Vacuum 128 (2016) 1–8

Contents lists available at ScienceDirect

Vacuum

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

Analysis of gas separation, conductance and equivalent single gas approach for binary gas mixture flow expansion through tubes of various lengths into vacuum

Dimitris Valougeorgis*, Manuel Vargas, Steryios Naris

Department of Mechanical Engineering, University of Thessaly, Pedion Areos, 38334 Volos, Greece

ARTICLE INFO

Article history:
Received 10 December 2015
Received in revised form
21 February 2016
Accepted 27 February 2016
Available online 28 February 2016

Keywords:
Vacuum gas dynamics
Gas mixtures
Gas separation
Conductance
DSMC

ABSTRACT

The steady-state binary gas mixture expansion through tubes of various lengths into vacuum is considered, focusing on the intensity of gas separation, the computation of conductance and the implementation of the equivalent single gas approach in terms of the mixture composition and its molar fraction in a wide range of the Knudsen number. The analysis is based on the dimensionless flow rates of He-Ne, He-Ar, He-Kr and He-Xe. Gas separation is characterized by the ratio of the dimensionless flow rates of the two species and it is increased as both the Knudsen number and the square root of the heavy over the light molar mass ratio of the components are increased. The gas mixture conductance is increased as the molar fraction of the light species is increased and it is bounded from below and above by the conductance of the heavy and light species respectively. The error introduced in the equivalent single gas approach is increased along with the difference between the molar masses of the species and the Knudsen number. These statements are valid for any tube length. Quantitative results are also provided. Practical guidelines, which may be useful in industrial applications and measurements under vacuum conditions, are deduced.

1. Introduction

Rarefied pressure driven gas mixture flows through tubes connecting two vessels are very common in industrial applications including flow setups in vacuum technology and gaseous microsystems. In general, the characteristics and properties of these flows are different than the corresponding ones in single gas flows. This is due to the fact that for flows far from local equilibrium, the mean molecular speed of each species of the mixture varies with respect to the mean molecular speed as well as to the bulk (macroscopic) velocity of the mixture. These relative velocities, which do not exist in single gases, result to gas flow separation, which greatly influences the overall flow description [1,2].

The binary gas mixture flow through long channels of various cross sections has been extensively studied, assuming fully developed flow conditions, in the whole range of the gas rarefaction. Based on the McCormack model [3], which is considered as a very reliable linear kinetic model, properly recovering all transport coefficients, the flow through circular tubes has been simulated in Ref. [4] and then, this approach has been extended to channels of rectangular, triangular and trapezoidal cross sections [5,6] including a comparison study between computational and experimental results [7]. The deduced flow rates of various gas mixtures have been accurately estimated and the presence of gas separation due to the higher speed of the light particles compared to the heavy ones has been outlined. A more focused investigation on the gas separation phenomenon has been reported in Ref. [8,9], where the pressure driven gas mixture flow through long tubes into vacuum has been considered. Some of the numerical results presented in Ref. [8] are very helpful in the analysis performed here and they are used to generalize, at some extend, the concluding remarks of the present work. Furthermore, the influence of the composition of the mixture and of its molar fraction has been recently thoroughly reviewed in Ref. [10] by presenting numerical results of some of the above works and by comparing with those of single gases. It is also pointed out that for mixtures with significantly different molecular masses, reliable results are obtained only through the solution of suitable kinetic equations modelling each specific gas mixture. All this work [3–10] is based however, on the assumption of fully

* Corresponding author.
E-mail address: diva@mie.uth.gr (D. Valougeorgis).

http://dx.doi.org/10.1016/j.vacuum.2016.02.015

developed flow and therefore, the deduced remarks refer to gas mixture flows through long capillaries via the infinite capillary theory.

Corresponding modelling work in capillaries of finite length is very limited due to the increased number of parameters defining the flow and the resulting high computational effort. The systematic description of the flow dependency on all involved parameters is computationally very intensive. The flow of two binary gas mixtures (He-Xe and Ne-Ar) through capillaries of various lengths has been investigated in Ref. [11], describing the effects of gas rarefaction, induced pressure difference and tube length on the flow rate and the macroscopic distributions.

More recently, in the framework of the European project EMRP IND12 [12], time-dependent binary gas flows through short capillaries have been investigated. In an effort to simulate the dynamic expansion process in a hybrid manner, extensive computations have been performed to obtain the steady-state flow rates of three binary gas mixtures (He-Ne, He-Ar, He-Kr) expanding through a specific aspect ratio tube into vacuum [13]. The computed flow rates are in a wide range of the reference Knudsen number and more important they are provided for many values of the molar fraction of the three mixtures. Also, the selected three mixtures represent well binary gas mixtures with small, moderate and large differences in their molecular masses. Therefore, these results are very useful in order to analyse the effect of gas composition and provide, if possible, general guidelines in the case of pressure driven binary gas mixture flow through short channels. This analysis has not been performed in Ref. [13] since the work was focusing on the development of a hybrid scheme and on the comparison with corresponding time-dependent experimental results.

