Numerical study of rarefied gas flows in microchannels with oscillating elements

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Abstract. This paper presents a numerical study of a free-molecular ($Kn > 10$) gas flow in two devices with high-frequency oscillating boundary: (1) flow in plane channel with a series of oscillating barriers. (2) flow in a channel with wall performing forced harmonic motion. All calculations were performed using simplified collision-free version of Event-Driven Molecular Dynamics method (EDMD). It was shown that high-frequency oscillations have a significant influence on the gas flow, and this influence depends on molecules characteristic thermal speed. Thus it was shown, that this influence will be different for gases with different molecular masses, which leads to gas separation effect.

1. Introduction

Constant development of microelectronics and microtechnology has lead to the emergence of many new applications of microelectromechanical systems (MEMS). Microdevices with moving parts can be distinguished as separate subclass among all MEMS devices with applications in various areas of microfluidics \cite{1-3}. Recently a series of works appeared devoted to microdevices utilizing surface acoustic waves (SAW) to separate solid microparticles with different sizes \cite{4-6}. Meanwhile, applications of MEMS with moving parts to rarefied gas dynamics problems are very rare.

Authors of this work were the first to discover a series of novel effects appearing for rarefied gas flow in microstructures with moving elements \cite{7-11}. The main idea here is that for gas flowing in free-molecular regime, the only thing affecting gas molecules motion is the number and pattern of gas-surface collisions. For instance, it was noted that for gas flowing in plane straight channel with diffuse reflection law used on the walls, the probability of molecule to pass through the channel decreases exponentially with the number of collisions. Thus for gas flows in microstructures with moving parts molecules passing probability (and, hence, mass flux) can change significantly when the ration of characteristic oscillation speed is compatible with characteristic thermal speed of molecules.

In this work we study the free-molecular gas flow in two devices: in microchannel with a series of oscillating barriers and in the channel with walls moving according to the harmonic law. It is shown that one can influence the conductivity of the channel for a given gas due to forced oscillations of parts the boundary. It is also explained how this effect can be used to separate gas mixtures.
2. Problem statements

First problem studies flow in a plane channel with diameter $D$ and a series of oscillating barriers (figure 1). Barriers have distance $L$ between them and oscillate with frequency $\omega$. Initial phases of barriers motion are chosen in such a way that common motion of barriers lowest point represent a travelling “pseudo-wave” with length $\lambda$. Characteristic wave speed $k$ of such motion is the product $\lambda \omega$.

![Figure 1. Geometry of the first problem. Channel with series of oscillating barriers.](image1)

Second problem studies rarefied gas flow in a curving channel (figure 2), having length $L$ and width $D$ in motionless state (i.e. when there are no oscillations and channel walls are straight). Channel wall are curving according to harmonic law with amplitude $A$, wave length $\lambda$ and wave speed $k$:

$$
y_{\pm} = y_{0,\pm} + A \sin \left( \frac{2\pi x - kt}{\lambda} + \psi \right), \quad y_{0,+} - y_{0,-} = D,
$$

(1)

index $\pm$ corresponds to upper and lower surfaces.

![Figure 2. Geometry of the second problem. Channel with wall curving according to harmonic law.](image2)

Interaction between gas molecule and solid surface was described in terms of Maxwell diffuse scattering model (model with full energy and momentum accommodation). This means that molecule comes in thermal equilibrium with the wall after collision and molecules velocity after collision has equilibrium Maxwell distribution with temperature of the wall. The problem is studied in isothermal case – temperature of the wall and gas at inlet are constant in space and time. The flow is considered free-molecular which means that collision between molecules are neglected. Molecules were simulated as material point with no internal degrees of freedom. Mass forces were not taken into account.

3. Solution procedure

Numerical algorithm was thoroughly discussed in authors works [7–11]. Assumption about free-molecular flow regime allows to ignore collisions between molecules and calculate molecules trajectories independently. This significantly simplifies numerical algorithm which can be treated as either collision-free version of event-driven molecular dynamics method (EDMD [12, 13]) or of direct simulation Monte-Carlo (DSMC) method.

Calculations for each molecule consisted of three stages. First, a molecule was created at inlet cross section with coordinates, velocity and starting time, sampled from corresponding physical distributions. Point of next collision with surface was calculated after that. New velocity was calculated at collision point according to scattering kernel and then a search for new collision point
started. Collision-reflection process was repeated until molecule left the channel through either inlet or outlet cross-section.

As a result of calculations for great number \( (N = 10^7) \) of molecules one obtains passing probability \( P \) as ratio of number of molecules that passed through the channel to the number \( N \) of all probe molecules. Evaluating \( P \) for different values of \( k \) – characteristic oscillations speed and \( c = \sqrt{2k_BT/m} \) – molecules characteristic thermal speed (here \( T \) is temperature, \( k_B \) – Boltzmann constant, \( m \) – mass of the molecule) one obtains profile \( P(k/c) \). Based on profile \( P(k/c) \) one can then evaluate \( \gamma(k) \) – coefficient of separation enhancement for a given pair of gases (for He-Ar mixture in this case).

4. Channel with barriers

Results of calculations for first problem are presented in Figure 3. Characteristic speed of oscillations in this case is the product of pseudo-wave length \( \lambda \) and barriers oscillation frequency \( \omega \). The main parameters of the study are also the distance between the barriers \( L \) and wavelength \( \lambda \) (determined under fixed \( L \) by the number of barriers and phase shift \( \Delta\phi \) between their motion laws). Results in figure 3(a) indicate that for small number of barriers separation enhancement can occur only for low values of \( L/D \). However, such close distances between neighboring barriers cannot be achieved in practice. Meanwhile increasing number of barriers (figure 3(b)) one can achieve enhanced separation even for higher values of \( L/D \). Moreover, increasing number of barriers and, hence, increasing pseudo-wave length \( \lambda \) one can achieve values of characteristic speed \( \lambda\omega \) comparable with characteristic thermal speed of molecules even for comparatively low values of frequencies \( \omega \) (about kHz). This fact means that it is possible to realize this effect in practice.

![Figure 3](image)

**Figure 3.** Simulation results in first problem. Dependence of coefficient \( \gamma \) on characteristic speed \( \lambda\omega \) for different values of ratios \( L/D \) (a) and \( \lambda/L \) (b).

5. Channel with curving walls

Second problem has more parameters and only main results are presented in Figure 4. It is shown that separation effect (nonmonotic \( P(k/c) \) profile) is observed only at ratios \( A/D \) (oscillation amplitude to channel diameter) around 0.2 (figure 4). Values of separation enhancement coefficient \( \gamma \) in case \( A/D = 0.2 \) are presented in figure 5(a). For higher and lower values of \( A/D \) separation effect vanishes (profiles become monotonic) but pumping effect is still observed, which means that for low and high values of \( A/D \) this device can be used as a vacuum gas pump. It is noted that with increasing wavelength \( \lambda \) separation effect is getting stronger but requires higher values of wave speed \( k \) to reach maximal effect (figure 5(a)). It is also noted that using longer channel also leads to more effective separation (figure 5(b)).
Figure 4. Simulation results in second problem. Profiles $P(k/c)$ for $L/D=10$ and different values of $\lambda/A$ (given in legend) and $A/D$. (a) $A/D=1.0$. (b) $A/D=0.5$. (c) $A/D=0.4$. (d) $A/D=0.2$. (e) $A/D=0.1$. (f) $A/D=0.01$.

Figure 5. Dependence of coefficient $\gamma$ on characteristic wave speed $k$ for different values of ratios $\lambda/A$ (a) and $L/D$ (b).

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