

Molecular simulation of thermal conductivity of rarefied gas nanosuspensions

Sergei Krasnolutskii^{1*}, *Eugene Lezhnev*^{1,2}, and *Valery Rudyak*^{1,2}

¹Novosibirsk State University of Architecture and Civil Engineering (Sibstrin), Theoretical Mechanics Department, 630008, Leningradskaya str. 113, Novosibirsk, Russia

²Kutateladze Institute of Thermophysics, Siberian Branch of the RAS, 630090, Ak. Lavrentieva ave. 1, Novosibirsk, Russia

Abstract. The thermal conductivity coefficient of rarefied gas nanosuspensions is modelled using kinetic theory and stochastic molecular modelling (SMM) method. Gas nanosuspensions based on rarefied argon with spherical zinc nanoparticles with diameters of 5, 10 and 20 nm at temperature of 300 K and atmospheric pressure are considered. The interactions of carrier gas molecules, a carrier gas molecule with a nanoparticle, and nanoparticles between themselves are described using Lennard-Jones, Rudyak–Krasnolutskii (RK) and Rudyak–Krasnolutskii–Ivanov (RKI) potentials respectively. It is shown that the thermal conductivity of the Ar-Zn gas nanosuspensions is lower than one of pure argon and decreases with an increase in the volume concentration of nanoparticles and a decrease in their size. In particular, the thermal conductivity of a gas nanosuspension with particles with a diameter of 5 nm at their volume concentration 0.001 drops by 8.2% compared to pure argon. The results obtained using both methods are consistent well.

1 Introduction

Gas nanosuspensions are nanofluids in which the carrier medium is gas. They can be used and are already done in various industrial technological processes, medicine, and are also important for environmental monitoring [1, 2]. Also, the problems of describing the combustion and detonation processes in gas nanosuspensions are quite relevant [3].

To model the gas nanosuspensions flows, it is necessary to know their transport coefficients, in particular, the coefficient of thermal conductivity. To date, the only method of determining the transport coefficients is an experiment. However, it is clear that in this way it is impossible to determine all possible transport coefficients for different external parameters. It is also impossible to provide experiments for gas nanosuspensions with particles from different materials in a wide range of their sizes and for different carrier gas. Therefore, it is required to have a theory and tools for calculating the transport coefficients of gas nanosuspensions. Classical theories [4, 5] created for the description of suspensions with macroscopic particles do not applicable for rarefied gas nanosuspensions because the particle size is much more than the free path length of the carrier gas molecules.

In paper [6] it was shown that Boltzmann kinetic theory can be used to describe the dynamics of ultra disperse rarefied gas suspensions and transport processes in them. Using this theory, we have modelled diffusion [7] and thermal diffusion [8] of nanoparticles in a rarefied gas, the effective viscosity of rarefied gas nanosuspensions [9], and influence of nanoparticle

material on transport coefficients [10]. It has been experimentally shown that the Cunningham–Milliken–Davies correlation [11] does not work well for determining the size of nanoparticles smaller than 10 nm by their diffusion coefficient, while the kinetic theory gives well results [12]. However, effective thermal conductivity of rarefied gas nanosuspensions has not yet been considered.

The molecular dynamics method is not actually applicable for modelling the transport coefficients of the rarefied gases and rarefied gas nanosuspensions. Therefore, the method of stochastic molecular modelling (SMM) has been developed [13, 14]. This method is intended, in particular, for calculating the transport coefficients in rarefied gases, their mixtures and gas nanosuspensions not only in the bulk, but in nanochannels of various shapes and porous media, for which it is difficult to solve the kinetic equation. In particular, using this method, the effective viscosity of rarefied gas nanosuspensions of Cu₂O in nitrogen, Zn in neon and U in hydrogen were simulated [15].

Thus, the purpose of this paper is to apply the kinetic theory and the SMM method to calculate the effective thermal conductivity coefficient of rarefied gas nanosuspensions. Gas nanosuspensions based on rarefied argon with spherical zinc nanoparticles at a temperature of 300 K and atmospheric pressure is considered. The size of nanoparticles was varied from 5 to 20 nm, and their volume concentration was varied from 0 to 10⁻³. The interactions of carrier gas molecules, a carrier gas molecule with a nanoparticle and nanoparticles between themselves are described using

*Corresponding author: sergius-l@mail.ru

Lennard-Jones, RK [16] and RKI [17] potentials, respectively.

