Mesoscopic two-phase model for describing apparent slip in micro-channel flows

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The phenomenon of apparent slip in micro-channel flows is analyzed by means of a two-phase mesoscopic lattice Boltzmann model including non-ideal fluid-fluid and fluid-wall interactins. The weakly-inhomogeneous limit of this model is solved analytically. The present mesoscopic approach permits to access much larger scales than molecular dynamics, and comparable with those attained by continuum methods. However, at variance with the continuum approach, the existence of a gas layer near the wall does not need to be postulated a priori, but emerges naturally from the underlying non-ideal mesoscopic dynamics. It is therefore argued that a mesoscopic Lattice Boltzmann approach with non-ideal fluid-fluid and fluid-wall interactions might achieve an optimal compromise between physical realism and computational efficiency for the study of channel micro-flows.

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The microscopic physics underlying fluid/solid interactions is fairly rich and complex, for it depends on specific details of molecular interactions as well as on the micro-geometrical details of the boundary. However, on a macroscopic scale, these details can often be safely ignored by assuming that the net effect of surface interactions is simply to prevent any relative motion between the solid walls and the fluid elements next to them. This is the so-called “no-slip” boundary condition, which forms the basis of mathematical treatments of bounded flows as continuum media \footnote{A review of experiments and numerics}. No-slip boundary conditions are extremely successful in describing a huge class of viscous flows. Yet, the evidence is that certain classes of viscous flows do slip on the wall. Recent advances in microfluidics experiments \footnote{A review of experiments and numerics}, as well as numerical investigations \footnote{A review of experiments and numerics}, have identified the conditions which seem to underlie the validity of the no-slip assumption. Namely: (i) single-phase flow; (ii) wetted surfaces and (iii) low levels of shear rates. Under such conditions, careful experiments have shown that fluid comes to rest within a few molecular diameters from the surface \footnote{A review of experiments and numerics}. Conditions (i-iii) are not exhaustive, though. For instance, partial slips of simple (Newtonian) flows, such as alkanes and water, is predicted by an increasing number of experiments \footnote{A review of experiments and numerics} and simulations \footnote{A review of experiments and numerics}, which can drive dynamic phase transitions. The only free parameter in the LBE is the strength of these non-ideal (potential energy) interactions. Hopefully, the present mesoscopic approach provides an optimal compromise between the need of including complex physics (phase-transition) not easily captured by a continuum approach, and the need of accessing experimentally relevant space-time scales which are out of reach to microscopic Molecular Dynamics (MD) simulations \footnote{A review of experiments and numerics}. In particular, at variance with the macroscopic approach, the gas film does not need to be postulated a priori, but emerges dynamically from the underlying mesoscopic description, by progressive switching of potential interactions. One major advantage of this formulation is that it allows to develop a simple and straightforward analytical interpretation of the results as well as of the effective slip length arising in the flow. This interpretation is based on the macroscopic limit of the model which can be achieved by a standard Chapman-Enskog expansion.

The lattice Boltzmann model used in this paper to describe multiple phases has been developed in \footnote{A review of experiments and numerics}. Since this model is well documented in the literature, here we shall provide only the basic facts behind it. We recall that the model is a minimal discrete version of the Boltzmann
that corresponds to the Maxwellian distribution in the

\[ f_l(x + c_l, t + 1) - f_l(x, t) = -\frac{1}{\tau} \left( f_l(x, t) - f_l^{eq}(x, t) \right) \]

where \( f_l(x, t) \) is the probability density function associated
to a mesoscopic velocity \( c_l \) and where \( \tau \) is a mean
collision time and \( f_l^{eq}(x, t) \) the equilibrium distribution
that corresponds to the Maxwellian distribution in the
fully continuum limit. The bulk interparticle interaction
is proportional to a free parameter, \( G_b \), entering the balance
equation for the momentum change:

