



# Molecular dynamics simulations of momentum and thermal diffusion properties of near-critical argon along isobars



Jakler Nichele<sup>a,b</sup>, Itamar Borges Jr.<sup>a,b</sup>, Alan B. Oliveira<sup>c</sup>, Leonardo S. Alves<sup>a,d,\*</sup>

<sup>a</sup> Defense Engineering Graduate Program, Military Institute of Engineering, 22290-270 Rio de Janeiro, Brazil

<sup>b</sup> Chemical Engineering Department, Military Institute of Engineering, 22290-270 Rio de Janeiro, Brazil

<sup>c</sup> Department of Physics, Federal University of Ouro Preto, 35400-00 Ouro Preto, Brazil

<sup>d</sup> Theoretical and Applied Mechanics Laboratory, Mechanical Engineering Department, Fluminense Federal University, 24210-240 Niterói, Brazil

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## ABSTRACT

Three basic diffusion properties of argon – shear viscosity, bulk viscosity and thermal conductivity – were studied in the neighborhood of the critical point using molecular dynamics (MD) and the Lennard-Jones potential energy function. MD simulations were performed along the  $1.0P_c$  and  $1.2P_c$  isobars. Green-Kubo relations and a Lennard-Jones pair potential were used. Four different sets of Lennard-Jones parameters were used. A comparison of computed shear viscosity and thermal conductivity values with data available from the National Institute of Standards and Technology (NIST) displayed a good agreement. Results for bulk viscosity indicated that values of this property cannot be neglected in this thermodynamic region, a result that violates the traditional and much-assumed Stokes hypothesis in classical fluid mechanics. Furthermore, it was shown that in the neighborhood of the critical region the bulk viscosity can have larger values than the shear viscosity.

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## 1. Introduction

Fluid dynamics and heat transfer models are strongly related to accurate values for transport coefficients. The Navier-Stokes equation [1] and the energy equation [2] incorporate for a given substance three transport coefficients that connect the physical dynamics of momentum and heat to three properties, namely, bulk viscosity, shear viscosity and thermal conductivity.

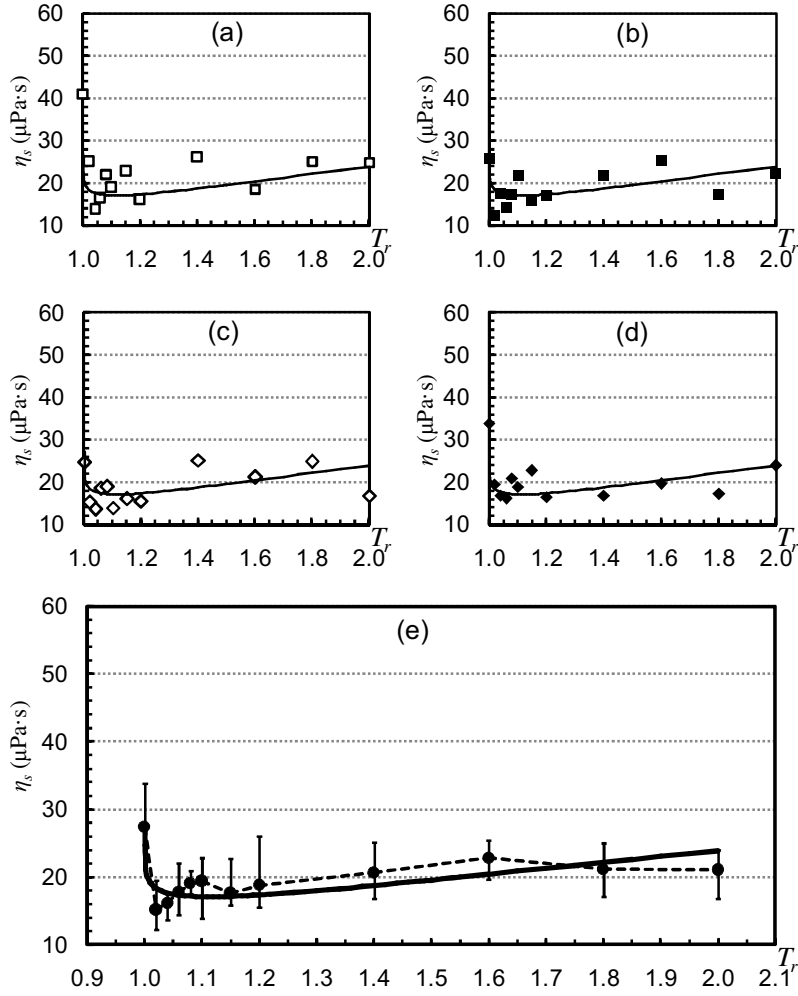
There are in the literature several data sets that collect experimental values of shear and thermal conductivity for simple substances. The electronic tables from the National Institute of Standards and Technology (NIST) [3], for instance, allow the solution of a great number of typical engineering problems. In these cases, the bulk viscosity is generally neglected based on the validity of Stokes hypothesis [4] even when the fluid is neither incompressible nor a monoatomic dilute gas [5]. Hence, bulk viscosity values are rarely found in tables, technical works and engineering projects, even though they are needed for the complete specification of the Navier-Stokes stress tensor.