2 The simulation techniques

The interaction of carrier gas molecules was described by the Lennard-Jones 6-12 potential

$$U = 4\varepsilon_1 \left[\left(\frac{\sigma_1}{r} \right)^{12} - \left(\frac{\sigma_1}{r} \right)^6 \right]$$

with parameters $\sigma_1 = 3.542 \text{ \AA}$, $\varepsilon_1 = 93.3 \text{ K}$ calculated from the viscosity coefficient of rarefied argon [18]. The RK potential [16] describing the interaction of carrier gas molecules with spherical nanoparticles of radius R has the following form

$$\Phi(r) = \Phi_9(r) - \Phi_3(r), \quad (1)$$

where

$$\begin{aligned} \Phi_9(r) &= C_9 \left\{ \left[\frac{1}{(r-R)^9} - \frac{1}{(r+R)^9} \right] - \frac{9}{8r} \left[\frac{1}{(r-R)^8} - \frac{1}{(r+R)^8} \right] \right\}, \\ \Phi_3(r) &= C_3 \left\{ \left[\frac{1}{(r-R)^3} - \frac{1}{(r+R)^3} \right] - \frac{3}{2r} \left[\frac{1}{(r-R)^2} - \frac{1}{(r+R)^2} \right] \right\}, \\ C_9 &= \frac{4\pi \varepsilon_{ij} \sigma_{ij}^{12}}{45 V}, \quad C_3 = \frac{2\pi \varepsilon_{ij} \sigma_{ij}^6}{3 V}. \end{aligned}$$

Here V is the volume per atom of a dispersed particle.

Potential parameters $\sigma_2 = 2.46 \text{ \AA}$, $\varepsilon_2 = 1040 \text{ K}$ were used for zinc atoms [19]. The geometric averages are used as combinational relations for calculating the parameters of the interaction potential of the atoms of the carrier gas and the dispersed particle

$$\sigma_{ij} = \sqrt{\sigma_{ii} \sigma_{jj}}, \quad \varepsilon_{ij} = \sqrt{\varepsilon_{ii} \varepsilon_{jj}}.$$

The effective thermal conductivity coefficient of the gas nanosuspension was calculated in the first approximation of the Chapman–Enskog method for spherically symmetric molecules and nanoparticles for which Eiken corrections do not need to be used [20,21]

$$\lambda_k = \frac{1 + Z_\lambda}{X_\lambda + Y_\lambda}, \quad (2)$$

where

$$\begin{aligned} X_\lambda &= \frac{x_1^2}{\lambda_1} + \frac{2x_1x_2}{\lambda_{12}} + \frac{x_2^2}{\lambda_2}, \\ Y_\lambda &= \frac{x_1^2}{\lambda_1} U^{(1)} + \frac{2x_1x_2}{\lambda_{12}} U^{(Y)} + \frac{x_2^2}{\lambda_2} U^{(2)}, \\ Z_\lambda &= x_1^2 U^{(1)} + 2x_1x_2 U^{(Z)} + x_2^2 U^{(2)}, \end{aligned}$$

$$U^{(1)} = \frac{4}{5} A_{12}^* - \frac{1}{12} \left(\frac{12}{5} B_{12}^* + 1 \right) \frac{m_2}{m_1} + \frac{1}{2} \frac{(m_1 - m_2)^2}{m_1 m_2},$$