\[ \frac{d(\rho u_i)}{dt} = F \equiv G_b \sum_l w_l \Psi(\rho(x)) \Psi(\rho(x + c_l)) c_l \]

being \( w_l \) the equilibrium weights and \( \Psi \) the potential
function which describes the fluid-fluid interaction trig-
erged by density variation. By Taylor expanding eq. (2)
one recovers, in the hydrodynamical limit, the equation
of motion for a non-ideal fluid with equation of state
\( P = c_s^2 (\rho - \frac{1}{2} G_b \Psi^2(\rho)) \), \( c_s \) being the sound speed velocity.
With the choice

\[ \Psi(\rho) = 1 - \exp(-\rho/\rho_0) \]

with \( \rho_0 = 1 \) a reference density, the model supports phase
transitions whenever the control parameter exceeds the
critical threshold \( G_b > G_c \). In our case, \( G_c = 4 \) for an
averaged density \( \langle \rho \rangle = \log(2) \).

We consider \( G_b \) as an external control parameter, with no
need of responding to a self-consistent temperature
dynamics. It has been pointed out \cite{30} that the SC model
is affected by spurious currents near the interface due to
lack of conservation of local momentum. This criticism,
however, rests on an ambiguous interpretation of the fluid
velocity in the presence of intermolecular interactions.
In fact, spurious currents can be shown to disappear com-
pletely once the *instantaneous* pre and post-collisional
currents are replaced by a time-average over a collisional
time. This averaged quantity is readily checked to fulfill
both continuity and momentum conservation equations
without leading to any spurious current \cite{31}. Let us now
consider the main result of this letter, namely the critical
interplay between the bulk physics and the presence of
wall effects. In fact, in order to make contact with exper-
iments and MD simulations, it is important to include
fluid-wall interactions, and notably a parametric form
of mesoscopic interactions capable of mimicking wett-
ability properties as described by contact angles between
droplets and the solid wall \cite{32}. This effect is achieved
by assuming that the interaction with the wall is rep-
resented as an external force \( F_w \) normal to the wall and
decaying exponentially \cite{28, 29}, i.e.

\[ F_w(x) = G_w \rho(x) e^{-|x-x_w|/\xi} \]

where \( x_w \) is a vector running along the wall location and
\( \xi \) the typical length-scale of the fluid-wall interaction.

Equation (3) has been previously used in literature by
using a slightly different LBE scheme to show how the
wetting angle depends on the ratio \( G_w / G_b \) in presence of
phase coexistence between vapor and liquid \cite{28}. Here
we want to study the opposite situation, i.e. the effects
of \( G_w \) when the thermodynamically stable bulk physics
is governed by a single phase. The main result is that
the presence of the wall may trigger a local phase co-
existence inducing the formation of a less dense phase
in the vicinity of the walls and an apparent slip of the
bulk fluid velocity profile extrapolated at the wall loca-
tion. Equations (1)-(3) have been numerically solved for
different values of the parameters \( G_b, G_w \) and \( \xi \) in a two
dimensional channel with periodic boundary conditions
in the stream-wise \( x \) direction, being \( y = 0 \) and \( y = L_y \)
the wall positions. The sign of \( G_w \) is such to give a re-
pulsive force for the liquid particles at the wall.

The flow is driven by a constant pressure gradient in the
\( x \) direction \( F_1 = \delta_{i,x} \partial_x P_0 \). No-slip boundary
conditions are used at the wall and for small Knudsen numbers,
i.e. in the large scale limit, the numerical solutions have
been checked against its weakly-inhomogeneous macro-
scopic hydrodynamic limit, namely:

\[ \partial_t \rho + \partial_i (u_i \rho) = 0 \]

\[ \rho \left[ \partial_t u_i + (u_j \partial_j) u_i \right] = -\partial_i P + \nu \partial_j (\partial_j \partial_j u_i) + F_i \]

\[ P = c_s^2 \rho - V_{eff}(\rho) \]

