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Lattice Boltzmann computations of micro channel and micro orifice flows

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RESUMEN

La filtración de micro flujos gaseosos puede complicarse por deslizamiento del flujo por el filtro y las partículas. El deslizamiento complica soluciones por Navier-Stokes. El método directo de simulación Monte Carlo y sus derivados aplican, pero son complejos. El método de redes de Boltzmann parece ofrecer ventajas en los regimenes de deslizamiento y transición. Para evaluar el método, cálculos de flujo fueron realizados en micro-canales y micro-orificios a diversos números de Reynolds y Knudsen. Se uso la aproximación de relajación temporal simple de las redes de Bhatnagar-Gross-Krook con el parámetro de relajación como responsable por las variaciones de densidad. Los resultados de perfiles de velocidad y distribución de presión para micro-canales concuerdan con la literatura. Los resultados para micro-orificios coinciden con otros cálculos a bajo número de Reynolds, pero difieren cuando el número de Reynolds incrementa. El método de redes de Boltzmann parece confiable para estos flujos, pero a elevados números de Reynolds pueden necesitarse modelos de relajación temporal más sofisticados.

ABSTRACT

Filtration in gas micro flows is an important problem complicated by possible slip flow for the filter media and the particles. Slip complicates Navier Stokes solutions. The direct simulation Monte Carlo method and its derivatives can be applied, but they are very complex. The lattice Boltzmann method appears to offer some advantages for such slip and transitional flows. To evaluate the method, it was used to compute micro-channel and micro-orifice flows for a range of Reynolds and Knudsen numbers. The Lattice Bhatnagar-Gross-Krook single relaxation time approximation was used with the relaxation parameter accounting for density variations. Velocity profile and pressure distribution results for micro-channels are in good agreement with the literature. The micro-orifice results agree well with other computations at low Reynolds numbers, but display deviations with increasing Reynolds number. The lattice Boltzmann method appears suitable for these flows, but more sophisticated relaxation time models may be needed for the higher Reynolds numbers.

Keywords: Lattice Boltzmann Equation, MEMS micro flows, microchannels, microfilters, and microfiltration.

NOMENCLATURE

c_s	speed of sound
d	molecular diameter
e	energy term in the Navier-Stokes equation
e_α	discrete particle velocity in the lattice Boltzmann method
f	single particle mass distribution function
$f^{(eq)}$	equilibrium distribution function
$\tilde{f}$	post-collision distribution function
h	orifice height
H	channel height
Kn	Knudsen number
k_B	Boltzmann constant
$\boldsymbol{l}$	orifice length
L	channel length
n	number density of gas molecules
$\boldsymbol{n}$	unit outward normal
p	pressure in the LBGK
P	pressure in the Navier-Stokes equation
R	gas constant
Re	Reynolds number
t	time
T	temperature
$\boldsymbol{u}$	fluid velocity
w_α	weighting factor in the LBGK
$\mathbf{x}$	spatial position vector

GREEK LETTERS

γ	adiabatic index
δ_t	time step
δ_x	space step
ε	a variable related to the square of the energy
ξ	particle velocity vector
κ	relaxation time
λ	mean free path
ν	kinematic viscosity
Π	pressure ratio in Poiseuille flow
ρ	fluid density
τ	dimensionless relaxation time in LBGK method

INTRODUCTION

The rapid development in the field of micro electromechanical systems (MEMS) has led to a wide range of applications. The fabrication methods for MEMS have been improved noticeably resulting in smaller dimensions and accurate geometries. Their utilization includes liquid, gas and liquid-gas environments. This advance in better fabricated devices and new applications of MEMS sometimes contrasts with the research that has been done to describe their physics. The characteristic dimension of these devices is of the order of 0.1 to 10 μm, and includes micro channels, micro pumps, micro valves, micro nozzles, flow sensors.

At this very small scale, a fluid particle can travel a relatively long distance and collide with a boundary before it collides with another fluid particle. The Knudsen number (Kn) represents this effect as the ratio of the mean free path of the fluid to a characteristic length of the flow. It is used to determine the flow regime over which the continuum (conventional viscous fluid flow analysis based on the Navier-Stokes equations, NS) or free molecular (atomistic analysis based on kinetic theory and the Boltzmann equation, BE) approaches are suitable.

Different mathematical approaches have been developed to describe fluid flows in different flow regimes. The continuum regime for the Navier-Stokes equation applies when $\mathrm{Kn} < 0.001$. The Navier-Stokes equation regime with slip-flow boundaries is valid from $0.001 < \mathrm{Kn} < 0.1$. The transitional regime occurs if $0.1 < \mathrm{Kn} < 10$ and the Burnett equations (a special analytical case of the Boltzmann equation subject to certain restrictions) can be used. Finally, the linearized Boltzmann equation applies for the free molecular regime after $\mathrm{Kn} \geq 10$, (Karniadakis & Beskok, 2002).

