Vacuum 128 (2016) 244–251

Contents lists available at ScienceDirect

Vacuum

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

Influence of the gas-surface interaction model on time-dependent rarefied gas simulations

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ARTICLE INFO

Article history:
Received 22 December 2015
Received in revised form
4 March 2016
Accepted 24 March 2016
Available online 2 April 2016

Keywords:
Rarefied gas dynamics
Time-dependent flow
DSMC
Hybrid modelling
Gas-surface interaction
Gas separation mechanism

ABSTRACT

In this paper, the influence of the gas-surface interaction on the time-dependent rarefied gas flow through a short tube into vacuum is investigated. Due to a significant scale separation, the flow is simulated using a hybrid scheme proposed by Vargas et al. [1, 2], in which the pressure change in the upstream chamber is coupled to the flow rate obtained by the Direct Simulation Monte Carlo (DSMC) computations. First, the influence of gas-surface interaction is demonstrated through comparison of DSMC simulation results obtained for different values of accommodation coefficients. The obtained dataset is then used to show how the boundary conditions can affect the time-dependent gas flow, even when applied on the small surface area of the device. It is argued that the domain of possible solutions is bounded by the cases of specular and diffuse scattering. Furthermore, it is investigated how this domain can be affected by measurement uncertainties present in the experimental setup. Next, the analysis of the gas-surface interaction is extended to binary mixtures. In the end, it is discussed how the obtained results can be used in order to improve the efficiency of gas separation mechanisms.

1. Introduction

Rarefied gas flows are a prominent feature in many industrial areas ranging from vacuum technologies to aerospace engineering. Particularly in the former, rapid pressure change of the gas is of significant practical interest. These include leak testing, CD/DVD metallization, surface coating, mass spectrometry and vacuum gauge testing, among others. In these applications, the flow field is mostly time-dependent, which significantly increases the complexity of the required computer simulations and experimental setups.

Recently, a hybrid approach for simulating time-dependent rarefied gas flows was introduced by Vargas et al. [2]. In their setup, the gas expands from a high pressure chamber towards a low pressure one through a conducting tube. Since in such a scenario the time scale of the gas flow through the tube is significantly lower than the time scale of the pressure change, the kinetic simulation of the entire domain becomes computationally prohibitive. In the introduced hybrid scheme, kinetic modelling (micro model) is employed only for a small region around the tube, while the gas behaviour in the rest of the domain is modelled using mass conservation principle together with the equation of state (macro model). The information from the micro model is fed into the macro model in the form of the mass flow rate through the tube, whereas the pressure change in the chambers is obtained from the equation of state.

In a follow-up study [1], the authors investigated the time-dependent rarefied gas flow of single gases and binary mixtures from an upstream vessel through a short tube into vacuum using the above-mentioned hybrid scheme. Through the comparison of their simulation results and the experimental data from the modified setup of [4–6], the authors reported a discrepancy of 10% for the gas pressure. The main cause of the discrepancy was attributed to the geometrical uncertainties of the flow configuration. For modelling gas-surface interaction, the diffuse scattering kernel was used.

Due to its simplicity and acceptable accuracy, the diffuse scattering kernel is broadly used for describing gas-surface interactions. Although it is an acceptable choice for many practical computations, it has been observed that in certain test cases the numerical data obtained by the diffuse kernel cannot match the corresponding experimental results (see e.g. Refs. [10–12]). More accurate simulations can be performed by using the diffuse-specular Maxwell kernel [23] or the Cercignani-Lampis (CL)

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http://dx.doi.org/10.1016/j.vacuum.2016.03.028
0042-207X/

kernel [7]. Unlike the Maxwell kernel, the CL kernel is able to reproduce physical lobular patterns for monatomic gases and it gives more accurate predictions of the flow field [10]. Furthermore, in different studies concerning the influence of the gas-surface interaction on the rarefied gas flow through a short channel [13] and tube [16] into vacuum, it has been shown that the mass flow rate strongly depends on the value of the tangential momentum accommodation coefficient (TMAC).

Here, a systematic study of the influence of gas-surface interaction on the time-dependent rarefied gas flow is carried out using the above-mentioned hybrid approach. A brief overview of the flow configuration and the hybrid scheme is given in §2. Next, the scattering kernels employed for modelling of the gas-surface interaction are described in §3. The results are presented and analysed in §4, where the influence of accommodation coefficients and geometrical uncertainties on the flow is investigated. In the end, some concluding remarks are given in §5.