where subscripts \( i, j \) run over the two spatial dimensions.
Above we have \( \nu = c_s^2 (\tau - 1/2) \) and \( P \) is the total pressure
consisting of an ideal-gas contribution, \( c_s^2 \rho \), plus the
so-called excess pressure, \( V_{eff} \), due to potential-energy
interactions. The expression of \( V_{eff} \) in terms of both \( G_b \)
and \( G_w \) reads:

\[
V_{eff}(\rho) = \frac{1}{2} G_b (1 - \exp(-\rho))^2 + G_w \int_0^\nu ds \rho(s) \exp(-s/\xi).
\]

Let us notice that the continuum equation \( \frac{\partial}{\partial y}(\rho u_y) = 0 \), which, because of the boundary conditions, implies \( \rho u_y = 0 \), i.e. \( u_y = 0 \) everywhere. Thus, in a homogeneous channel along the stream-wise direction, the velocity \( u_x \) satisfies the equation

\[
\nu \partial_y (\rho \partial_y u_x) = -\partial_x P_b.
\]  

In the new variable, \( y' = y - H \), where \( H = L_y/2 \), we may express the solution of \( 5 \) as:

\[
\frac{u_x}{\nu} = -\int_{y'}^H \frac{s \partial x P_0}{\nu \rho(s)} ds.
\]  

Using \( 6 \) and assuming that density variations are concentrated in a smaller layer of thickness \( \delta \) near the wall, we can estimate the mass flow rate \( Q_{eff} \) for small \( \delta \) as:

\[
\frac{Q_{eff}}{Q_{pois}} = 1 + \frac{3}{2} \frac{\Delta \rho_w}{\rho_w} \frac{\delta}{H}
\]  

where \( Q_{pois} \) corresponds to the Poiseuille rate \( 2 \partial_x P_0 H^3/3 \nu \) valid for incompressible flows with no-slip boundary conditions. In equation \( 7 \), the quantity \( \Delta \rho_w \) is defined as the difference between \( \rho \) computed in the center of the channel and \( \rho_w \) computed at the wall. The effective slip length is then usually defined in terms of the increment in the mass flow rate \( 17 \):

\[
\lambda_s \sim \delta \frac{\Delta \rho_w}{\rho_w}
\]  

This is the best one can obtain by using a purely continuum approach. The added value of the mesoscopic approach here proposed consists in the possibility to directly compute the density profile, and its dependency on the underlying wall-fluid and fluid-fluid physics. To this purpose, we consider the momentum balance equation in \( 4 \) for the direction normal to the wall, \( i = y \). Since \( u_y = 0 \), we simply obtain \( \partial_y P = 0 \), i.e.

\[
c^2 \partial_y \rho - 2G_b(1 - \exp(-\rho)) \exp(-\rho/\xi) - G_w \rho e^{-y/\xi} = 0.
\]

Let us first study the effects of the wall in \( 12 \) by setting \( G_b = 0 \). One can easily obtain \( \log(\rho(y)/\rho_w) = \frac{s^2}{c_s^2} (1 - \exp(-y/\xi)) \), which enables us to estimate \( \Delta \rho_w = \rho_w (\exp(\xi G_w/c_s^2) - 1) \). Using \( 8 \), we obtain for the effective slip-length:

\[
\lambda_s \sim \xi e^\xi G_w/c_s^2 \quad [G_b = 0].
\]  

We now turn our attention to the non trivial interference between bulk and wall physics whenever \( G_b > 0 \). Defining the bulk pressure as: \( P_b = c_s^2 \rho - \frac{1}{2} G_b (1 - \exp(-\rho))^2 \), we can rewrite equation \( 11 \) to highlight its physical content as follows:

\[
\log \left( \frac{\rho(y)}{\rho_w} \right) = \xi G_w (1 - e^{-y/\xi}) / \partial P_b / \partial \rho
\]  

where the bulk effects appear only through the following term:

\[
\frac{\partial P_b}{\partial \rho} = \frac{1}{\log(\rho(y)/\rho_w)} \int_0^\nu \partial P_b \frac{d \rho}{\partial \rho} \rho.
\]  