In general, the Boltzmann equation (BE) can be used to describe a flow in any of the flow regimes. The BE is derived rigorously from Newton's laws in the low-density limit. The evolution of a velocity distribution function is characterized by the BE through molecular transport and binary intermolecular collisions. However, it is almost impossible to solve the integro-differential Boltzmann equation analytically. The BE may be approximated with several approaches, including the Burnett equations mentioned previously. One scheme, the Lattice Boltzmann Equation (LBE), has been investigated extensively in the past fifteen years or so. In the LBE the Boltzmann equation is simplified and solved based on the interactions of particle moving with restricted velocities and speeds on a discrete lattice. Many researchers have studied the LBE in the continuum regime with satisfactory results for a variety of fluid flow cases; see Yu et al., (2003). In contrast, little research has been carried out in order to develop the LBE beyond the continuum regime. The approach is attractive, for it is not based upon a continuum assumption and computations with it promise to be more efficient than those with such techniques as Direct Simulation Monte Carlo approaches. Some good progress in the development of the LBE in the slip and transitional regimes has been made by Nie et al. (2002) and by Lim et al. (2002).

This work deals with a study of the LBE in the slip regime. A simple single relaxation time approximation of the LBE (Qian, 1992), called the Lattice Bhatnagar-Gross-Krook model (LBGK) originally designed for continuum flow is implemented. In order to simulate micro-channel and micro-orifice flow, modifications suggested by Nie et al. (2002) are introduced in the LBGK model. The results of this implementation are then compared with results from the unified flow model developed by Karniadakis & Beskok (2002). Their model uses the compressible NS equations for the slip and transitional regimes.

Special attention is focused on the flow passing a micro-orifice. As will be explained later, micromachined membranes with perforations are used as micro-filters in some MEMS applications (Yang et al., 2001). The simplified simulation model consists of a single orifice in a long periodic channel. Imtiaz & Beskok (2001) simulated micro-filter flow using a spectral element implementation of the compressible NS equations with higher order velocity slip and temperature jump boundary conditions. Their results show that the compressibility and rarefaction effects become very important for gas micro flow in the slip and transitional regimes. Thus, if the LBGK is intended to be used for micro flow simulations it has to reproduce the compressibility effects in gas micro flows in the slip and transitional regime. The goal of the present work was to determine the LBE responds at this limit.

THEORETICAL FORMULATION AND NUMERIC IMPLEMENTATION

In the BE, the central variable of interest is a one-particle probability distribution function $f(\mathbf{x},\mathbf{e},t)$, where $\mathbf{x}$ denotes the particle's coordinate in the physical space, and $\mathbf{e}$ is the particle's velocity. For the Boltzmann equation, the state of monatomic gases is described by this probability distribution function, which represents the number of particles in the six-dimensional phase space $d\mathbf{x}d\mathbf{e}$ at time t. A simplified version of the BE can be expressed as

$$\frac{\partial f}{\partial t} + \mathbf{e} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{e}} = Q(f, f_*) \quad (1)$$

where **F** is an external body force. The first term in the left-hand-side of the BE represents the rate of change of the density distribution function of particles in the phase space. The second term in the left-hand-side is the convection of molecules across a fluid volume by particle velocity **e**. The convection of particles across the velocity space as a result of the external force **F** is shown by the third term of the left-hand-side of the BE. Particle collisions are represented by the right-hand-side of the BE (collision term) as

$$Q(f, f^*) = \int_{R^3} \int_{S^+} |\mathbf{E} \cdot \mathbf{n}| \left[f(\mathbf{x}, \mathbf{e}_*') f(\mathbf{x}, \mathbf{e}') - f(\mathbf{x}, \mathbf{e}_*) f(\mathbf{x}, \mathbf{e}) \right] B \mathbf{n} d\mathbf{e}_* \quad (2)$$

The above equation represents collisions of two molecules with post-collision velocities **e** and **e**$_*$, and corresponding pre-collision velocities **e'** and **e'**$_*$. The integration is performed over the three dimensional velocity space R^3 and the hemisphere S^+, that includes the region in which the particles move after the collision.

The classical approach to solving the BE analytically consists of a simplification of the collision term. Many methods have been developed following this approach, with the method of Bhatnagar, Gross and Krook (BGK) (Bhatnagar et al., 1954) the most popular. In the BGK method the collision term is approximated as

$$Q_{BGK}(f, f^*) = e_* (f_{loc} - f) \quad (3)$$

where e_* is the collision frequency, which is assumed to be independent of the particle velocity **e**. However, e_* is a function of spatial coordinates and time. According to Karniadakis and Beskok (2002) the BGK, for a full solution of the BE, is only accurate for isothermal flows.

