of viscosity is η_r = 1.900 while at T = 300 K it is η_r = 1.450.
And second, the choice of pressure is a necessary condition for correct comparison of the transport coefficients of the carrier fluid and nanofluid. This is consistent with experimental practice.

6 Achnoledgements

References

1. Mahbubul I.M., Saidur R., Amalina M.A. Latest developments on the viscosity of nanofluids. *International J. Heat and Mass Transfer*, 2012, **55**, 874-885.
2. Hosseini S.Sh., Shahrjerdi A. and Vazifeshenas Y. A review of relations for physical properties of nanofluids. *Australian J. Basic and Applied Sciences*, 2011, **5**(10), 417-435.
3. Rudyak V.Ya. Viscosity of nanofluids. Why it is not described by the classical theories. *Advances in Nanoparticles*, 2013, **2**, 266-279.
4. Rudyak V.Ya., Belkin A.A., Tomilina E.A., Egorov V.V. Nanoparticle friction force and effective viscosity of nanofluids. *Defect and Diffusion Forum*, 2008, **273-276**, 566-571.
5. Rudyak V.Ya., Belkin A.A. and Egorov V.V. On the effective viscosity of nanosuspensions. *Technical Physics*, 2009, **54**(8), 1102-1109.
6. Rudyak V.Ya., Dimov S.V., Kuznetsov V.V. and Bardakhanov S.P. Measurement of the viscosity coefficient of an ethylene glycol-based nanofluid with silicon dioxide particles. *Doklady Physics*, 2013, **58**(5), 173-176.
7. Rudyak V.Ya., Dimov S.V. and Kuznetsov V.V. About dependence of the nanofluid viscosity coefficient on the temperature and size of the particles. *Technical Physics Letters*, 2013, **39**(17), 53-59.
8. Timofeeva E.V., Smith D.S., Yu W., France D.M., Singh D., Routbo J.L. Particle size and interfacial effects on thermo-physical and heat transfer characteristics of water-based α-SiC nanofluids. *Nanotechnology*, 2010, **21**(21), 215703. doi:10.1088/0957-4484/21/21/215703.
9. He Y., Jin Y., Chen H., Ding Y., Cang D. and Lu H. Heat transfer and flow behavior of aqueous suspensions of TiO_2 nanoparticles (nanofluids) flowing upward through a vertical pipe. *Int. J. Heat Mass Transfer*, 2007, **50**(11-12), 2272-2281.
10. Nguyen C.T., Desgranges F., Roy G., Galanis N., Marer T., Boucher S. and Mintsa H. Temperature and particle-size dependent viscosity data for water-based nanofluids – Hysteresis phenomenon. *Int.*

J. Heat and Fluid Flow, 2007, **28**, 1492-1506.

11. Rudyak V.Ya., Krasnolutskii S.L. About viscosity of rarefied gas suspensions with nanoparticles. *Doklady Physics*, 2003, **48**(10), 583–586.

12. Rudyak V.Ya., Krasnolutsky S.L. Effective viscosity coefficient for rarefied gas nanosuspensions. *Atmosphere and Ocean Optics*, 2004, **17**(5), 468–475.

13. Rudyak V., Dimov S., Krasnolutskii S., Ivanov D. Effective viscosity of the nanofluids: Experimental studying and molecular dynamics simulation. *Technical Proceedings of the 2013 NSTI Nanotechnology Conference and Expo. NSTI-Nanotech*, 2013, **2**, 370-373.

14. Rapaport D.C. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, 1995. 549 p.

15. Norman G.E., Stegailov V.V. Stochastic Theory of the Classical Molecular Dynamics Method. *Mathematical Models and Computer Simulations*, 2013, **5**(4), 305-333.

16. Rudyak V.Ya., Krasnolutskii S.L. The interaction potential of dispersed particles with carrier gas molecules. *Rarefied Gas Dynamics XXI. Proc. 21st Int. Symp. on RGD*. Toulouse, Gépadués-Éditions, 1999, **1**, 263–270.

17. Rudyak, V.Ya., Krasnolutskii, S.L. Kinetic description of nanoparticle diffusion in rarefied gas. *Doklady Physics*, 2001, **46**(12), 897-899.

18. Rudyak V.Ya., Krasnolutskii S.L. and Ivanov D.A. The Interaction Potential of Nanoparticles. *Doklady Physics*, 2012, **57**(1), 33-35. doi:10.1134/S1028335812010053

19. Schofield P. Computer simulation studies of the liquid state. *Comput. Phys. Comm.*, 1973, **5**(1), 17-23.

20. Hirschfelder J.O., Curtiss Ch.F. and Bird R.B. *Molecular Theory of Gases and Liquids*. Wiley, New York, 1954.

21. Arefyev K.M. *Transport processes in gases and plasma*. Leningrad, Energoatomizdat, 1983, 127 p.

22. Heinz H., Vaia R.A., Farmer B.L., Naik R.R. Accurate Simulation of Surfaces and Interfaces of Face-Centered Cubic Metals Using 12−6 and 9−6 Lennard-Jones Potentials. *J. Phys. Chem. C*, 2008, **112**(44), 17281–17290. DOI: 10.1021/jp801931d

23. M.P. Allen, D.J. Tildesley, *Computer Simulation of Liquids*, University Press, Oxford, 1987.

24. Rudyak V.Ya., Belkin A.A., Ivanov D.A., Egorov V.V. The simulation of transport processes using the method of molecular dynamics. Self-diffusion coefficient. *High Temperature*, 2008, **46**(1), 30-39.

25. Rudyak V.Ya. *Statistical Aerohydromechanics of Homogeneous and Heterogeneous Media. Vol. 2: Hydromechanics*. Novosibirsk, Novosibirsk State University of Architecture and Civil Engineering, 2005, 468 p.

26. Batchelor G.K. The effect of Brownian motion on the bulk stress in a suspension of spherical particles. *J. Fluid Mech.*, 1977, **83**(1), 97-117.

27. Rudyak V.Ya., Krasnolutskii S.L., Ivanov D.A. Molecular dynamics simulation of nanoparticle diffusion in dense fluids. *Microfluidics and Nanofluidics*, 2011, **11**(4), 501-506. DOI: 10.1007/s10404-011-0815-4.