Vacuum 109 (2014) 246–252

Contents lists available at ScienceDirect

Vacuum

journal homepage: www.elsevier.com/locate/vacuum

Ab initio simulation of rarefied gas flow through a thin orifice

Felix Sharipov*, José L. Strapasson

Departamento de Física, Universidade Federal do Paraná, 81531-990 Curitiba, Brazil

ARTICLE INFO

Article history:
Received 27 January 2014
Received in revised form
25 March 2014
Accepted 28 March 2014
Available online 5 April 2014

Keywords:
Rarefied gas
Orifice flow
Direct simulation Monte Carlo
Ab initio potential

ABSTRACT

A rarefied gas flow through a thin orifice is calculated for the three noble gases, helium, argon and krypton, applying the direct simulation Monte Carlo method based on the *ab initio* potential. The calculations have been carried out over the whole range of the gas rarefaction and for several values of the pressure ratio with the numerical error less than 0.5%. A comparative analysis showed that the relative difference of the flow rate based on the *ab initio* potential from that obtained for the hard sphere molecular model depends on many factors, namely, gas species, pressure ratio, gas rarefaction and gas temperature. Among the gases considered here, the difference for helium is smallest and does not exceed 0.7%. The deviation for krypton is largest and reaches 1.4%. A relative deviation of the flow rate due to the temperature variation is within 0.9%. A comparison of the axial distributions of density, temperature and bulk velocity shows that the Mach discs for the *ab initio* potential are stronger than those for the hard sphere model.

1. Introduction

Rarefied gas flow through a thin orifice represents a great practical interest due to its wide application in vacuum technology [1], microfluidics [2], electronic microscopy [3], spacecraft design [4], gas flow metrology [5,6] and other technologies. Such a gas flow is also of a great scientific interest because of its simple formulation and small number of parameters determining its solution. That is why it was pointed out as a benchmark problem by the paper [7] where numerical and experimental results on the orifice flow of rarefied gas were compiled and compared. The comparison was performed between results obtained by the direct simulation Monte Carlo (DSMC) method [8] in the work [9] and those obtained from the BGK model equation by the discrete velocity method in Ref. [10]. These numerical results are in a good agreement with experimental data reported in Refs. [11–13]. The maximum disagreement between all these results reaches 5%. However, the experimental technique reported in the paper [6] allows to measure the mass flow rate through short tubes with an uncertainty of better than 0.02%. Thus, numerical methods of rarefied gas dynamics must be constantly improved in order to meet the practical requirements to predict the flow rate through orifices, slit, short tubes and channels with a higher precision.

The model kinetic equations, i.e. some simplifications of the Boltzmann equation, used in Refs. [10,14–17] are powerful tools to solve a large range of practical problems, but their uncertainty is about 5% so that more accurate results can be obtained on the basis of the exact Boltzmann equation applied in Refs. [18,19] or by the DSMC technique used in Refs. [9,20–27]. The results reported in all these papers are obtained for the hard sphere (HS) molecular model. This model has many advantages such as the simplicity of its implementation and nonnecessity to specify the gas species and its temperature for calculations carried out in dimensionless quantities. On the other hand, this model provides a non-physical dependence of gas viscosity on the temperature. In order to correct this dependence, the variable hard sphere (VHS) model was proposed [8]. This model changes the total cross section of molecular collisions, but it does not change the deflection angle distribution. Like the HS model, it is simple to implement, but it requires to specify the gas and its temperature. In this sense, the VHS model is less advantageous than the HS model. Thus, it is very important to know the uncertainty of the HS model because of its simplicity, its universality and because of the abundance of data in the open literature based on this model. As was shown in Refs. [28,29], this molecular model provides results for simple one-dimensional problems with an accuracy of few percent, but the accuracy of the HS model in two-dimensional flows such as flows through orifices and slits is still unknown.

Recently, a technique to implement an arbitrary intermolecular potential into the DSMC method was proposed in Ref. [30]. The computational time based on this technique is of the same order as

* Corresponding author.
E-mail addresses: sharipov@fisica.ufpr.br (F. Sharipov), jlstrapasson@fisica.ufpr.br (J.L. Strapasson).

http://dx.doi.org/10.1016/j.vacuum.2014.03.027
0042-207X/

that based on the HS model. As an example, some calculations were carried out for the Lennard-Jones potential which contains some unknown parameters usually extracted from experimental data. In order to avoid the use of such adjustable parameters, the *ab initio* (AI) potential calculated for practically all noble gases and their mixtures, see e.g. Refs. [31–34], can be applied. An implementation of this potential into the DSMC [35] made this method completely free from adjustable parameters extracted from experiments.

The aim of the present paper is to study the influence of intermolecular potential on the orifice flow of rarefied gas. To achieve this purpose, numerical simulations of such a flow are performed by the DSMC technique based on the AI potential for three noble gases, viz., helium (He), argon (Ar) and krypton (Kr). Moreover, the same simulation is carried out for the HS molecular model in order to estimate its uncertainty in the problem in question.

2. Statement of the problem

Consider an orifice in an infinitesimally thin partition, which separates two semi-infinite containers. One of them contains a gas at a pressure p_0, while the other container is maintained at a smaller pressure $p_1 < p_0$. The temperatures of the gas in both containers are equal to T_0. We are going to calculate the mass flow rate $\dot{M}$ through the orifice and the flowfield in the containers.