The LBE is designed to solve the kinetic behavior of a particle with different number of speeds and velocities in two or three dimensional square or cubic lattices. For the scope of this study, the three speeds and nine velocities on a two dimensional square lattice, known as D2Q9 and first introduced by Qian (1992), is used. The kinetics of the particle for its velocity distribution function $f(\mathrm{x}, \xi, \mathrm{t})$ is solved by LBE. Here, **x** is the spatial position vector, ξ is the particle velocity vector, and t is the time. The evaluation of the hydrodynamic moments of f yields the macroscopic quantities. Many scientists have used this kinetic model, in which the single relaxation-time-approximation technique was first introduced by Bhatnagar et al. (1954) in the solution of the Boltzmann Equation:

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla f = -\frac{1}{\kappa}(f - f^{(0)}), \quad (4)$$

where κ is the relaxation time and $f^{(0)}$ is the Maxwell-Boltzmann distribution function, also known as the equilibrium distribution function. The viscosity can be estimated as $v = \kappa \mathrm{RT}$, in which R is the ideal gas constant and T is the gas temperature.

He and Luo (1997) proposed a way to solve Eq. (4) numerically, discretizing it in the context of the conservation laws in velocity space using a finite set of velocity vectors $\{\xi_\alpha\}$ as

$$\frac{\partial f_\alpha}{\partial t} + \xi_\alpha \cdot \nabla f_\alpha = -\frac{1}{\kappa}(f_\alpha - f_\alpha^{(eq)}) \quad (5)$$

here again, $f_\alpha(\mathrm{x}, \mathrm{t}) \equiv f(\mathrm{x}, \xi, \mathrm{t})$ is the distribution function associated with the ath discrete velocity ξ_α, and $f^{(eq)}$ is the equilibrium distribution function in this discrete velocity space. Equation (5) is called the discrete velocity model (DVM). In particular, for the case of the D2Q9 model (Figure 1) the discrete velocity set $\mathbf{e}_\alpha$ is

$$\mathbf{e}_0 = 0,$$

$$\mathbf{e}_\alpha = c\left(\cos(\alpha - 1)\frac{\pi}{4}, \sin(\alpha - 1)\frac{\pi}{4}\right)$$

for $\alpha = 1,3,5,7,$

$$\mathbf{e}_\alpha = \sqrt{2}c\left(\cos(\alpha - 1)\frac{\pi}{4}, \sin(\alpha - 1)\frac{\pi}{4}\right) \quad (6)$$

for $\alpha = 2,4,6,8,$

where: $c = \delta x / \delta t$ is the lattice constant
δ_t = time step.

In this context, the equilibrium distribution function can be represented as

$$f_\alpha^{(eq)} = \rho w_\alpha \left[1 + \frac{3}{c^2}\mathbf{e}_\alpha \cdot \mathbf{u} + \frac{9}{2c^4}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u} \cdot \mathbf{u}\right] \quad (7)$$

where: $w_\alpha = \begin{cases} \frac{4}{9}, \alpha = 0, \\ \frac{1}{9}, \alpha = 1,3,5,7, \\ \frac{1}{36}, \alpha = 2,4,6,8, \end{cases}$

are the weighting factors.

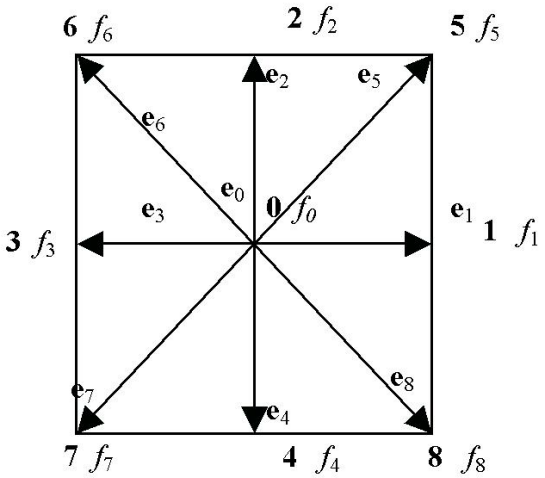

Figure 1. A two dimensional nine velocity lattice model.

The density and the momentum fluxes can be estimated by

$$\rho = \sum_{\alpha=0}^{8} f_\alpha = \sum_{\alpha=0}^{8} f_\alpha^{(eq)}, \tag{8}$$

and

$$\rho \mathbf{u} = \sum_{\alpha=0}^{8} \mathbf{e}_\alpha f_\alpha = \sum_{\alpha=0}^{8} \mathbf{e}_\alpha f_\alpha^{(eq)} \tag{9}$$

If the velocity of sound in this model is assumed to be $c_s = c/\sqrt{3}$, then the equation of state for ideal gases becomes

$$p = \rho c_s^2 . \tag{10}$$

The DVM can be solved using any standard numerical method such as finite difference. It is important to point out that the use of the finite difference technique requires special care when $\kappa \ll 1$ for low viscosity flows (Yu et al., 2003). However, in the Lattice Boltzmann model, Eq. (5) is solved by fully discretizing it with time step δt and space step $\delta x = e_\alpha \delta t$ as follows

$$f_\alpha(\mathbf{x}_i + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}_i, t) = \frac{1}{\tau}\left[f_\alpha(\mathbf{x}_i, t) - f_\alpha^{(eq)}(\mathbf{x}_i, t)\right] \tag{11}$$

where: $\tau = \lambda/\delta t$
$\mathbf{x}_i$ = a point in the discretized physical space.