Equation \( 12 \) highlights two results. First, the effect of the bulk can always be interpreted as a renormalization of the wall-fluid interaction by

\[
G_w^R \equiv G_w/\frac{\partial P_b}{\partial \rho}.
\]  

Second, as it is evident from \( 13 \), one must notice that near the bulk critical point where \( \partial P_b / \partial \rho \to 0 \), the renormalizing effect can become unusually great. In other words, the presence of the wall may locally push the system toward a phase transition even if the bulk physics it is far from the transition point. As a result, the effective slip length in presence of both wall and bulk non-ideal interactions can be estimated as:

\[
\lambda_s \sim \xi \exp(\xi G_w^R).
\]

In Fig. \( 14 \) we show \( \rho(y) \) for different values of \( G_b \) and \( G_w = 0.03 \), \( \xi = 2 \) as obtained by numerically integrating equations \( 14 \). The numerical simulations have been carried out by keeping fixed the value of \( \rho = \frac{1}{L_y} \int_0^L \rho(s) ds = \log(2) \). As one can see, while \( G_b \to G_c = 4 \), the density difference \( \Delta \rho_w \) between the
We plot the momentum profile $\langle \rho u_z \xi \rangle$ normalized to its center channel value $(\langle \rho u_z \xi \rangle)_c$ as a function of the distance from the wall $y$ normalized to the channel height $L_w$. The results of numerical simulations $\square$ with $G_h = 3.5$, $G_w = 0.08$ and $\xi = 2$ are compared with the analytical estimate (continuous line) obtained solving equations 9 and 6. To highlight the rarefaction effect, the parabolic fit in the center channel region (dotted line) is also plotted. Inset: estimate of the apparent slip length in the channel obtained the same parabolic fit as in the main figure.

We have shown that for large scale separation, the parabolic profile at low approach is reached. For a quantitative check, we have numerically integrated equations 13 and 14 for a given value $\langle \rho \rangle = \log(2)$. The analytical estimate for $\rho u_z$ is compared with the numerical results in Fig. 3. This is a stringent test for our analytical interpretation. The result is that the analytical estimate is able to capture the deviations from a pure parabolic profile at approaching the wall region, where rarefaction effects are present. The crucial point in our analysis is that, even for very small $G_w$, a large apparent slip can occur in the channel if $G_h$ is close to its critical value; i.e. the limit $G_w \to 0$ and $G_h \to G_h^c$ do not commute. For example, let us consider the case when $G_w \sim \epsilon \ll 1$, $\xi \sim \epsilon$ and $G_h \to G_h^c - \xi^3$, we obtain $\frac{\partial \rho u_z}{\partial y} \sim \epsilon^3$ and therefore, equation 14 predicts that $\lambda_s \sim O(1)$ for $\epsilon \to 0$. The wall effect, parametrized by $G_w$ and $\xi$, can act as a catalyzer in producing large apparent slip. Most of the results shown in Figs. 1 and 2 are in close agreement with the MD numerical simulations $\square$. Our analysis points out that, close to the wall, one can observe a “local phase transition” triggered by the presence of the wall itself. In summary, we have shown that a suitable form of the Lattice Boltzmann Equation can be proposed in order to simulate apparent slip in microchannel. Slip boundary conditions arise spontaneously because, close to the wall, a “gas” layer is formed. If the system is close to a state where coexistence of different phases (liquid and gas) are thermodynamically achievable, then, macroscopic slip effects can result. We have shown that for large scale separation, the model reduces to a continuum set of hydrodynamical equations which explains the qualitative and quantitative behavior of the mass flow rate in terms of the model parameters, i.e. $G_h$ and $G_w$.
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