$$\begin{aligned} U^{(2)} &= \frac{4}{5} A_{12}^* - \frac{1}{12} \left(\frac{12}{5} B_{12}^* + 1 \right) \frac{m_1}{m_2} + \frac{1}{2} \frac{(m_1 - m_2)^2}{m_1 m_2}, \\ U^{(Y)} &= \frac{4}{5} A_{12}^* \frac{(m_1 + m_2)^2}{4m_1m_2} \frac{\lambda_{12}^2}{\lambda_1\lambda_2} - \frac{1}{12} \left(\frac{12}{5} B_{12}^* + 1 \right) - \\ &\quad - \frac{5}{32A_{12}^*} \left(\frac{12}{5} B_{12}^* - 5 \right) \frac{(m_1 - m_2)^2}{m_1 m_2}, \\ U^{(Z)} &= \frac{4}{5} A_{12}^* \left[\frac{(m_1 + m_2)^2}{4m_1m_2} \left(\frac{\lambda_{12}}{\lambda_1} + \frac{\lambda_{12}}{\lambda_2} \right) - 1 \right] - \\ &\quad - \frac{1}{12} \left(\frac{12}{5} B_{12}^* + 1 \right), \end{aligned}$$

$$\lambda_i = \frac{25}{32} \frac{(\pi m_i k T)^{1/2}}{\pi \sigma_{ii}^2 \Omega_{ii}^{(2,2)*} (T_i^*)} \frac{3k}{2m_i},$$

$$\lambda_{12} = \frac{25}{32} \frac{(2\pi m_{12} k T)^{1/2}}{\pi R^2 \Omega_{12}^{(2,2)*} (T_{12}^*, \sigma_{12}^*)} \frac{3k}{4m_{12}},$$

$$A_{12}^* \equiv \frac{\Omega_{12}^{(2,2)*}}{\Omega_{12}^{(1,1)*}}, \quad B_{12}^* \equiv \frac{5\Omega_{12}^{(1,2)*} - 4\Omega_{12}^{(1,3)*}}{\Omega_{12}^{(1,1)*}}.$$

Here x_1, x_2 are the molar fractions of the components, index 1 refers to a carrier gas, and index 2 refers to nanoparticles, $\sigma_{22} = 2R$ is the diameter of the dispersed particle, $T_i^* \equiv kT/\varepsilon_{ii}$, $\Omega_{ij}^{(l,r)*}$ are the reduced Ω -integrals [20, 21].

In general, the transport coefficients of the fluids are determined by the fluctuation-dissipation theorems (FDTs) [22]. These FDTs are known in the literature as Green–Kubo formulas [23–25]. According to FDTs, the transport coefficients are time integrals of two-time correlation functions of the corresponding dynamic variables. The equivalence of the formulas for the transport coefficients of the kinetic theory of gases to the Green–Kubo formulas is proved in [26, 27]. The calculation of correlation functions requires information about the dynamic variables of the system being modelled at successive moments of time. In a rarefied gas and in a rarefied gas nanosuspension the interaction of molecules does not contribute to the transport coefficients and to the equation of state. The corresponding contributions appear only in the so-called nonideal gas [28]. For this reason, to model the transport coefficients of a rarefied gas nanosuspension, it is sufficient to have data on the dynamic variables of its molecules and particles only in the velocity space.

Modelling by the SMM method was carried out as follows. In accordance with the given mass density of gas (or numerical one) the molecules are distributed uniformly over the simulation volume. Their velocities are played out according to the Maxwell distribution with a given temperature. Since the equilibrium state of the system was modelled, the total momentum should be zero. To do this, a special procedure is carried out, described in [14]. At the initial time t , all molecules and nanoparticles are listed in some arbitrary order. By changing the order of the particles in this list, we will get different phase trajectories. Thus, at time t , the particles have velocities $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$ and coordinates $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$. Then the calculation time t_s of the phase trajectory is divided in intervals $\tau_i = \sigma_1/v_{i\alpha}$, here $v_{i\alpha}$ is

the maximum modulo velocity of gas molecules of the system at a given time. The formation of the list at the first-time step ($t + \tau_1$) begins with the consideration of particle (molecule) 1. To check the collision of particle 1 during the time τ_1 with any other, a random number u is generated, evenly distributed over the interval $[0;1]$. If it turns out to be less than the average probability of a collision, then a collision will occur. Let, for certainty, consider a nanoparticle (for the gas molecules, the formulas are similar). The collision probability is determined by means of the kinetic theory [20, 21] and has the following form

$$P_\tau = 4\tau_1 n_2 (2R)^2 \sqrt{\frac{\pi k_B T}{m_2}} + 2\tau_1 n_1 d_{12}^2 \sqrt{\frac{2\pi k_B T}{m_1}} = P_2 + P_{12}, \quad (3)$$

where $d_{12} = R + \sigma_1/2$, R is the radius of the dispersed particle, n_α is the numerical density of the carrier gas or nanoparticles.