This is the so called Lattice Boltzmann Equation (LBE) with the Bhatnagar-Gross-Krook (BGK) approximation (LBGK), and it is solved numerically through the collision and streaming steps respectively as

$$\tilde{f}_\alpha(\mathbf{x}_i, t + \delta t) = f_\alpha(\mathbf{x}_i, t) - \frac{1}{\tau}\left[f_\alpha(\mathbf{x}_i, t) - f_\alpha^{(eq)}(\mathbf{x}_i, t)\right] \tag{12}$$

and

$$f_\alpha(\mathbf{x}_i + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}_i, t) = \tilde{f}_\alpha(\mathbf{x}_i, t + \delta t) \tag{13}$$

where: $\tilde{f}_\alpha$ = post-collision state.

The equivalent NS-viscosity derived from Eq. (10) can be expressed as

$$\nu = (\tau - \tfrac{1}{2})\, c_s^2\, \delta t. \tag{14}$$

Equation (14) requires that $\tau > \tfrac{1}{2}$ in all LBE computations. In addition, τ cannot be greater than 2 in order to maintain numerical stability (Qian, 1992). Also to fulfill stability criteria, the actual value of the viscosity ought to be $O(0.1)$ in computations at moderate Reynolds number, according to Succi (2001).

LATTICE BOLTZMANN EQUATION FOR MICRO FLOWS

The relaxation time τ normally remains constant during the computational procedure. As noted in the previous section, τ also defines the viscosity ν in the incompressible limit. However, in very long micro channels, the density variation can be large along the channel, even though the variation of the local density is small (Karniadakis and Beskok, 2001). In order to account for this density variation and its effect on the kinematic viscosity, ν, Nie et al. (2002) replaced the relxation time τ with τ' in the following manner

$$\tau' = \frac{1}{2} + \frac{1}{\rho}(\tau - \frac{1}{2}) \tag{15}$$

Then, the viscosity can be rewritten as

$$\nu = c_s^2\,(2\tau - 1)/(2\rho) \tag{16}$$

which suggests a constant dynamic viscosity $\mu = \rho\nu$.

In classical kinetic theory ν is linearly proportional to λ, under the assumption of a hard sphere gas; thus, the mean free path can be redefined in the LBE as

$$\mathrm{Kn} = A\frac{(\tau - 0.5)}{\rho H} \tag{17}$$

where H = is the characteristic length of the flow domain.

COMPRESSIBLE NAVIER-STOKES EQUATIONS (UNIFIED MODEL)

The LBE micro-channel and micro-orifice simulations performed

in this work are compared to computational results from the unified flow model of Karniadakis & Beskok (2002), as the micro flow literature lacks experimental results for micro-channels or micro-orifices at conditions relevant to this study. Comparisons to atomistic simulation models such as molecular dynamics (MD) and direct simulation Monte Carlo method (DSMC) are not considered, for these models are designed mainly to simulate rarefied gases at high Kn numbers (highly transitional and free molecular flows). Therefore, the unified flow model of Karniadakis and Beskok seems to be the best alternative, since it has been proven to be highly accurate in the description of micro-channel and micro-orifice flows (Imtiaz & Beskok, 2001). The unified model of Karniadakis and Beskok has been compared with the DSMC and with some experimental data of velocity and pressure measurements in micro-channel flow. This model is based on the compressible NS equation with velocity scaling laws and consideration of rarefied effects. The authors claim to have accomplished excellent approximations for gas flows in micro pipes and micro channels in the whole Knudsen regime.

In their micro-channel model, Karniadakis & Beskok (2002) were able to non-dimensionalize the velocity profile as a function only of the y coordinate to the channel height and the Knudsen number as follows

$$U^*(y,Kn) = U(x,y)/\overline{U}(x) = \left[\frac{-\left(\frac{y}{h}\right)^2 + \frac{y}{h} + \frac{Kn}{1-\mathbf{b}Kn}}{\frac{1}{6} + \frac{Kn}{1-\mathbf{b}Kn}} \right] \quad (18)$$

In equation (18), **b** represents a constant that defines the order of accuracy of the method for the velocity slip boundary condition. In this case, **b** can take values of 0, –1 and –2, the last one being the highest order model. Since, the LBE method for micro-flows used here is thought to be highly accurate in the slip regime, **b** = –2 is selected as a higher-order model for comparison purposes.

