Simulation of free-molecular and transition multicomponent gas flow through the system of filaments with different temperatures

A N Yakunchikov\(^1,2,3\) and V V Kosyanchuk\(^1,2,3\)

\(^1\) Faculty of mathematics and mechanics, Lomonosov Moscow State University, Moscow, Russia
\(^2\) Institute of Mechanics of Lomonosov Moscow State University, Moscow, Russia
\(^3\) Mechanical Engineering Research Institute of the Russian Academy of Sciences, Moscow, Russia

E-mail: art-ya@mail.ru

Abstract. This work studies plane transition flow (Kn = 0.1–10) of a mixture of noble gases in the system, consisting of several rows of stretched filaments having different temperatures. Problem statement studying equilibrium state in closed system is considered. Calculations were performed using method of event-driven molecular dynamics (EDMD). It is shown that temperature difference leads to gas separation effect, which can be thereafter enhanced by increasing the number stages (rows of filaments).

1. Introduction
First studies of rarefied gas flows induced by temperature differences started more than a century ago [1, 2]. This effect (referred to in literature as “thermal transpiration”) was utilized by Knudsen to construct his gas pump without moving parts [3, 4]. Nowadays, this method of creating pressure difference attracts the interest of researchers due to rapid development of technology of nano/ micro-electromechanical systems (NEMS / MEMS). Numerous versions of pump geometries were proposed [5–7], including multistage micropumps [8].

The flow of gaseous mixtures in such systems was studied numerically and experimentally [9, 10] and the effect of separation of the components with different molecular masses was shown. To date, prototypes of gas separation microdevices have been created on the basis of a nonisothermal membrane [11, 12] and on the basis of a lattice of plates with different temperatures [13]. In this paper, we consider the possibility of creating a gas separating device based on the lattice of threads (filaments) kept at different temperatures.

2. Problem statement
A plane problem about the flow of a mixture of five gases (He, Ne, Ar, Kr, Xe) in a system consisting of several rows of stretched filaments having different temperatures was considered. Equilibrium is studied state in the system (see figure 1), where one end is closed and another one is connected to a reservoir with constant parameters – pressure \(p_0\), temperature \(T_0\) and composition \(x_{0i}\) (\(x_{0i}\) – is the molar concentration of component in reservoir).
A system consisting of four stages of filaments was simulated. Each state contains two rows of filaments – cold one with temperature $T_0$ and hot one with temperature $T_1$. Geometry of the problem is defined by $h$ – distance between rows in one stage (see figure 2), $L$ – distance between stages and $d$ – diameter of a filament. Minimal distance between surfaces of neighboring filaments is denoted by $g = h - d$. Dimensions of the problem in directions perpendicular to $x$ – axis were assumed much greater than listed parameters and thus symmetry conditions were used on $y$ – bounds. Simulations were performed for 24 different configurations ($L/d = 5, 10, 15, 20, 25, 30, 35, 40$; $h/d = 1.25, 1.5, 2$) for Knudsen numbers $Kn_L = \lambda/L = 0.1 - 0.8$ и $Kn_g = \lambda/g = 4 - 15$. Molar concentrations at open end were set equal ($x_{0i} = 0.2, i = 1,...,5$) in all simulations.

3. Calculations and results
Problem was solved using the method of event-driven molecular dynamics (EDMD) [14]. Strengths of the developed EDMD approach are meshless structure, deterministic (non-stochastic) implementation of intermolecular collisions (unlike in Direct Simulation Monte-Carlo method) and reduction of computational time compared to classical molecular dynamics simulations. Interaction between gas molecules and solid surface was described in terms of Maxwell scattering kernel with full energy and momentum accommodation.