So if $u < P_2$ then a collision will occur with another nanoparticle j selected randomly from the $(N - 1)$ remaining ones. In this case the velocities of the collided particles are changed using the conserve equations. If $P_2 \leq u < (P_2 + P_{12})$ then the gas molecule j is selected for the collision. After next nanoparticle or molecule is randomly selected, their velocities change in accordance with conservation laws.

Movement under the influence of the Lennard-Jones potential, RK (1) or RKI [17] occurs in the plane defined by the vectors $\mathbf{r}_{j1} = \mathbf{r}_j - \mathbf{r}_1$ and $\mathbf{v}_{j1} = \mathbf{v}_j - \mathbf{v}_1$ and begins at a distance of $0 \leq b \leq \sigma/2$ (b is the aiming parameter). In this case, the angular momentum $M = m|\mathbf{r}_{j1} \times \mathbf{v}_{j1}| = mv_{j1}b$ relative to the centre of the field and the kinetic energy $E = mv_{j1}^2/2$ are preserved. The scattering angle of the particle is calculated as follows

$$\theta_0(b) = \int_{r_m}^{\infty} \frac{Mdr}{2\sqrt{2mr^2(E - U(r)) - M^2}}$$

Then the angle of deviation will be equal to $\chi = \pi - 2\theta_0(b)$. To obtain a vector in three-dimensional space, we need to construct orthonormal basis vectors in the interaction plane. First of them is defined in an obvious way $\mathbf{e}_v = \mathbf{v}_{j1}/|\mathbf{v}_{j1}|$. The second one is determined based on the process of obtaining the orthogonal Gram-Schmidt basis $\mathbf{r}_1 = \mathbf{r}_{j1} - \mathbf{r}_{j1}(\mathbf{r}_{j1} \cdot \mathbf{e}_v)/r_{j1}^2$. Normalizing it, we get $\mathbf{e}_n = \mathbf{r}_1/|\mathbf{r}_1|$. Then the desired vector will be a linear combination of the basis vectors $\mathbf{e}_\chi = \mathbf{e}_n \sin\chi - \mathbf{e}_v \cos\chi$. Having this vector obtained, we find the velocities of the particles after the collision

$$\mathbf{v}'_1 = \mathbf{v}_1 + \frac{2(\mathbf{v}_{1j} \cdot \mathbf{e}_\chi)\mathbf{e}_\chi m_j}{(m_1 + m_j)},$$

$$\mathbf{v}'_j = \mathbf{v}_j - \frac{2(\mathbf{v}_{1j} \cdot \mathbf{e}_\chi)\mathbf{e}_\chi m_1}{(m_1 + m_j)}.$$

If the generated number turned out to be greater than the average probability of collision, the particle 1 does

not collide in the time interval τ_1 and its velocity remains equal to \mathbf{v}_1 . If it collides with a particle or molecule j , then the velocities 1 and j will change in the original list. Similarly, all remaining particles are processed sequentially. As a result, a new list of velocities $(\mathbf{v}'_1, \mathbf{v}'_2, \dots, \mathbf{v}'_N)$ is formed.

Then the second-time step ($t + \tau_2$) is determined and all procedure described repeats. The next list of the particles and molecules velocities is formed. This procedure is repeated until the calculation time is over. The result is a complete set of velocities of the molecules and particles of the system at successive times, which can be used to calculate correlation functions of the corresponding FDT.

The coefficient of thermal conductivity of the pure medium is determined by the following FDT

$$\lambda_{s0} = \frac{k_B}{3VT^2} \int_0^{\tau_p} \chi_0(t) dt, \quad (4)$$

where

$$\chi_0(t) = \langle \mathbf{j}(0) \cdot \mathbf{j}(t) \rangle, \quad \mathbf{j}(t) = 0.5 \sum_{\alpha,i} m_{\alpha,i} v_{\alpha,i}^2 \mathbf{v}_{\alpha,i}.$$

Here V is the volume of the simulation cell, k_B is the Boltzmann constant, $\chi_0(t)$ is the autocorrelator of heat flux.

