Bulk viscosity of gaseous argon from molecular dynamics simulations

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Bulk viscosity of dilute argon gas is calculated using molecular dynamics simulations in the temperature range 150–500 K and is found to be proportional to density squared in the investigated range of densities 0.001–$1\,\mathrm{kg\,m^{-3}}$. Comparison of the results obtained using Lennard–Jones and Tang–Toennies models of pair interaction potential reveals that the value of bulk viscosity coefficient is sensitive to the choice of the pair interaction model. Inclusion of Axilrod–Teller–Muto three-body interaction in the model does not noticeably affect the values of the bulk viscosity in dilute states, contrary to the previously investigated case of dense fluids.

I. INTRODUCTION

Bulk viscosity of fluids (also known as volume viscosity, or second viscosity) is a transport coefficient which corresponds to the irreversible part of the resistance of fluids to compression or expansion [1]. Recognized for a long time as an independent coefficient [2, 3], bulk viscosity manifests itself in various phenomena which involve compressible fluid flows, ranging from sound adsorption and dispersion [4] to shock wave structure [5, 6] and its interaction with bubbles [7] and vortices [8], supersonic [9, 10] and hypersonic [11] flows, combustion [12, 13], acoustic streaming [14, 15], separation of emulsions [16], longitudinal rheology [17], Rayleigh–Taylor instability [18], turbulent flows [19, 20] and capillary flows [21]. Despite vast range of applications, not many reviews dedicated to bulk viscosity of fluids have been published so far [22–24].

In dilute molecular gases, bulk viscosity arises due to the relaxation of internal degrees of freedom [23, 25]. For some molecular fluids it is predicted to be much larger than shear viscosity [26]. In contrast to molecular gases, monoatomic gases have no rotational and vibrational degrees of freedom, and electron excitations can be neglected unless thermal energy is comparable with electronic excitation energy. In absence of internal degrees of freedom bulk viscosity originates from the structural relaxation due to rearrangement of atoms during compression and rarefaction of the fluid [24]. The experimental data on bulk viscosity is most accurately obtained from measurements of acoustic absorption [27]. The experimental values of bulk viscosity have been reported for neon [28], argon [29–37], krypton [35–38] and xenon [35–37, 39]. Theoretical approaches to the bulk viscosity of simple fluids in their dense states, based on statistical mechanics and kinetic theory, require pair distribution function or other structural data of the fluid as their inputs [40–45], and are strongly dependent on the accuracy of these inputs [46, 47]. Predictive power of such theories decreases at high densities [48], therefore increasing the role of computer simulations. Simulations of bulk viscosity of liquid noble gases modeled by Lennard–Jones potential were carried out using Green–Kubo formula [49]

and modified Einstein relation [50] in a wide range of states, including the states close to the freezing line [51] and metastable states [52].

At low densities, the appropriate theoretical approach to describe the bulk viscosity of simple fluids is provided by kinetic theory of gases. The simplest model based on Boltzmann equation, which takes into account only two-body collisions between particles, predicts zero value of bulk viscosity [53], thus making it necessary to take into account higher-order collisions [54, 55]. Since bulk viscosity of monoatomic gases is determined by many-particle collisions, it has small value and is difficult to measure experimentally. Currently, the only source of experimental data on the bulk viscosity of monoatomic gases is the work of Madigosky on argon [33].

In the present work, we compute the values of the bulk viscosity coefficient obtained using molecular dynamics simulation of dilute argon gas. In addition to reporting these values, we aim to answer the following questions:

A. How bulk viscosity of argon gas depends on its density?

B. What is the effect of many-body interactions?

C. Can interatomic interaction be approximated by Lennard–Jones potential?

The motivation behind each of these questions is detailed in the following subsections.

A. Density dependence

The dependence of bulk viscosity of gases, μ, on their density, ρ, can be expressed in form of a 'virial' expansion [56]:

$$\mu(\rho) = \mu_0 + \mu_1\rho + \mu_2\rho^2 + \dots \qquad (1)$$

The bulk viscosity virial coefficients μ_0, μ_1, μ_2 etc. contain the contributions of binary, ternary, quaternary etc. collisions and, generally, depend on temperature. Higher-order contributions in Eq. (1) are known to diverge

[57, 58]. Nevertheless, the truncated virial expansion can be used at sufficiently low densities [59].