The solution of the problem is determined by two main parameters: the pressure ratio p_1/p_0 and the gas rarefaction δ defined as

$$\delta = ap_0/(\mu_0 v_0), \quad v_0 = \sqrt{2k_B T_0/m}, \tag{1}$$

where a is the orifice radius, μ_0 is the shear viscosity at the temperature T_0, v_0 is the most probable molecular speed at the same temperature, m is the molecular mass of the gas, and k_B is the Boltzmann constant. Note, the limit $\delta \to 0$ corresponds to the free-molecular (or collisionless) regime of the flow, while the opposite limit ($\delta \to \infty$) describes the hydrodynamic regime.

The results on the flow rate will be given in terms of the reduced flow rate defined as

$$W = \dot{M}\big/\dot{M}_0, \quad \dot{M}_0 = \sqrt{\pi}a^2 p_0/v_0, \tag{2}$$

where $\dot{M}_0$ is the mass flow rate in the free molecular regime ($\delta \to 0$) in the limit $p_1/p_0 \to 0$. Thus, for an arbitrary pressure ratio, the dimensionless flow rate W reads

$$W = 1 - p_1/p_0, \quad \text{at } \delta \to 0. \tag{3}$$

The solution of the problem in question is also determined by the gas-surface interaction law. As was shown in Refs. [9,15], the influence of this factor on the slit and orifice rates is negligible so that the diffuse scattering of gaseous particles on the partition walls is assumed.

3. Potential

As it has been mentioned above, the three noble gases He, Ar, and Kr are considered here. The AI potentials for these gases were calculated in Refs. [31,33] and can be written down as

$$U(r) = E_h\left[Ae^{-a_1R-a_2R^2} - \sum_{n=3}^{8}\frac{C_{2n}}{R^{2n}}\left(1 - e^{-bR}\sum_{k=0}^{2n}\frac{(bR)^k}{k!}\right)\right], \tag{4}$$

where $E_h = 4.35974417 \times 10^{-18}$ J is the Hartree energy, $R = r/a_0$, $a_0 = 5.2917721092 \times 10^{-11}$ m is the Bohr radius. The parameters A, a_1, a_2, b, and C_n are reported in Ref. [31] for He and Ar and in Ref. [33] for Kr. Their values are summarized in Table 1. Moreover, the distance r_0 corresponding to the zero potential, i.e. $U(r_0) = 0$, and the well-depth of the potentials, i.e. $\varepsilon = -\min\{U\}$, are given in Table 1.

4. Numerical scheme

The DSMC method described in the book [8] is used here. An application of this method to the orifice flow is given in details in Ref. [9] so that only its modifications will be given in this section.

4.1. Deflection matrix

To apply a potential like that given by Eq. (4), it should be cut off, i.e. a maximum impact parameter b_m when a collision happens must be assumed. Once a pair of particles is selected for collision, their velocities are changed according to the classical theory of binary collision. The deflection angle χ determining the direction of the relative velocity g after a collision depends on the dimensionless kinetic energy of collision defined as

$$E = mg^2\big/4\varepsilon, \tag{5}$$

where ε is given in Table 1 for each gas species. According to the technique proposed in Ref. [30], the deflection angle χ for a binary collision is precalculated and stored in computer memory. The regularly distributed values of the energy are considered, i.e.

$$E_j = (j - 0.5)E_m/N_e, \tag{6}$$

where $1 \le j \le N_e$, E_m is the maximum energy defined by Eq. (5) and N_e is an integer. The impact parameter values b_i are distributed as

$$b_1 = b_m\big/\sqrt{2N_b}, \quad b_i = \sqrt{b_{i-1}^2 + b_m^2\big/N_b}, \tag{7}$$

where N_b is an integer. Thus, the matrix χ_{ij} is calculated for N_e values of the energy E defined by Eq. (5) and for N_b values of the impact parameter b. To choose the deflection angle χ_{ij} from the precalculated matrix for a specific collision, the following rules are used

$$i = N_b R_n + 1, \quad j = (E/E_m)N_e + 1, \tag{8}$$

where R_n is a random number and E is dimensionless energy (5) of this collision, i.e. the index i is chosen randomly from the range $1 \le i \le N_b$ and the index j corresponds to the discrete value E_j close-in to the energy E in the specific collision.

The values of E_m, b_m, N_e and N_b used in the present work are given in Table 2. The reduced temperature $T^* = k_B T/\varepsilon$ is also given in this table in order to show that $E_m > 20T^*$ as was recommended in Ref. [30].

Table 1
Parameters for the *ab initio* potential given by Eq. (4).

	He, Ref. [31]	Ar, Ref. [31]	Kr, Ref. [33]
A	6.62002	82.9493	109.66
a_1	1.88553	1.45485	1.32512
a_2	0.0639819	0.0379929	0.0404
b	1.85822	1.62365	1.40
C_6	1.46098	63.7520	120.14
C_8	14.1179	1556.46	3565.02
C_{10}	183.691	49,437.9	364,467.0
C_{12}	3.26527×10^3	2.07289×10^6	0
C_{14}	7.64399×10^4	1.105297×10^8	0
C_{16}	2.27472×10^6	7.24772×10^9	0
r_0/a_0	5.007	6.375	6.781
ε/k_B (K)	10.631	139.53	199.4