However the gas nanosuspension is the two components medium. In order to calculate the thermal conductivity coefficient of the gas nanosuspension, it is necessary to exclude the contribution due to the mutual movement of its components. The corresponding FDT has the following form

$$\lambda_s = \frac{k_B}{3VT^2} \int_0^{\tau_p} \chi'(t) dt, \quad (5)$$

where

$$\chi'(t) = \langle \mathbf{j}'(0) \cdot \mathbf{j}'(t) \rangle,$$

$$\mathbf{j}'(t) = 0.5 \sum_{\alpha,i} m_{\alpha,i} v_{\alpha,i}^2 (\mathbf{v}_{\alpha,i} - \mathbf{v}_{\alpha,c}),$$

$$\mathbf{v}_{\alpha,c} = \frac{1}{N_\alpha} \sum_{\alpha,i} \mathbf{v}_{\alpha,i}.$$

Here $\mathbf{v}_{\alpha,c}$ are the velocities of the centre of mass of the carrier gas and nanoparticles.

The observed variables are obtained in SMM method (as in molecular dynamics method) averaging calculated data over ensemble of the independent phase trajectories. In presented data the average of the thermal conductivity coefficient is carried out over 1000 independent phase trajectories.

3 Simulation results

First, both methods described above were used to simulate the thermal conductivity coefficient of pure

argon at an atmospheric pressure of 101325 Pa and a temperature of 300 K. Simulation with the kinetic theory (3) gave $\lambda_k = 0.01784 \text{ W/(mK)}$. Using the SMM method, the thermal conductivity of pure argon was modelled as follows. The simulation cell contained 10143 argon atoms. 500 independent phase trajectories continuing of 80 mean free times per each were calculated. Averaging along the trajectories the coefficient (7) gave $\lambda_s = 0.01735 \text{ W/(mK)}$. Experimental value of thermal conductivity of pure argon at the same pressure and temperature is $\lambda_e = 0.01777 \text{ W/(mK)}$ [29]. Thus, the error in calculating the thermal conductivity coefficient of pure argon in the first approximation of the kinetic theory does not exceed 0.4 %; and by the SMM method does not 2.7 %. The typical error of the experimental measure of the thermal conductivity coefficient is 1–3 %. Kinetic theory gives slightly overestimated values of the thermal conductivity coefficient in comparison with the experimental data, while the SMM method, on the contrary, somewhat underestimates them.

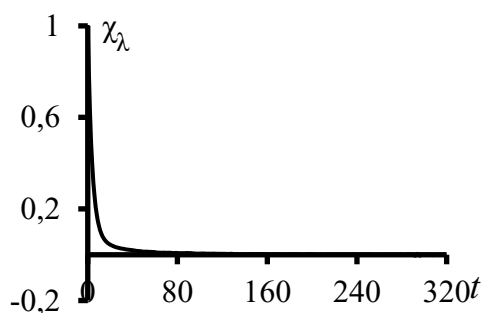


Fig. 1. The evolution of the normalized autocorrelation function of heat flux.

Then the thermal conductivity coefficient of the Ar-Zn gas nanosuspensions with nanoparticles of diameter 5, 10 and 20 nm at their volume concentrations of 5, 8 and $10 \cdot 10^{-4}$ were calculated by the kinetic theory and SMM method at the same pressure and temperature. The advantage of the SMM method is the possibility of studying the mechanisms of the transport processes. In particular, the SMM method permits to study the evolution of the correlation functions in formulas (4) or (5). As an example, we will describe in more detail the calculation of thermal conductivity of an argon-based gas nanosuspension with zinc particles with a diameter of 10 nm with volume concentration of $\phi = 5 \cdot 10^{-4}$. The simulation cell contained 198824 argon molecules and one nanoparticle. 1000 trajectories of 320 mean free times each were calculated. Figure 1 shows the evolution of the autocorrelation function of heat flux normalized by its value at the initial time $\chi_\lambda = \chi'(t)/\chi'(0)$ (see formula (5)). This autocorrelation function damps exponentially with character time of the order of several free path times. This behaviour corresponds the kinetic theory of rarefied gases and rarefied gas nanosuspensions in particular.