The low-density limit of bulk viscosity, given by μ_0, is zero for monoatomic gases [53]. In systems with only repulsive interactions the density expansion starts with the ρ^2 term [59–61]. However, in systems with attractive interactions the presence of the non-zero term proportional to ρ is not excluded due to possible existence of bound states [62, 63]. Simulations of Lennard–Jones fluid by Meier et al. [50] give bulk viscosity proportional to ρ at low densities, while the experimental values of bulk viscosity measured for argon by Madigosky [33] are proportional to ρ^2, although the gas was not dilute in both these cases. The question on the low-density behaviour of bulk viscosity remains open.

In order to recover the density dependence of the bulk viscosity of dilute gas, we carry out molecular dynamics simulations at very low (down to 10^{-3} kg m^{-3}) densities.

B. Many-body interaction

Total potential energy of a system of N identical atoms, $U(r_1, \ldots, r_N)$, can be expanded as a sum of n-body interactions [64], u_n:

$$U(r_1, \ldots, r_N) = \sum_{i<j}^{N} u_2(r_i, r_j) + \sum_{i<j<k}^{N} u_3(r_i, r_j, r_k) + \ldots \tag{2}$$

Thermodynamic properties of the system with many-body interactions can often be determined using a model system with an appropriate effective pair potential [65] which may depend on the thermodynamic state of the system and the thermodynamic property to be described [66]. Such coarse-graining procedure, based on Henderson theorem [67], is not necessarily applicable for non-equilibrium and inhomogeneous systems. Many-body interactions may affect transport and interfacial properties of the fluids, as reported for self-diffusion coefficient [68], shear viscosity [68–71], bulk viscosity [69, 70, 72], thermal conductivity [69, 70], and gas-liquid surface tension [73, 74]. In particular, many-body interatomic interactions were found to play a significant role in formation of bulk viscosity in dense argon fluid [72].

In dilute gases, many-particle collisions are seldom. However, using the kinetic theory of gases to calculate the term in the bulk viscosity expansion (1) proportional to ρ^2, described by the virial coefficient μ_2, would require considering at least four-particle collisions. The collision integral would contain terms up to those corresponding to four-body interaction. Thus, the influence of many-body interactions on dynamics of many-particle collisions and, consequently, on the values of bulk viscosity may be not small.

Numerical analysis of the collision integral is difficult even in the case of of triple collisions [54] and three-body

interactions [55]. For this reason, in order to study the effect of three-body interaction on bulk viscosity we resort to molecular dynamics simulations.

C. Pair potential

Although it is a common practice to represent inter-particle interaction in argon is by Lennard-Jones pair potential,

$$u_{\text{LJ}}(r) = 4\epsilon_{\text{LJ}} \left[\left(\frac{\sigma_{\text{LJ}}}{r} \right)^{12} - \left(\frac{\sigma_{\text{LJ}}}{r} \right)^{6} \right] \tag{3}$$

(with the parameters ϵ_{LJ} and σ_{LJ} corresponding to the depth of the potential well and the distance at which the potential is zero, respectively), it is known that Lennard–Jones potential is only an approximation to real interaction in noble gases. Accurate interatomic potentials have been obtained for argon using ab initio quantum chemical calculations [75, 76]. Experimental results obtained for argon at large pressures are better explained if a larger steepness of interaction potential at small interatomic separation distances is taken into account [77, 78]. Moreover, the effect of many-body interactions on thermodynamic properties can be substantial [79–81].

Nevertheless, the account of triple-dipole and dipole-dipole-quadrupole dispersion interactions was shown to move the effective potential of liquid argon towards Lennard-Jones form [82], and indeed, using Lennard–Jones potential with the values of the parameters ϵ_{LJ} and σ_{LJ} not necessarily corresponding to genuine pair interaction describes thermodynamic properties of dense noble gases with good accuracy [83]. The role of many-body interaction, however, decreases with decrease in density, so that the effective pair potential becomes closer to the actual pair potential. As a result, using ab initio pair potential yields better prediction of thermophysical properties of argon at low densities [84].