Figure 3 illustrates simulation results for the case of geometry when ratio $Kn_L/Kn_g$ of Knudsen numbers in chamber and between neighboring filaments has maximal value. Temperature between stages of filaments has linear profile with jump near surface of filaments and pressure is increasing with each next stage. Resulting pressure at the closed end of the system is approximately 2 times higher than the initial pressure in the reservoir. Number densities of the components increase as $1/T$ in the direction of the cold side of the chamber between the stages, and in the stages themselves concentrations decrease abruptly. The difference in molar concentrations is produced exactly in the chambers between the stages, and inside each stage (between neighboring rows) composition remains practically unchanged.
Figure 3. Temperature, pressure, number density and molar concentration of components for geometry \( L/d = 40, \ g/d = 0.25 \) for \( Kn_L = 0.1, \ Kn_g = 15 \).

The authors gave a qualitative physical explanation for this result by considering the stationary problem of heat transfer between two surfaces of different temperatures in two different regimes (free-molecular and continuum regime). That allowed to put forward a phenomenological hypothesis that the strongest separation effect is when the flow regime inside a stage approaches free-molecule limit, and the flow in the chamber between stages approaches continuum one. This hypothesis was completely confirmed by the results of EDMD simulations.

4. Conclusion
A plane problem about the transitional flow (\( Kn = 0.1–10 \)) of a mixture of five noble gases in a system consisting of several rows of stretched filaments having different temperatures was studied. Pressure, temperature, density and molar concentration distributions were obtained. Temperature between stages of filaments has linear profile with jump near surface of filaments and pressure is increasing from stage to stage. As a result, pressure produced at the closed end of the system is approximately 2 times higher than the initial pressure in the reservoir. It is shown that under the influence of the temperature difference the effect of mixture separation arises. Number densities of the components increase in the direction of the cold side of the chamber between the stages, and in the stages themselves
concentrations decrease abruptly. It is shown that the difference in molar concentrations is produced exactly in the chambers between the stages, and inside each stage (between neighboring rows) composition remains practically unchanged. The strongest effect of separation is achieved under condition that flow regime inside a stage approaches free-molecule limit, and the flow regime in chambers is close continuum one.

Acknowledgments
The research was carried out using the equipment of the shared research facility of HPC computing resources at Lomonosov Moscow State University [15]. This work is supported by the Russian Science Foundation (grant № 17-71-10227).

References
[1] Maxwell J C 1879 Philos. Trans. R. Soc. London 170 231–56
[2] Reynolds O 1879 Philos. Trans. R. Soc. London 170 727–845
[3] Knudsen M 1909 Ann. Phys. 336 205–29
[4] Knudsen M 1910 Ann. Phys. 338 1435–48
[5] Aoki K, Degond P, Mieussens L, Takata S and Yoshida H 2008 Multiscale Model. Simul. 6 1281–316
[6] Bond D M, Wheatley V and Goldsworthy M 2014 Int. J. Heat Mass Transf. 76 1–15
[7] Bond D M, Wheatley V and Goldsworthy M 2016 Int. J. Heat Mass Transf. 93 1038–58
[8] Gupta N K, An S and Gianchandani Y B 2012 J. Micromechanics Microengineering 22 105026
[9] Naris S, Valougeorgis D, Kalempa D and Sharipov F 2004 Phys. A Stat. Mech. its Appl. 336 294–318
[10] Kosuge S and Takata S 2008 Eur. J. Mech. B/Fluids 27 444–65
[11] Matsumoto M, Nakaye S and Sugimoto H 2016 AIP Conference Proceedings 1786 080011
[12] Nakaye S, Sugimoto H, Gupta N K and Gianchandani Y B 2015 Eur. J. Mech. B/Fluids 49 36–49
[13] Sugimoto H and Abe T 2008 AIP Conference Proceedings (AIP) 1084 1123–8
[14] Yakunchikov A and Kosyanchuk V 2018 Comput. Fluids 170 121–7
[15] Sadovnichy V, Tikhonrovav O, Voevodin V and Opanasenko V 2013 Contemp. High Perform. Comput. From Petascale Towar. Exascale 283–307