A nonlinear pressure variation is expected along long micro-channels in contrast to the linear pressure variation in laminar Poiseuille flows at very small, no-slip Knudsen numbers. Karniadakis & Beskok (2002) present a non-dimensional equation for this pressure distribution along the channel and it will be used for comparison to the LBE method results of the present study for micro-channels. The equation is expressed as

$$\tilde{P}^2 - 1 + 2(6+\tilde{\alpha})\frac{2-\sigma_v}{\sigma_v}Kn_0(\tilde{P}-1) + 2(6b+\tilde{\alpha})\frac{2-\sigma_v}{\sigma_v}Kn_0^{\,2}\log_e\left(\frac{\tilde{P}-bKn_0}{1-bKn_0}\right) = B(1-x/L) \quad (19)$$

where :

$\tilde{P}(x) = P(x)/P(0)$,

B = has to have a value such that $\tilde{P}(0) = P_i/P_0 = \Pi$

MICRO-CHANNEL SIMULATION RESULTS

In this implementation, a channel with a ratio of height to length of 100 (L/H>>1) was used to simulate the velocity and pressure profiles using 20 lattice units in the y-coordinate and 2000 in the x-coordinate. A schematic of the computational domain is shown in Figure 2. The bounce-back boundary condition is applied at the bottom and top plates (Zieger, 1993). The density redistribution in the first lattice column is applied for the inlet/outlet pressure-difference boundary condition (Succi, 2001). The Knudsen number was selected to be 0.0194 in this implementation to be consistent with the literature.

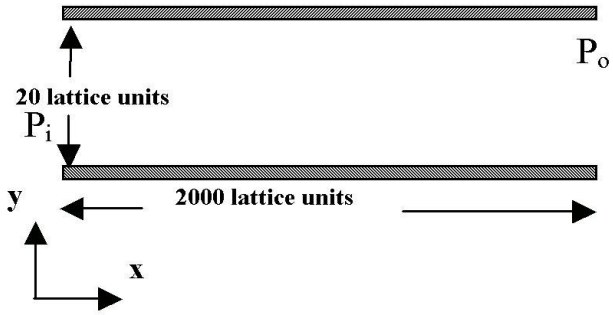

Figure 2. Schematic of Poseiuille flow in a micro-channel with L/H=100, and Π=2.0.

The results of the present implementation for the velocity profiles are compared with Eq. (18) and are shown in Figure 3, for a pressure ratio Π of approximately 2.0. From Figure 3 one can notice that the present LBGK simulation over predicts the velocity profile when compared with Eq. (18) at the middle of the channel's height. The greatest deviation is approximately 8.74% at the maximum velocity value. Note

$\Pi = P_i/P_0$

P_i, P_0 = pressure at inlet and outlet respectively.

that there is a gap in the prediction of the velocity between the first and the last fluid nodes and the wall nodes. In this simulation, the solid wall nodes correspond to $y = 0$ and $y = 19$. The next-to-wall fluid nodes are $y = 1$ and $y = 18$. As a result, the slip velocity is not well predicted for this LBGK simulation. Since Eq. (17) limits the number of lattice units in the y-coordinate, it is not possible for this LBGK scheme to refine the number of grid points near the wall, which presumably would lead to a better agreement with Karniadakis & Beskok (2002). Despite the existence of grid refinement schemes for the regions near the wall, they are only applicable to the continuum LBGK model; see (Chen et al., 1996), (Mei et al., 2000), (Verberg and Ladd, 2000), and (Verberg and Ladd, 2002).

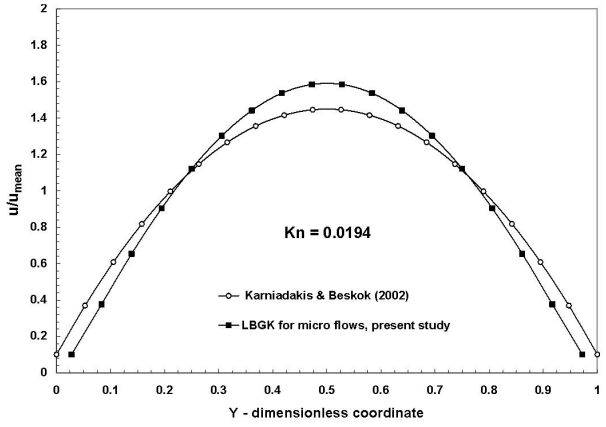

Figure 3. Non-dimensionalization of the velocity profile with the mean velocity along the channel height. The LBGK results correspond to the outlet nodes.