However, in the neighborhood of the critical point, availability of transport coefficient data is scarce. Moreover, theory and experiment display anomalies in the behavior of some thermodynamic and transport properties, usually appears as a divergence towards infinite or zero depending on the property [6–10]. In particular, the high compressibility of near-critical fluids reduces the accuracy of experimental measurements. For this class of fluids, bulk viscosity data are even more limited since the acoustic absorption of sound waves – the most used experimental technique [11,12] – is subject to high levels of error. To overcome this drawback, Brillouin scattering was developed as a promising technique to measure bulk viscosity, though it is still not widely known and used [13].

In order to overcome the aforementioned experimental limitations, an interesting possibility is performing molecular simulations that can suitably model the near-critical state and compute transport coefficients. One of these methods is equilibrium molecular dynamics (MD) [14–16]. In this approach, fundamental thermophysical properties such as energy, temperature, pressure can be determined from specific averages of the dynamic evolution of an ensemble of molecules. Other properties are obtained using relations from thermodynamics and statistical mechanics including time correlations, e.g., transport properties [17]. This method is useful in the investigations of phase diagrams [18] and chemical reactions [19]. In the framework of MD, particle tra-

\* Corresponding author at: Defense Engineering Graduate Program, Military Institute of Engineering, 22290-270 Rio de Janeiro, Brazil.

E-mail address: [leonardo.alves@mec.uff.br](mailto:leonardo.alves@mec.uff.br) (L.S. Alves).



**Fig. 1.** Shear viscosity computed using  $10^4$  argon atoms in the MD simulation for  $P=1.0P_c$  in a range of reduced temperatures from 1.0 to 2.0 using the Lennard-Jones potential with different parameters pairs – (a) [25], (b) [26], (c) [29], (d) [30] – and (e) the average values with error bars.

jectories in phase space defined by positions and velocities are computed from the forces resulting from an interaction potential energy between pairs of atoms and molecules. The most employed model for non-bonded particles is the Lennard-Jones (L-J) potential [20]. It has a simple mathematical expression and leads to accurate results notably in the study of noble gases. The L-J has already been used to compute transport properties of supercritical fluids far from their critical points, transport properties of near-critical fluids using other approaches and other properties [21–26].

In this work, we investigated transport properties of near-critical argon using equilibrium MD. The present simulations are based on Green-Kubo theory and use four different versions of argon Lennard-Jones potentials available in the literature. The importance of investigating argon in this work is twofold. First, it is the most abundant noble gas in the atmosphere. Second, it is an important substance employed for calibration purposes in laboratories because it is chemically inert and has a low cost. The present results were compared with available experimental data, which allows one to estimate their range of applicability. Due to the scarcity of bulk viscosity experimental values, especial emphasis was given to this transport property in such a way that they can be used in simulations of compressible fluid flow [27] as well as heat transfer problems [28].

## 2. Fundamentals

### 2.1. Molecular dynamics and the Lennard-Jones potential

The basis of the MD technique is the computational simulation of Newton’s equation of motion for a set of interacting moving particles. For a system consisting of argon atoms in a regular box, only interactions between pairs of non-bonded atoms were considered. In other words, many-body interactions are not considered explicitly.

A pair potential suitably models the interactions between atom pairs. The simplest realistic model for this purpose is the L-J 12-6 potential. It is a two parameters model given by Eq. (1)

$$U_{LJ}(r_{ij}) = \begin{cases} 4\epsilon \left[ \frac{\sigma}{r_{ij}}^{12} - \frac{\sigma}{r_{ij}}^6 \right], & r_{ij} \leq r_c \\ 0, & r_{ij} > r_c \end{cases} \quad (1)$$

where  $\epsilon$  is the depth of the potential well,  $\sigma$  is the zero-energy distance,  $r_{ij}$  is the distance between particles  $i$  and  $j$ , and  $r_c$  is a cut-off distance that plays an important role in reducing the computational cost. To use this potential it is necessary to correct the computed value of the potential in order to include the small energies resulting from long-range interactions farther than  $r_c$  [20]. The 12-exponent term models repulsion effects while the 6-exponent

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