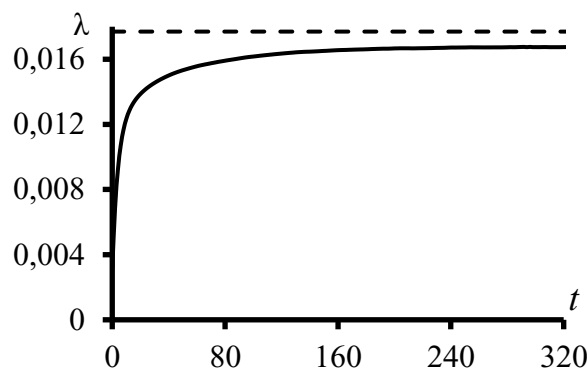


Fig. 2. Dependence of thermal conductivity coefficient [W/(m·K)] of Ar-Zn gas nanosuspension (solid line) on integration time (mean free path time).

Figure 2 shows the evolution (in units of mean free path time) of the thermal conductivity coefficient (5) of the Ar-Zn gas nanosuspension (solid line). The dashed line shows the value of the thermal conductivity coefficient of pure argon. The value obtained of the thermal conductivity coefficient is $\lambda_s = 0.01718 \text{ W/(m \cdot K)}$. It is important to note that the difference between the thermal conductivity coefficient with the diffusion contribution λ_{s0} (4) and without the diffusion contribution λ_s (5) is insignificant and amounts to only 10^{-4} %.

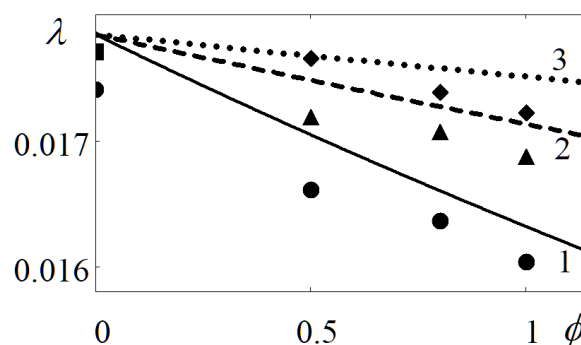


Fig. 3. Dependence of thermal conductivity coefficient [W/(m·K)] of gas nanosuspensions on volume concentration of nanoparticles ($\phi \cdot 10^3$).

As mentioned above the thermal conductivity of the Ar-Zn gas nanosuspension was also simulated using kinetic theory. Rarefied gas nanosuspensions based on argon with spherical zinc particles with diameters of 5, 10 and 20 nm at a temperature of 300 K and atmospheric pressure were considered. The volume concentration of nanoparticles varied from 0 to 10^{-3} . The simulation results are shown in Figure 3. Here solid (1), dashed (2) and dotted (3) lines show the dependence of the thermal conductivity coefficient of the gas nanosuspensions on the volume concentration of nanoparticles with diameters of 5, 10, and 20 nm respectively.

Experimental data for the thermal conductivity of pure argon at the same pressure and temperature are shown by a black rectangle (see $\phi = 0$ in Figure 3). The thermal conductivity of the Ar-Zn gas nanosuspension with nanoparticles with diameters of 5, 10 and 20 nm calculated by the SMM method is shown in Figure 3 by circles, triangles and rhombuses, respectively.

We see that the thermal conductivity of the Ar-Zn gas nanosuspension is lower than the thermal conductivity of pure argon and decreases with an increase in the volume concentration of nanoparticles. The second important conclusion is that the smaller the size of the nanoparticles the lower the thermal conductivity of the gas nanosuspension at the same volume concentration of nanoparticles and the more it differs from the thermal conductivity of the pure carrier gas.

