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Multiscale simulation of non-isothermal microchannel gas flows

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ABSTRACT

This paper describes the development and application of an efficient hybrid continuum-molecular approach for simulating non-isothermal, low-speed, internal rarefied gas flows, and its application to flows in Knudsen compressors. The method is an extension of the hybrid continuum-molecular approach presented by Patronis et al. (2013) [4], which is based on the framework originally proposed by Borg et al. (2013) [3] for the simulation of micro/nano flows of high aspect ratio. The extensions are: 1) the ability to simulate non-isothermal flows; 2) the ability to simulate low-speed flows by implementing a molecular description of the gas provided by the low-variance deviational simulation Monte Carlo (LVDSMC) method; and 3) the application to three-dimensional geometries. For the purposes of validation, the multiscale method is applied to rarefied gas flow through a periodic converging-diverging channel (driven by an external acceleration). For this flow problem it is computationally feasible to obtain a solution by the direct simulation Monte Carlo (DSMC) method for comparison: very close agreement is observed. The efficiency of the multiscale method, allows the investigation of alternative Knudsen-compressor channel configurations to be undertaken. We characterise the effectiveness of the single-stage Knudsen-compressor channel by the pressure drop that can be achieved between two connected reservoirs, for a given temperature difference. Our multiscale simulations indicate that the efficiency is surprisingly robust to modifications in streamwise variations of both temperature and cross-sectional geometry.

1. Introduction

Designers of microfluidic devices are in need of computational tools that can be used to analyse problems that involve rarefied gas flows in complex micro geometries. Numerical simulation of the gas flow through such geometries is, however, extremely challenging. Conventional continuum fluid dynamics (CFD) becomes invalid or inaccurate as the characteristic scale of the geometry (e.g. the channel height, h) approaches the molecular mean free path, λ [1,2]. When $\lambda/h \gtrsim 0.1$, the error in solutions obtained from CFD may be significant, and we must consider the fluid for what it is: a collection of interacting particles. However, the computational expense of simulating the flow of a rarefied gas in high-aspect-ratio micro geometries (i.e. ones that are long, relative to their cross section) using a particle method, such as the direct simulation Monte Carlo (DSMC) method [2], can be prohibitively high [3,4]. The computational intensity of the particle method

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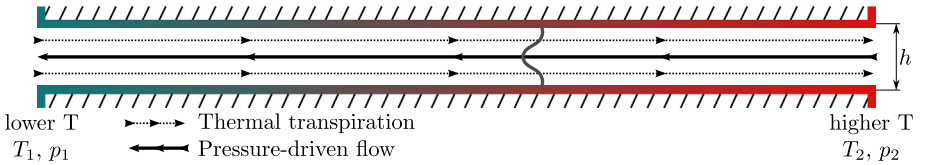

Fig. 1. Thermal transpiration and opposing pressure-driven flow.

is greater still when simulating low-speed microfluidic devices where there are only small deviations from equilibrium, characterised by extremely low Mach numbers and weak temperature gradients.

To simulate the flow of a rarefied gas in micro geometries of high aspect ratio, processes need to be resolved simultaneously over both the smallest and largest characteristic length scales of the geometry: the problem is multiscale in nature. To tackle this, the internal-flow multiscale method (IMM) [3] has been developed. The IMM facilitates the coupling of conventional continuum theory and a suitable particle method, via mass and momentum flux conservation. This coupling allows us to take advantage of the simplicity and efficiency of continuum theory, and the accuracy of the particle method. The IMM is iterative, involving a bidirectional and indirect exchange of information between the continuum domain and a number of spatially-distributed particle subdomains, until convergence is obtained.

Recently, the IMM has been extended to treat compressible internal rarefied gas flows [4], but limited to isothermal problems and relatively high-speed flows. The DSMC method was used to provide the molecular description of the gas transport, and thus low-speed near-equilibrium flows could not be simulated efficiently. This is because, at low speeds, the number of samples required to obtain an acceptable signal-to-noise ratio is intractable.

