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Time-dependent rarefied gas flow of single gases and binary gas mixtures into vacuum

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ABSTRACT

Time-dependent flows of single gases and binary gas mixtures with various molar fractions from a chamber through a short tube into vacuum are examined by simulations and experiments. The main goal is the comparison of the flow behaviour between pure gases and binary mixtures including the investigation of the gas separation effect. The simulations are based on an explicit hybrid scheme, coupling at each time step the tube flow rate estimated from a database accordingly constructed via a DSMC solver to the gas pressure in the chamber obtained by a mass conservation equation. Computational results describing the expansion process in terms of the temporal evolution of pressure in the chamber as well as of the total and species flow rates through the tube are reported. Comparison between computational and the corresponding deduced experimental pressures deduces a difference of about 10% which may be explained by accumulation of uncertainties in the time sequence. The binary gas mixture pressure evolution curves are always bounded by the corresponding ones of the components of the mixture flowing as single gases and the tube conductance varies in the opposite direction to that of the weighted mean of the component molar masses. Gas separation is monotonically increased as we move from the viscous towards the free molecular regime, while the rate with which gas separation is increased has a maximum in the transition regime. The equivalent single gas approach provides a reasonable estimate provided that the molar fraction of the light gas and the ratio of heavy to light molar mass are not too high.

1. Introduction

Industrial applications under various vacuum conditions, where the involved gas transport changes with time, include coating processes involving load locks like CD/DVD metallization or bottle coating, drying processes, leak detection, processes in MEMS, etc. Despite their frequent occurrence, time-dependent rarefied gas flows have attracted limited attention, both computationally and experimentally. This is attributed to the increased computational effort (the time dimension is added) and to the more demanding and expensive experimental work (rapid changes of pressure and temperature in time).

Recently, there has been some effort in simulating time-dependent rarefied gas flows through capillaries of circular cross-section. Based on the linearized Bhatnagar–Gross–Krook kinetic model equation, the unsteady fully developed flow in long tubes has been modelled [1], while the Direct Simulation Monte Carlo (DSMC) method has been applied to simulate the transient flow of a rarefied gas through an orifice [2] and a short tube [3]. In all cases, the upstream and downstream boundary conditions remain constant with respect to time and therefore the time needed to reach steady-state conditions is in the order of microseconds (μs). These prototype flow configurations are mainly of theoretical interest, since in typical fast industrial vacuum processes the characteristic times are in the millisecond or second range.

The Physikalisch–Technische Bundesanstalt (PTB) has developed a calibration facility, where the response and relaxation times of vacuum gauges due to rapid pressure changes can be measured [4,5]. This is realized by gas expansion from a high pressure upstream vessel to a low pressure downstream vessel via an exchangeable duct and a very fast opening valve. The time scale of

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these expansions is similar to fast industrial applications. In this study we investigate how flows of single gas species compare with binary mixtures in such gas expansions.

Simulating this flow configuration solely on kinetic principles is computationally impractical due to the size of the computational domain, which must include the whole volume of the two chambers, in connection with the required very small time step. By taking advantage of the specific characteristics of the flow to introduce acceptable simplifications in modelling, we may greatly reduce the computational effort.

A general approach has been introduced to model the time-dependent flow through a long tube connecting the two chambers [6]. The results include the tube pressure variation in time and space as well as the pressure variation in the two chambers and are valid in the whole range of the Knudsen number. However, this approach is limited to flow configurations where the capillary is very long and the volumes of the capillary and the chambers as well as the corresponding characteristic times are of the same order.

The evolution of the flow through short tubes connecting two chambers has been recently modelled in a hybrid manner [7]. At each time step, based on kinetic theory, a steady-state flow configuration is solved to estimate the amount of gas passing through the tube (micro model) and then the pressure in the two vessels is updated by applying the mass conservation principle and the equation of state (macro model). It is noted that the steady-state kinetic flow rates at each time step are obtained from an adequately dense kinetic database which has been pre-constructed for this purpose and whenever needed interpolation is performed. Based on this approach, the variation of the pressure in the chambers and of the flow rate through the tube with respect to time is provided for several configurations. The theoretical background and a detailed description on the advantages of such hybrid type simulations are given in Ref. [8], where several multi-scale methodologies are analysed. Similar methodologies exploiting time scale separation in a simple manner have also been implemented before in unsteady molecular flows related to filling, exhaust and pumpdown times in pipes and vacuum systems [9] as well as in micro-actuators modelling [10,11].