In this study, we investigate the effect of approximating pair interaction with Lennard–Jones potential upon the values of bulk viscosity in low-density states.

II. INTERACTION MODELS

In order to obtain answers to the questions set in the Introduction, we consider three models of interatomic interaction:

(i) Lennard–Jones pair potential,

(ii) ab initio pair potential

(iii) ab initio pair potential + three-body interaction.

In model (i) we use Lennard–Jones potential, Eq. (3), with the values of the parameters $\epsilon_{\text{LJ}}/k_B = 116.79$ K and $\sigma_{\text{LJ}} = 0.33952$ nm provided by Rutkai et al. [83].

We describe pair interaction in models (ii) and (iii) by the following modification of the Tang–Toennies poten-

Parameter	Unit	Value
A	K	4.61330146×10^7
a_1	$(\text{nm})^{-1}$	-2.98337630×10^1
a_2	$(\text{nm})^{-2}$	-9.71208881
a_{-1}	nm	$2.75206827 \times 10^{-2}$
a_{-2}	$(\text{nm})^2$	$-1.01489050 \times 10^{-2}$
b	$(\text{nm})^{-1}$	4.02517211×10^1
C_6	$\text{K}\,(\text{nm})^6$	$4.42812017 \times 10^{-1}$
C_8	$\text{K}\,(\text{nm})^8$	$3.26707684 \times 10^{-2}$
C_{10}	$\text{K}\,(\text{nm})^{10}$	$2.45656537 \times 10^{-3}$

TABLE I. Parameters of the modified Tang–Toennies potential function (4), taken from Ref. [75].

tial function [85] presented by Jäger *et al.* [75]:

$$u_{\text{TT}}(r) = A \exp\left(a_1 r + a_2 r^2 + \frac{a_{-1}}{r} + \frac{a_{-2}}{r^2}\right)$$
$$- \sum_{n=3}^{8} \frac{C_{2n}}{r^{2n}} \left[1 - e^{-br} \sum_{k=0}^{2n} \frac{(br)^k}{k!}\right]. \quad (4)$$

We use the values of the parameters A, a_n, b and C_n obtained for argon by Jäger *et al.* [75] and listed in Table I. The higher-order dispersion coefficients are determined using the recursion formula [75, 85]:

$$C_{2n} = C_{2n-6} \left(\frac{C_{2n-2}}{C_{2n-4}}\right)^3, \quad n \geq 6. \quad (5)$$

Various models of three-body interactions in argon have been reported, including triple-dipole [86–88] and higher-order [89] dispersion as well as other (exchange and induced polarization) contributions [79, 90–93]. In model (iii) we use triple-dipole dispersion interaction, derived by Axilrod and Teller [94] and Muto [95], which decays more slowly with inter-particle separation than the exchange, induced-polarization, and higher-order dispersion contributions, and is therefore the most significant many-body contribution for gases. Axilrod–Teller–Muto interaction is described by formula

$$u_3(r_{12}, r_{23}, r_{31}) = \nu \frac{1 + 3\cos\gamma_1 \cos\gamma_2 \cos\gamma_3}{r_{12}^3 r_{23}^3 r_{31}^3}, \quad (6)$$

where the r_{ij} are the lengths of the sides, γ_i are the angles of the triangle formed by three argon atoms, and ν is triple-dipole interaction coefficient. We use the value $\nu = 7.353 \times 10^{-108}$ J m^9 reported for argon by Kumar and Meath [88].

III. SIMULATION DETAILS

Computations were carried out using LAMMPS package [96] for molecular dynamics simulation in combination with the OCTP package [97] for on-the-fly computation of bulk viscosity. We used the equilibration and

bulk viscosity computation procedures described by Jamali *et al.* [97]. The values of the bulk viscosity coefficient were extracted from fluctuations of kinetic pressure, which were sampled in microcanonical (NVE ensemble) over a time period of 5 ps. To enhance statistics, each simulation was run for 4×10^5 production time steps, with time step set to 0.25 fs.