2. Hybrid modelling

In this section, a brief overview of the hybrid scheme will be given, while all additional information about the scheme and flow configuration can be found in Refs. [1,2]. The system under consideration consists of two cylindrical chambers connected via a short tube (schematic view given in Fig. 1) and it is identical to the one investigated in Ref. [1]. The gas in the upstream chamber is initially at pressure $p_0 = 1000$ Pa and temperature $T = 295$ K, while the downstream chamber is held at vacuum. The reported volumes of the upstream and downstream chambers are 3.1 ℓ and 185 ℓ, respectively, and the connecting tube has the length $L = 0.4962 \pm 0.01$ mm and diameter $D = 2R = 1.0113 \pm 0.005$ mm. Hence, the tube volume is negligible compared to the volume of the chambers. This causes a significant scale separation of the characteristic flow times through the tube and inside the reservoir. In other words, the time step necessary to resolve the flow through the tube would be many orders of magnitude smaller compared to the gas relaxation time in the upstream chamber. For this reason, a full kinetic description of the gas expansion would be computationally impractical. The computational efficiency can be improved by implementing the hybrid scheme [2], in which the kinetic description is employed solely for the quasi-steady gas flow through the tube (micro model). Then, the relaxation of the gas in the upstream chamber is described by using the equation of state together with the mass conservation principle (macro model).

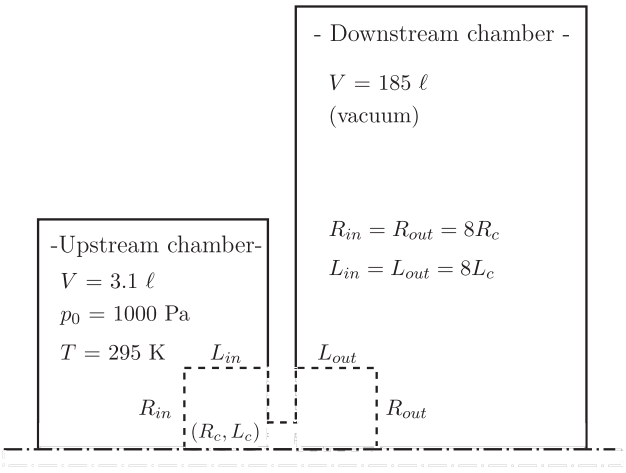

Fig. 1. Schematic of the gas expansion setup of [1]. Dashed line outlines the area where DSMC is employed.

The derivation of the macro model is discussed first. The following formulation is laid down for the general case of the binary gas mixture and simplified expressions for the single gas can be readily deduced. Since only expansion of monatomic gases is investigated, the gas state in the upstream chamber can be described by the ideal gas law

$$p_i(t)V = N_i(t)\Re T \ (i \in \{1,2\}), \tag{1}$$

where $p_i(t)$ and $N_i(t)$ are the partial pressure and number of moles of species i at time t, respectively, $\Re$ is the universal gas constant with the value of 8.314 J/mol/K and V is the chamber volume. The total pressure $p(t)$ and total number of moles $N(t)$ in the mixture are obtained by summing the respective values of these quantities for each species. The pressure is assumed to be uniform in the entire upstream chamber. Furthermore, since the gas expansion is not very rapid, the temperature of the gas T is assumed to remain constant throughout the process, which is verified by measurements (see Ref. [1]).

The amount of the lighter species in the mixture is specified by the molar fraction

$$C(t) = \frac{N_1(t)}{N_1(t) + N_2(t)} = \frac{p_1(t)}{p_1(t) + p_2(t)} \tag{2}$$

and the degree of gas rarefaction is determined by the rarefaction parameter

$$\sigma(t) = \frac{p(t)R}{\mu(t)v(t)}, \tag{3}$$

where $\mu(t)$ is the mixture viscosity, $v(t) = \sqrt{2\Re T/M(t)}$ is the most probable molecular velocity and $M(t)$ is the molar mass of the mixture. Note that the value of the rarefaction parameter is inversely proportional to the Knudsen number.

The amount of gas in the upstream chamber decreases in time due to the outflow through the tube. The temporal evolution of the number of moles of species i in the upstream chamber is expressed as

$$\frac{dN_i}{dt} = -\dot{N}_i(t), \tag{4}$$

where $\dot{N}_i(t)$ is the molar flow rate of species i through the tube. Differentiation in time of the ideal gas law (1), together with the mass conservation Eq. (4), results in the pressure evolution equation of the form

$$\frac{dp_i}{dt} = -\dot{N}_i(t)\frac{\Re T}{V}, \tag{5}$$

which directly links the change of pressure in the upstream chamber to the molar flow rate through the tube. As an additional remark, the downstream chamber is maintained at vacuum during the expansion process.

The molar flow rate through the tube is estimated by using an appropriate kinetic description of the pressure driven flow. Rarefied gas flow through a cylindrical tube has been extensively studied in the past as one of the benchmark cases for validation of different kinetic schemes [15,16–21]. In the present study, simulations have been performed by using the 'No Time-Counter' version of Bird's DSMC method [3] for hard sphere molecules. The computational domain consists of the tube of radius $R_c = 0.50565$ mm and length $L_c = 0.4964$ mm ($L_c/R_c \approx 1$), together