In the present work, the flow rate database provided in Ref. [13], as well as additional results for the flow rates of He-Xe, which are obtained in the present work, along with associated data for long tubes in Ref. [8], are all implemented in order to establish certain rules describing the properties of steady-state rarefied binary gas mixture flows. More specifically, the issues of the intensity of gas separation, the computation of conductance and the range of validity of the equivalent single gas approach are analyzed in terms of the binary gas mixture composition and its molar fraction in a wide range of gas rarefaction. The effect of the tube aspect ratio is also examined. Practical guidelines, which may be useful in industrial applications and measurements under vacuum conditions, where binary gas mixtures are the working fluids, are deduced.

2. Flow configuration with input parameters and output quantities

Consider the steady-state binary gas mixture flow through a tube of length L and radius R, connecting two vessels denoted by A and B. The gas pressures P_A, P_B and temperatures T_A, T_B at the two vessels (far from the connecting tube) are maintained constant with $P_A > 0$, $P_B = 0$ and $T_A = T_B$. The flowing gas mixtures are He-Ne, He-Ar, He-Kr and He-Xe assuming hard sphere molecules and purely diffuse gas-surface interaction. The molecular masses of the components are: $m_{He} = 4.0026$ g/mol, $m_{Ne} = 20.1797$ g/mol, $m_{Ar} = 39.9480$ g/mol, $m_{Kr} = 83.7980$ g/mol, $m_{Xe} = 131.293$ g/mol. The quantities at vessel A, far upstream of the tube inlet, are taken as the reference ones. This flow configuration, with $P_B/P_A = 0$ and $L/R = 1, 5, 10$ is characterized by two more parameters.

The first one is the reference molar fraction

$$C_A = n_{1A}/(n_{1A} + n_{2A}) \tag{1}$$

where n_{1A} and n_{2A} are the reference molar number densities of species 1 and 2 respectively of the binary mixture in the upstream vessel, far from the tube inlet, while $n_A = n_{1A} + n_{2A}$ is the corresponding reference number density of the mixture. It is noted that index 1 always refers to the light species, i.e. to He, while index 2 always refers to the heavy species, i.e. depending upon the specific mixture to Ne, Ar, Kr or Xe. Thus, $C_A \in [0,1]$ denotes the molar fraction of the light species and $1 - C_A$ the molar fraction of the heavy one. The reference molar mass of the mixture is $m_A = C_A m_1 + (1 - C_A) m_2$, where m_1 and m_2 are the molar masses of the species, with $m_1 \le m_A \le m_2$. The downstream molar fraction C_B in binary gas mixture flows into vacuum is part of the solution.

The second one is the reference gas rarefaction parameter given by

$$\delta_A = \frac{P_A R}{\mu_A \upsilon_A}, \tag{2}$$

where $\mu_A = \mu_A(T_A, C_A)$ is a reference viscosity and $\upsilon_A = \sqrt{2R^* T_A / m_A}$ is a reference molecular speed ($R^* = 8.314$ J/mol/K is the global gas constant). Alternatively the reference Knudsen number, defined as $Kn_A = (\sqrt{\pi}/2)/\delta_A$, may be applied.

The output quantities of major importance in the present work are the molar flow rates of the two species J'_α, $\alpha = 1,2$ and the corresponding dimensionless flow rates defined as

$$J_\alpha = \frac{J'_\alpha}{\pi R^2 n_A \upsilon_A} = 2 \int_0^1 n_\alpha u_\alpha r dr \tag{3}$$

where $r = r'/R$, while n_α and u_α are the dimensionless number densities and axial velocities respectively. The flow rates J_α of the components as well as the total flow rate of the mixture $J = J_1 + J_2$ remain constant at each cross section along the tube.

The analysis is based on the flow rates J_1 and J_2 as well as on the conductance of each species through the tube, which is related to the flow rates according to [13].

$$Q_\alpha = J_\alpha \pi R^2 \upsilon_A, \ \alpha = 1, 2. \tag{4}$$

The total conductance is $Q = Q_1 + Q_2$. In some cases, working with the conductance, which is of major practical importance in vacuum technology, instead of the flow rates, provides a more clear view and an easier implementation of the deduced guidelines in technological applications.

3. Gas separation, conductance and equivalent single gas approach

The described steady-state pressure driven binary gas mixture flow configuration has been simulated in Ref. [13] via a DSMC solver for the specific tube aspect ratio $L/R = 1$. The binary gas mixtures of He-Ne, He-Ar and He-Kr have been considered. The flow rates J_1 and J_2 have been computed for all three mixtures with $\delta_A = 0$, 0.1, 0.5, 1, 5, 10, 50, 100 and $C_A = 0$, 0.125, 0.25, 0.375, 0.5, 0.675, 0.750, 0.875, 1. This kinetic database presented in the Table 3 of [13] serves perfectly the needs of the present analysis and it is accordingly used.

In addition, in order to generalize the output of the present work to channels of various lengths, results are also provided here for the binary gas mixture of He-Xe flowing through a tube of $L/R = 1$, 5 and 10 into vacuum. Computations have been performed with the same DSMC solver as for the other three mixtures and the computed J_1 and J_2 are tabulated for various values of δ_A and C_A in Table 1. This new set of results will also be used in connection to the corresponding He-Xe flow rates for long channels reported in Ref. [8]. It is noted that in all cases