We modified LAMMPS to include Tang-Toennies pair interaction, Eq. (4), and Axilrod–Teller–Muto three-body interaction, Eq. (6) [98]. The cutoff radius for all pair interactions was set to $6.5\sigma_{\text{LJ}}$. The potential for a triplet of atoms was calculated only if all three distances r_{12}, r_{23}, r_{31} between the three atoms satisfied $r_{ij} < r_{c_2}$. In addition, the product of the three distances was required to satisfy $r_{12}r_{23}r_{31} < r_{c_3}^3$ to exclude from calculation the triplets with small contribution to the interaction [99]. We set the cutoff values for three-body interactions to $r_{c_2} = 6.5\sigma_{\text{LJ}}$ and $r_{c_3} = 3.5\sigma_{\text{LJ}}$.

For each of the three potential models described in Section II, we carried out simulations of the system at the densities $\rho = 0.001$, 0.01, 0.1 and 1 kg m^{-3} and the temperatures $T = 150$, 200, 300 and 400 K. We ran the same simulation sets with 16384 and 32000 particles and did not observe systematic dependence of bulk viscosity on the number of particles in the simulation box for all interaction potentials and state points.

In order to compare our results with the experimental data by Madigosky [33], we additionally carried out simulations at $T = 234.55$ K of the system with *ab initio* + three-body interaction at the densities 0.01, 0.1, 1 and 10 kg m^{-3}.

IV. RESULTS

Figure 1 presents the results of the molecular dynamics simulation for the dependence of the ratio of bulk viscosity to the square of density for the potential model (iii) (*ab initio* pair + three-body interaction), described in Section II. The data was computed at $T = 234.55$ K with 32000 particles in the simulation box. We do not show error bars in Figure 1 because each point corresponds to a single simulation run which, according to the results of Pranami and Lamm [100], is not sufficient for obtaining a reliable estimate of the statistical uncertainty.

Figure 1 also shows the experimental values by Madigosky [33] obtained at higher densities. Modelling of the system with many-body interactions at such high densities was not undertaken in this work as it would require considerable computational resources. Nevertheless, experimental data by Madigosky [33] manifest ρ^2 dependence of bulk viscosity consistent with our results. The deviation of the experimental data from low-density dependence is observed only at very large densities when the gas is no longer dilute.

We have observed the results, similar to those shown in Figure 1, for all other temperatures, potential models, and system sizes we explored, without systematic depen-
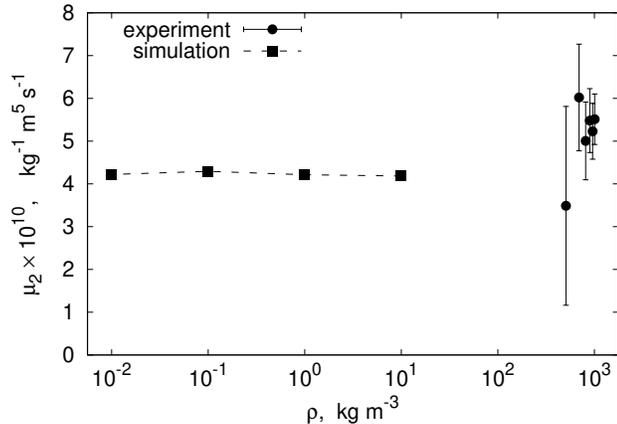
FIG. 1. Dependence of the ratio of bulk viscosity to the square of density at temperature 234.55 K. Bulk viscosity is obtained from molecular dynamics simulation using the potential model (iii), described in Section II (squares), and from experimental work by Madigosky [33] (circles). The dashed line is a guide to the eye.
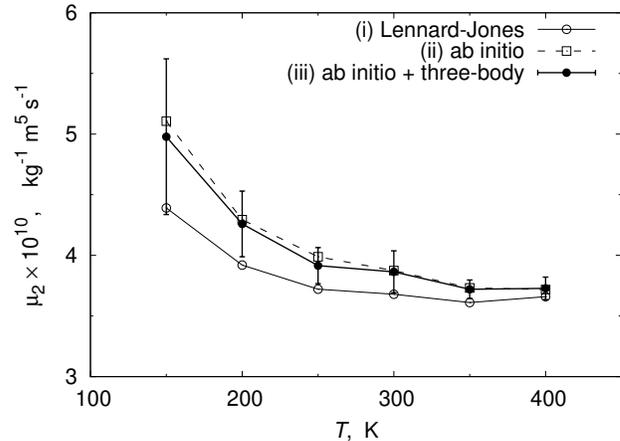
FIG. 2. Temperature dependence of the second bulk viscosity virial coefficient calculated using Eq. (7) for three potential models described in Section II: (i) Lennard–Jones pair interaction (3), (ii) Tang–Toennies pair interaction (4), and (iii) Tang–Toennies pair interaction (4) plus Axilrod–Teller–Muto three-body interaction (6). Error bars are shown only for model (iii), mean squared deviation for other models has similar magnitude. Other lines are drawn to guide the eye.