A similar analysis is presented in Figure 4, which compares the deviations of the streamwise pressure from the linear pressure distribution. It is customary to express the curvature in the pressure distribution in relation to its deviation from the corresponding linear pressure drop, $(P - P_l) / P_0$ along the channel length, where $P_l = P_0 + (P_i - P_0)(1\text{-}X)$. The fourth term of the right hand side of Eq. (16) can be neglected when $Kn=0.0194$. It is easy to observe the difference between the values from Eq. (19) and the present results obtained with the LBGK for micro flows. The present LBGK model overestimates the deviation in comparison with model of Karniadakis & Beskok (2002). It seems that the LBGK simulation results tend to make the deviation curve taller, although the maximum deviation remains at approximately $X = 0.58$. The LBGK at this point over-predicts the model of Karniadakis & Beskok by about 23%. One reason for this behavior may be that the

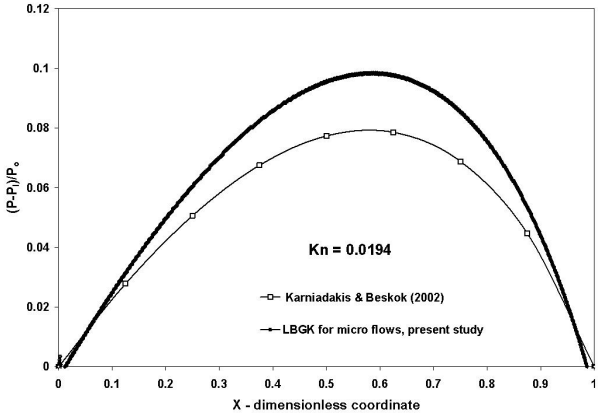

Figure 4. Deviations from linear pressure profile for $\Pi = 2.0$.

density redistribution boundary condition (Succi, 2001) used to reproduce the pressure-difference boundary condition seems to fail near to the inlet/outlet locations. It is suspected that other types of boundary condition schemes, such as the extrapolation method, will lead to better results (Chen et al., 1996). Nevertheless, the density redistribution scheme does provide a good approximation to the deviation from the linear pressure profile.

MICRO-ORIFICE SIMULATION RESULTS

One way to collect micron-size particles or biological agents from air is to use micro-machined membranes with a micron-size array of perforations (Yang et al., 1999). The typical hole sizes for this type of filter ranges from $1\mu m$ to $12\mu m$ with membrane thickness, l, from $1\mu m$ to $3\mu m$. Experimental and numerical simulations of the performance of such filtering membranes have been reported for these geometries.

The prime objective in evaluating LBGK for filter predictions is to observe in detail the flow's behavior passing the micro filter holes. The analysis can be performed considering only one hole, assuming that the effects are repeated throughout an array of micro filter holes. Imtiaz & Beskok (2001) performed similar simulations, as mentioned previously. They used the two-dimensional spectral element algorithm μFlow, which solves the unsteady compressible NS equations subject to higher-order velocity slip and temperature jump boundary conditions. In their simulations they fixed the height h to thickness ratio of the hole opening $(h/l = 1.5)$. The opening factor β, which is the ratio of the hole-area to the total filter area, was also kept constant ($\beta = 0.6$). The ratio of channel length to height has a constant value of 17. Figure 5 presents a schematic of the computational domain used in the current study to match the Imtiaz & Beskok geometry. Table (1), shows the geometry values that correspond to Figure 5. The term H_{ref} denotes the characteristic length used to estimate the reference Knudsen

TABLE 1. Dimensions of the micro-orifices used in this study.

H_{ref}	Dimensions (μm)		
	H	h	*l*
2 microns	2	1.2	0.8

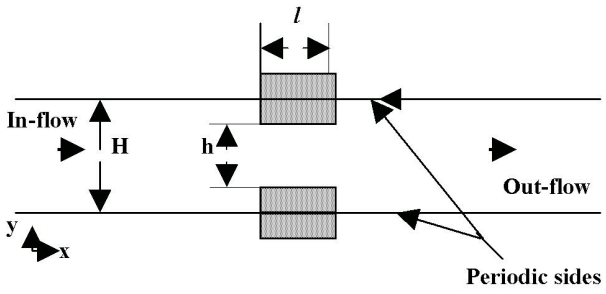

Figure 5. Schematic of the micro-filter model. Important length scales are identified on the figure.

number. In the Imtiaz & Beskok study, the flow domain was discretized using 360 non-uniform quadrilateral spectral elements. They utilized an 8th-order Gauss-Lobatto-Legendre polynomial expansion in each direction.

For the present LBGK computations, the 2μm channel height case requires 20 lattice units in the y-direction and 340 in the x-direction in order to be keep the same length to height ratio used by Imtiaz & Beskok (2001). LBGK simulation results with the 2μm channel height case are used for comparison with the micro-filter simulations of Imtiaz & Beskok. Simulations are performed with four different Reynolds numbers.

Periodicity was assumed in the streamwise direction, and bounce-back boundary conditions are applied for the filter walls (Ziegler, 1993). The density redistribution boundary condition induces the flow through the hole (Succi, 2001). Successive variations of the acceleration term in this LBGK implementation were used to match the desired Reynolds number. Since, the LBM is an unsteady flow solver, the time history of the velocity is observed at three critical points of the computational domain to ensure steady state in computations. The first location is placed at L/4, around 100 lattice units before the obstruction. The second location is approximately at the middle of the orifice. Finally, the third location was situated at L/2.