In this paper, we present two extensions to the IMM that enable: a) non-isothermal and b) near-equilibrium flows to be modelled. We apply this extended IMM to study the phenomenon of thermal transpiration, and its application to Knudsen compressors (also known as Knudsen pumps) [5]: solid-state thermal molecular pumps which operate by exploiting thermal transpiration.

Thermal transpiration (thermal creep) is a rarefied gas effect, whereby a slip flow is generated at a surface in response to a streamwise variation in temperature. Importantly, and counter-intuitively, flow is driven from lower temperature to higher temperature regions. Fig. 1 illustrates the steady-state flow field in a channel with height comparable to the molecular mean free path, which connects two reservoirs; one with temperature T_1 and pressure p_1, and the other with temperature T_2 and pressure p_2. In this steady state, the net mass flow rate through the channel is zero. The transient processes that result in this steady-state condition are not captured by the IMM, but are briefly described here for clarity. Initially, with zero tangential wall-temperature gradient, $p_1 = p_2$. As a tangential wall-temperature gradient is applied, fluid is transported by thermal transpiration into the reservoir with high temperature. This raises the pressure in the high-temperature reservoir, creating a pressure gradient opposing the thermal transpiration. This pressure gradient continues to develop until it is sufficient to fully balance the flow due to thermal transpiration, resulting in zero mass flow rate (see Fig. 1). To achieve a large pressure drop $(p_2 - p_1)$, the flow resistance must be high, and so typically the aspect ratio of the channel must be high.

2. Multiscale and numerical methodology

The internal-flow multiscale method (IMM), which was developed for high-aspect-ratio geometries, uses particle-based 'micro subdomains', covering the full cross section of the channel or tube. These subdomains are distributed in the streamwise direction with a spacing sufficient to resolve any streamwise variation in the simulation geometry and flow variables within it. This subdomain placement is illustrated in Fig. 2(b), for a generic internal-flow geometry, Fig. 2(a). The geometry of each subdomain represents the cross-sectional geometry of the macro domain at that point locally.

Application of the IMM requires that a degree of length-scale separation exists between hydrodynamic variation along streamlines (i.e. in the s-direction, see Fig. 2(a)) and microscopic processes transverse to the flow direction (in x- and y-directions). For this scale separation to exist, the section geometry (and the wall boundary conditions) must vary slowly in the streamwise direction. A dimensionless number indicating the degree of such scale separation can be expressed:

$$S = \min\left\{ \left|\frac{\mathrm{d}L_y}{\mathrm{d}s}\right|^{-1}, \left|\frac{\mathrm{d}L_z}{\mathrm{d}s}\right|^{-1}, \left|\frac{L_y}{\phi}\frac{\mathrm{d}\phi}{\mathrm{d}s}\right|^{-1}, \left|\frac{L_z}{\phi}\frac{\mathrm{d}\phi}{\mathrm{d}s}\right|^{-1}, \left|\frac{R_y}{L_y}\right|, \left|\frac{R_z}{L_z}\right| \right\}, \tag{1}$$

where L_y and L_z are length scales in the transverse directions that characterise the cross-section geometry, ϕ is a flow variable (e.g., density, temperature or pressure), and R_y and R_z are the radii of curvature of the centre streamline. Provided $S \gg 1$, it can safely be assumed that, in small streamwise sections of the tube/channel, streamwise flow variations are effectively negligible and the walls are approximately parallel to the centre streamline (and consequently all other local streamlines). This is referred to by Borg et al. [3] as a *local parallel-flow assumption*, and it allows for the simulation domain to be represented by streamwise-periodic subdomains with exactly parallel walls, as depicted in Fig. 2(b). Depending on the type of molecular solver utilised, these subdomains can be three-dimensional (with a small but finite dimension in the s-direction) as illustrated in Fig. 2(b), or two-dimensional, as is the case in this paper, where the subdomains are cross-sectional slices with no dimension in the s-direction.