dence of μ/ρ^2 on ρ. We therefore conclude that $\mu \sim \rho^2$ at low densities, so that the ratio plotted in Figure 1 corresponds to the bulk viscosity second virial coefficient, μ_2, defined by Eq. (1). On that account, we shall calculate μ_2 using formula

$$\mu_2 = \frac{\mu}{\rho^2}, \qquad (7)$$

and averaging the results at different values of the (small) density and (large) number of particles, keeping track of mean square deviations. Figure 2 presents the temperature dependence of μ_2, calculated in this way, for all three potential models.

The results are different for Lennard–Jones and Tang–Tonnies pair potentials, and the difference increases with decrease in temperature. We conclude that modeling interatomic interaction with Lennard–Jones potential underestimates bulk viscosity, and more accurate models must be used in modeling bulk viscosity of argon gas in dilute states.

On the other hand, the change in the results due to Axilrod–Teller–Muto three-body interactions is within the statistical uncertainty. We therefore conclude that many-body interactions can be neglected in modeling bulk viscosity of dilute argon gas, so it should be sufficient to include only pair interactions in theoretical and numerical models.

For reference, we present in Table II the numerical values of the bulk viscosity second virial coefficient from the most accurate potential model we investigated, model (iii). These data can be used to calculate bulk viscosity, according to Eq. (7), as $\mu = \mu_2\rho^2$.

Temperature , K	$\mu_2 \times 10^{10}$, $kg^{-1} m^5 s^{-1}$	$\Delta\mu_2 \times 10^{10}$, $kg^{-1} m^5 s^{-1}$
150	4.97	0.64
200	4.26	0.27
250	3.92	0.15
300	3.86	0.17
350	3.72	0.08
400	3.73	0.09

TABLE II. Second bulk viscosity virial coefficient, μ_2, and corresponding mean squared deviation , $\Delta\mu_2$, calculated at different temperatures for the potential model (iii), described in Section II.

V. CONCLUSION

We have used molecular dynamics simulations to compute bulk viscosity of dilute argon gas at the densities of 0.001, 0.01, 0.1 and $1\,kg\,m^{-3}$ and the temperatures of 150, 200, 300 and 400 K. We investigated three models of interatomic interaction:

(i) Lennard–Jones pair potential,

(ii) Tang–Toennies *ab initio* pair potential, and

(iii) Tang–Toennies *ab initio* pair potential + Axilrod–Teller–Muto three-body interaction,

and established the following results:

A. Bulk viscosity of dilute argon gas is proportional to density squared in the investigated range of densities, not following the $\sim \rho$ dependence predicted by

Hammer and Oppenheim [62] for systems with attractive interactions and observed by Meier et al. [50] in more dense states.

B. Many-body interactions do not noticeably affect bulk viscosity in dilute states, contrary to the previously investigated case of dense fluids [72].

C. Using Lennard–Jones interaction model in dilute

states leads to underestimation of bulk viscosity of argon and, therefore, more accurate models of pair interaction should be used for quantitative predictions of bulk viscosity.

The results of this work can potentially facilitate further theoretical and computational studies of dynamic properties of noble gases and their mixtures.

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