Figure 6 shows a comparison of the x-velocity component from the results obtained by Imtiaz & Beskok(2001) with the present study for the 2μm channel height case. It is important to note that the Reynolds numbers do not match exactly due to the fact that Re cannot be set to a specific value in this LBGK implementation, due to the density redistribution boundary condition. Nevertheless, the comparison given in Figure 6 does give a good measure of the difference between the LBGK method for micro flows and the compressible NS for nearly identical Reynolds numbers. From Figure 6 it is evident that as the flow approaches the constriction, it experiences acceleration, reaching its maximum velocity at approximately the middle of the orifice. After the flow passes the orifice, it begins to slow down and the velocity become nearly constant after around L/X = 6.4. Lower constant velocities are experienced before the obstruction. The LBGK method for micro flows approximates almost exactly to the compressible NS at low Reynolds number. Figure 6 shows that at Re = 2.99 both curves are almost identical. However, as the Reynolds number increases the deviation between the methods increases as well. It seems that the LBGK under-estimates the velocity profile. The LBGK with Re = 4.77 starts to under-predict velocities when compared with the compressible NS at Re = 4.39. As Re increases the under-prediction becomes more evident, with the LBGK results at Re = 8.96 under predicting the velocity by approximately 9.2% at the maximum velocity point.

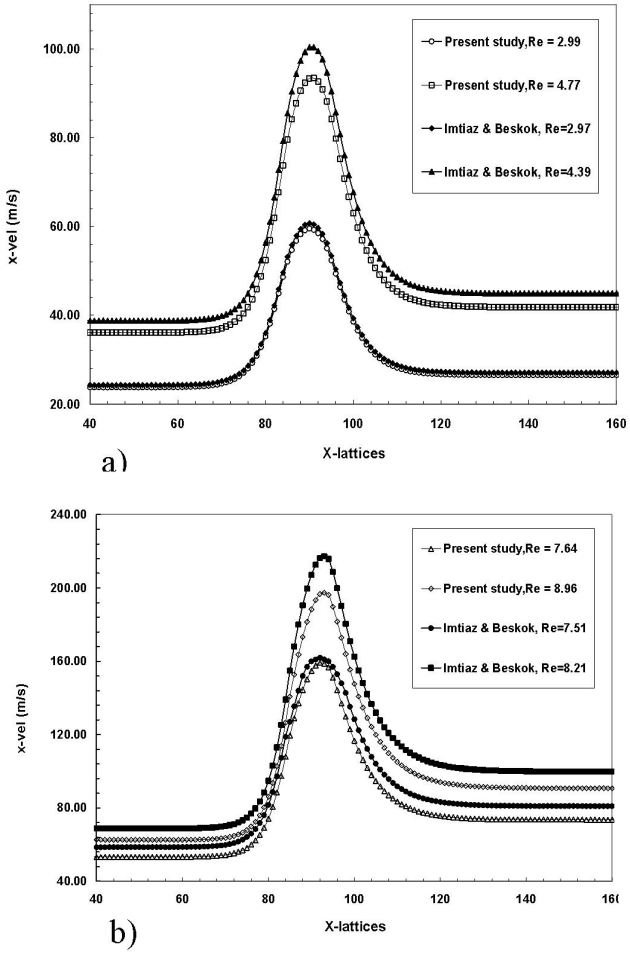

Figure 6. Comparison of streamwise velocity variation, for the 2im characteristic channel height, at a) low and b) high Reynolds number in the streamwise direction (zoomed around the orifice location).

One reason for this deviation is the fact that a velocity increase is responsible for altered density variations along the orifice. As will be explained later, the pressure drop through the orifice is proportional to this density variation. Thus, higher velocities mean higher density variation which increases the compressibility effects along the orifice.

Since the LBGK for continuum flows was originally designed to solve nearly incompressible flows, it seems that applications of the LBGK to micro flows may be susceptible to high compressibility effects. Another reason for the differences may be the small number of lattice units in the y-direction affecting the accuracy of the LBGK method. Up to now, there has been little in the literature about the development of any grid refinement technique for the LBGK for micro flows, although there are many techniques available for LBGK in the continuum regime (i.e., Filippova & Hanel, 1998 and Dazhi et al., 2002).

Figure 7 illustrates the density variations along the channel obtained with LBGK for micro flows. Here, it is shown that increased density variations occur at higher Reynolds numbers.