4 Analysis of the thermal conductivity coefficient

The thermal conductivity coefficient of binary mixtures (2) can be expanded in a series in molar fraction of the second component x_2 . In particular, with a small molar fraction of this component, we obtain

$$\lambda_k(x_2) \approx \lambda_1 \times \left(1 + \frac{2x_2}{1+U^{(1)}} \left[1 + U^{(Z)} - \frac{\lambda_1}{\lambda_{12}} (1 + U^{(Y)}) \right] \right). \quad (6)$$

The nanoparticles have a much larger size and mass compared to the molecules of the carrier gas. Therefore in formula (6) the following small parameters are introduced

$$s \equiv \frac{\sigma_1}{\sigma_2} \equiv \frac{\sigma_1}{2R_p}, \quad \mu \equiv \frac{m_1}{m_2}, \quad \alpha \equiv \frac{s^3}{\mu}, \quad (7)$$

where α is the ratio of the density of the nanoparticle material to the "density" of the carrier gas molecule.

To understand the value of the coefficient λ_k in comparison with the coefficient λ_1 (light gas) one needs to determine the sign of the coefficient for the molar fraction of the second component x_2 in (6)

$$\begin{aligned} & \left[1 + U^{(Z)} - \frac{\lambda_1}{\lambda_{12}} (1 + U^{(Y)}) \right] \approx 1 + \\ & + \frac{2\sqrt{2}}{15} \frac{A_{12}^*}{\Omega_{12}^{(2,2)*}} \Omega_{11}^{(2,2)*} \frac{\alpha}{s} - \frac{\sqrt{2}}{4} \frac{\Omega_{12}^{(2,2)*}}{\Omega_{11}^{(2,2)*}} \frac{1}{s^2} + \\ & + \frac{5\sqrt{2}}{4 \cdot 32} \frac{1}{\Omega_{11}^{(2,2)*}} \frac{\Omega_{12}^{(2,2)*}}{A_{12}^*} \left(\frac{12}{5} B_{12}^* - 5 \right) \frac{\alpha}{s^5}. \quad (8) \end{aligned}$$

With large ratios of nanoparticle diameters to the diameters of carrier gas molecules corresponding to small values of the parameter s at comparable densities, expression (8) has a negative sign mainly due to the last term. Therefore the thermal conductivity of the gas nanosuspension is lower than the thermal conductivity of the carrier gas. In the case of a mixture of heavy and light nonpolar gases, expression (8) will also be negative. The thermal conductivity of the mixture of light and heavy gases (at low concentration of the heavy gas) has the thermal conductivity lower than the light gas.

The physical reason for the decrease in the thermal conductivity of the gas nanosuspension compared to pure carrier gas is a decrease in the free path of the

carrier gas molecules due to scattering on nanoparticles. The same reasons lead to a decrease in the thermal conductivity of a mixture of heavy and light nonpolar gases compared to pure light one.

5 Conclusion

In this paper, the thermal conductivity of a rarefied gas nanosuspension was simulated by two fundamentally different methods, while using the same interaction potentials. In the absence of the possibility of experimental verification, kinetic theory is actually used as a tool for testing the SMM method. Early the kinetic was experimentally tested [12].

We calculate the relative difference between the thermal conductivity of gas nanosuspension and pure gas by the two methods mentioned above. Thermal conductivity coefficient of argon-based gas nanosuspension with zinc particles of 5 nm diameter and volume concentration $\phi = 5 \cdot 10^{-4}$ calculated using kinetic theory is $\lambda_k = 0.01704$ W/(m · K). Consequently, the thermal conductivity coefficient of this gas nanosuspension decreased by 4.5% compared to pure argon calculated also using kinetic theory. On the other hand, the thermal conductivity coefficients of the same gas nanosuspension $\lambda_s = 0.01661$ W/(m · K) and pure argon calculated using the SMM differ by 4.3%. One can see that both methods showed almost the same decrease in the thermal conductivity of the gas nanosuspension compared to pure gas. Furthermore, the accuracy of the SMM method can be growth increasing the number of use nanoparticles and molecules or/and the number of the phase trajectories used.

Thus the calculations data using the kinetic theory and the SMM method are qualitatively consistent, showing a decrease in the thermal conductivity of a gas nanosuspension compared to pure carrier gas. The simulation results qualitatively correspond to experimental data on the thermal conductivity of mixtures of light and heavy nonpolar gases [18].

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