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# Numerical Study of Gas Separation of Pressure-Driven Binary Mixture Flows Through a Microchannel

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**Abstract.** The gas separation phenomenon of the pressure-driven binary mixture (helium–argon) flows in a microchannel is investigated numerically over a wide range of Knudsen numbers using the discrete unified gas kinetic scheme. The effects of inlet/outlet pressure ratio and Knudsen number on gas separation are studied numerically. It is found that the separation is strengthened with the increase of pressure ratio, and exhibits different trends under different rarefied conditions. The degree of gas separation changes nonlinearly with the outlet Knudsen number and exhibits a maximum in the transitional regime. In particular, we find that the relative pressure deviation and the velocity ratio between light species helium and heavy species argon can be served as indicators for gas separation under different working conditions. Finally, the phenomenon of Knudsen minimum is observed for the light species and gas mixture in the transition regime, but it does not appear for the heavy species within the considered Knudsen number range ($\leq 10$).

**AMS subject classifications**: 76M12, 76P05, 82B40
**Key words**: Gas separation, discrete unified gas kinetic scheme, pressure-driven flow, microchannel.

## 1 Introduction

Rarefied gas mixture flows in a microchannel have attracted increasing attention in various fields, including micro-electromechanical systems (MEMSs) [1–4], membrane technology [5–9], and shale gas production [10, 11].

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Since there are complex microscopic interactions between gas molecules of different species besides those from the same species, some distinctive non-equilibrium phenomena (e.g., barodiffusion, diffusion slip, and separation effect, etc.) appear in gas mixture flows compared with single-species gas flows [12–19]. Many flow properties and non-equilibrium phenomena can be well understood by the investigation of flows in channels, despite their relatively simple geometry.

An important research topic is to investigate the gas separation, which was first observed in the flows of binary gas mixtures driven by a pressure gradient in a long microtube, where the species with different molecular masses have different mean velocities, leading to a non-uniform distribution of mole fraction in the tube [20]. Several MEMSs devices have been designed to either enhance or reduce gas separation for practical applications, i.e., gas separators [21–24] or micro-mixers [25, 26], where gas mixtures were studied in microchannels. Because of the small length scale of MEMS devices, the degree of non-equilibrium is described by the Knudsen number (Kn) defined as the ratio of the molecular mean free path to the channel height. According to Kn, the flow is commonly classified into the continuum ($\mathrm{Kn}<0.001$), slip ($0.001\leq \mathrm{Kn}<0.1$), transition ($0.1\leq \mathrm{Kn}<10$), and free molecular ($\mathrm{Kn}\geq 10$) flow regimes.

The gas separation phenomenon of binary mixtures in microchannels can be analyzed theoretically for the continuum regime (where no separation occurs) and the free-molecular regime (where each species is equivalent to single-species gas) [27–29]. However, the gas separation is not well-characterized in the rarefied (slip/transitional) regimes with Kn ranging from 0.01 to 10, where the Navier–Stokes equations fail to work [30]. On the other hand, the Boltzmann equation or simplified kinetic models can be adopted for describing such flow configurations [31]. For example, Sharipov and Kalempa [13, 32] investigated the binary gas mixture flowing into the vacuum through a long tube numerically, and found the molar fraction and rarefaction at the inlet of the tube have a crucial influence on the separation and flow rate. Szalmas and Valougeorgis [33] showed the discrepancy of overall mass flow rate could reach as high as 10% if the gas separation effect was not considered, indicating the non-negligible effect of gas separation. Further, Szalmas et al. [34] conducted a comparative study on pressure-driven binary gas flows through a long microchannel. Valougeorgis et al. [35] analyzed the separation effect of flows through microtubes and reported that the gas separation depends on the flow rate ratio of the two species. The aforementioned studies indicate that gas rarefaction and compressibility effects have a major influence on gas separation, but it remains unclear how separation varies with these parameters. Recently, some researchers investigated the effect of different Kn numbers and pressure ratios on gas separation using the lattice Boltzmann method (LBM)-based model for mixtures [36–38]. They focused on the time evolution of the smallest/average molar fraction in the channel, the molar fraction distribution in the channel, and the volumetric flow rates, respectively. However, they only studied flows in the slip and early transition regimes due to the limitations of the model. Based on the above literature review, it can be seen that previous studies on gas separation are limited to parts of the flow regimes. There is an urgent need to investigate