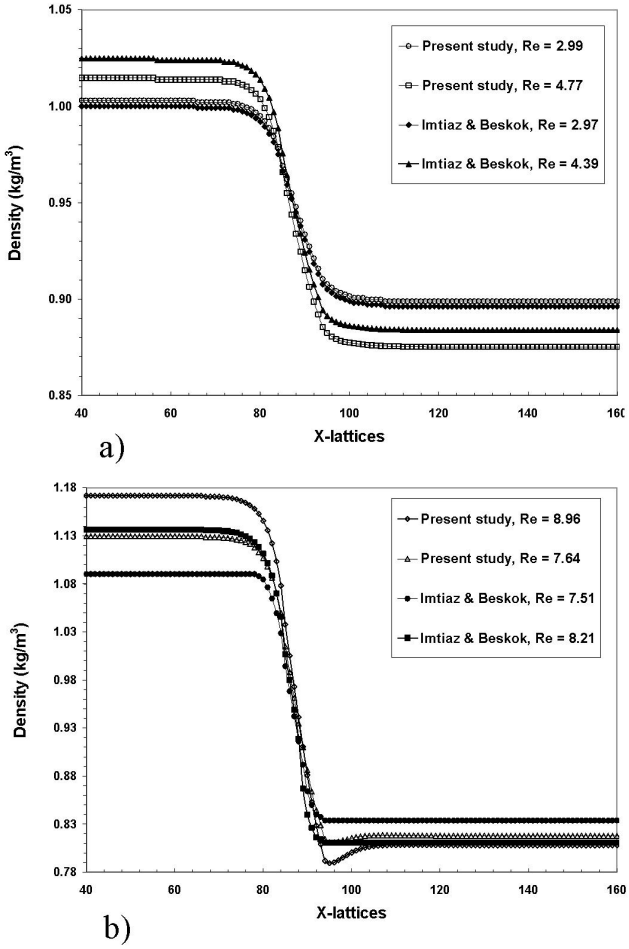

Fig. 7 Density variation along the channel, for the $2\mathrm{im}$ characteristic channel height, at a) low and b) high Reynolds numbers in the streamwise direction (zoomed at the orifice location).

According to Karniadakis & Beskok (2002), this is a direct indicator of the compressibility effects. The $\mathrm{Re} = 2.99$ case presents around 10% density drop along the constriction, while for $\mathrm{Re} = 8.962$, the density variation is greater that 28%. The effect of the Re number on the density variation can also be appreciated in the cases of $\mathrm{Re} = 4.775$ and $\mathrm{Re} = 7.649$. In the four cases, the fluid density remains at its maximum value until just before the constriction. After the fluid passes the constriction, the density drops and reaches its minimum value at this orifice edge.

The cases with $\mathrm{Re} = 7.64$ and $\mathrm{Re} = 8.96$ have a short recovery region after the constriction; the fluid density increases its value and then become constant. In the other two cases, with smaller Re numbers, the fluid density reaches its minimum value after the constriction and then becomes constant. These last behaviors are consistent with the findings of Imtiaz & Beskok (2001), which suggests again that the LBGK for micro flows may become inaccurate at higher Reynolds numbers (i.e, at $\mathrm{Re} \geq 7.649$).

In Nie et al.'s (2002), LBGK model for micro flows, the density variation along the channel is carried out through Eq. (15). However, this correction of the relaxation time comes with some limitations. First of all, Nie et al. do not specify Reynolds number limits for model stability and accuracy. It is suspected that the dependency on the relaxation parameter may limit the stability and accuracy of the LBGK method for micro flow simulations. In addition, while the model allows compressible flow simulations, isothermal conditions still are assumed in the scheme.

CONCLUSIONS

A LBGK model has been tested in the slip regime. In general, the LBGK for micro flows implemented in this study, approximates well the compressible NS model by Karniadakis & Beskok (2002) in the slip regime for micro-channel flows, and the corresponding results of Imtiaz & Beskok (2001) for micro-orifice simulation. The following points summarize the most important findings of this study:

- The LBGK for micro flows in micro channels agrees with the unified flow model results of Karniadakis & Beskok for slip regime simulations.
- The velocity distribution along the channel height is well predicted by the LBGK for micro flows. The maximum difference between the models is below 9.0%. The slip velocities at the wall are still negligible for these conditions.
- The deviations from the linear pressure profile are over predicted for the case of the slip regime at high Knudsen numbers with the LBGK for micro flows though the shape of the deviation is well predicted. The maximum difference between the two models is less than 23%.
- The LBGK for micro flows in micro orifices agrees with the Imtiaz & Beskok simulations at low Reynolds numbers.
- The velocity is under-predicted (about 9.2% of deviation at Re = 8.96) by the LBGK for micro flows at higher Reynolds numbers.

- The density and pressure differences along the orifice are greater at higher Re numbers, and LBGK for micro flows become less accurate at higher Re numbers as compressibility effects increase.

Finally, this study has demonstrated the promising potential of the LBE approach for micro flow applications. However more research needs to be done in order to improve the method. Special attention must be devoted to developing a micro flow LBE model with a multi-relaxation scheme to replace the single relaxation time approach of the current model. The multi-relaxation scheme approach will allow local grid refinements and yield a more accurate representation of the slip velocity near the solid walls. Comparisons of such a method would be suitable for Reynolds numbers higher than the ones presented in this work once a proper grid refinement can be accomplished.

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