In the present work, the hybrid modelling approach introduced in Ref. [7] is implemented to computationally investigate the time-dependent flow of various single gases and binary gas mixtures from an upstream vessel through a very short tube into high vacuum. The flow characteristics of pure gases and binary mixtures are compared and the effect of gas separation is analysed. The investigation is accompanied with corresponding experimental work performed at the modified PTB dynamic gas expansion facility [4,5]. The detailed flow configuration and parameters are given in Section 2. Then, the modelling procedure, with the involved micro and macro models are presented in Section 3, while the experimental set-up with the associated measurement procedure are described in Section 4. The obtained results are presented and discussed in Section 5. Finally, in Section 6 some concluding remarks are provided. The Appendix includes the computational data related to the micro model.

2. Flow configuration and parameters

The system under consideration is shown in Fig. 1 and consists of two chambers denoted by A and B, which are connected by a short tube of length L and radius R. The two containers have large but finite volumes V_A and V_B, with $V_A \ll V_B$, while the volume of the capillary V_C is negligibly small compared to the volume of the chambers ($V_C \ll V_A$).

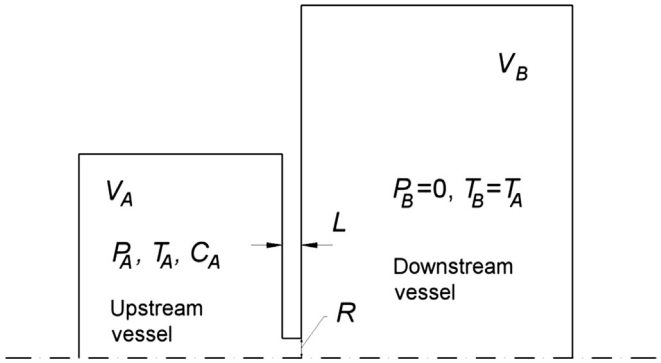

Fig. 1. View of the investigated set-up with geometrical and flow parameters.

In chamber A, at time $t = 0$, the state of a single gas is defined by its initial pressure $P_A^{(0)}$ and temperature $T_A^{(0)}$, connected by the equation of state written as

$$P_A^{(0)} V_A = N_A^{(0)} R^* T_A^{(0)}, \tag{1}$$

where $N_A^{(0)}$ is the initial number of moles in container A and $R^* = 8.314$ J/mol/K is the global gas constant. In the case of a binary gas mixture its initial state is defined by the initial pressure and temperature plus the molar fraction given by Ref. [12]

$$C_A^{(0)} = \frac{N_{1A}^{(0)}}{N_{1A}^{(0)} + N_{2A}^{(0)}} = \frac{P_{1A}^{(0)}}{P_{1A}^{(0)} + P_{2A}^{(0)}}. \tag{2}$$

Here, $N_{iA}^{(0)}$ and $P_{iA}^{(0)}$, with $i = 1, 2$, are the initial number of moles and partial pressure respectively of the each component in container A, while the initial total number of moles is given by $N_A^{(0)} = N_{1A}^{(0)} + N_{2A}^{(0)}$ and similarly the initial total pressure is $P_A^{(0)} = P_{1A}^{(0)} + P_{2A}^{(0)}$. The molar masses of the two species are m_1 and m_2 ($m_1 < m_2$), while the initial molar mass of the mixture is defined as [12]

$$m_A^{(0)} = C_A^{(0)} m_1 + \left(1 - C_A^{(0)}\right) m_2. \tag{3}$$

Therefore, $C_A^{(0)}$ actually refers to the molar fraction of the light species and for $C_A^{(0)} = 1$ and 0 the corresponding states of the single light and heavy gas respectively are recovered.

Furthermore, initially the gas rarefaction in chamber A is characterized by the initial Knudsen number defined as

$$Kn_A^{(0)} = \frac{\sqrt{\pi}}{2} \frac{\mu_A^{(0)} \upsilon_A^{(0)}}{P_A^{(0)} R} \tag{4}$$

where $\upsilon_A^{(0)} = \sqrt{2R^* T_A^{(0)} / m_A^{(0)}}$ is the initial molecular velocity of the gas and $\mu_A^{(0)}$ is the gas viscosity at temperature $T_A^{(0)}$ and molar fraction $C_A^{(0)}$. In the case of a single gas, $\upsilon_A^{(0)}$ corresponds to the most probable velocity. In chamber B, the pressure is taken equal to zero.

Then, the valve at the inlet of the tube rapidly opens and the time-dependent gas expansion between the two vessels evolves. In the downstream vessel B we assume $P_B = 0$ all the time, since its volume is much larger than the volume of vessel A and the vacuum pump is connected to vessel B. The molar flow rate denoted by $\dot{N}(t)$ gradually decreases, as the pressure difference between the two vessels is reduced asymptotically tending to zero.