Generalized hydrodynamic model for fluid flows: From nanoscale to macroscale

Zhaoli Guoa,b
National Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China

T. S. Zhaoa and Yong Shi
Department of Mechanical Engineering, The Hong Kong University of Science and Technology, Kowloon, Hong Kong

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At the macroscale, the hydrodynamics of a fluid can be well described by conventional hydrodynamic models such as the Navier-Stokes equations. However, as the flow passage is shrunk down to the nanometer size, the micro-interaction between the fluid and the confined solid walls becomes significant, and the conventional hydrodynamic model will become insufficient for describing such a flow system. In this work, we propose a generalized hydrodynamic model that is derived from a recently developed kinetic model for strong inhomogeneous fluid systems [Guo, Zhao, and Shi, Phys. Rev. E 71, 035301(R) (2005)]. We show that the present model can reduce to other hydrodynamic models in certain limits, and can be used for flows ranging from nanoscale to macroscale. Based on this generalized model, the static and dynamic behaviors of several simple fluid systems are studied. It is shown that at a small scale, the results predicted by the generalized hydrodynamic model are in agreement with those simulated by the molecular dynamic and the Monte Carlo methods, while for flow systems at a large scale, the results agree with those by the Navier-Stokes equations. © 2006 American Institute of Physics. [DOI: 10.1063/1.2214367]

I. INTRODUCTION

Although it is well understood that the hydrodynamic behaviors of a fluid at the macroscopic scale can be described by the continuum hydrodynamic models such as the Navier-Stokes equations, it is still a challenging task to model and simulate micro- and nanoscale fluid systems, which is important for both fundamental researches and practical applications in material science, chemistry, biology, and many other subjects. Particularly, with the growing interest in miniaturization of both microelectromechanical systems and nanoelectromechanical systems, fluid flows in small scales have received increased attention over the last decade.

As a fluid flows through a device of the nanometer size, the effect of interaction between the fluid molecules and the solid wall molecules is much more significant than in its bulk case. Usually, the fluid-wall interaction will induce a strong inhomogeneity in the fluid, featured with the layered fluid molecules adjacent to the solid wall, and strong fluctuations in the fluid density in the near-wall region. Owing to this inhomogeneity, the equilibrium and dynamic behaviors of the fluid may become significantly different from those at the macroscopic scale. Under such cases, the conventional hydrodynamic models, e.g., the Navier-Stokes equations, will become invalid since the inhomogeneity is usually neglected in these models.1,2 Therefore, one must resort to more elaborate models into which the microscopic interactions are incorporated appropriately in order to study these small scale flows. Up to date, the most powerful, and perhaps the most widely used tools for studying such fluid systems are the molecular dynamic (MD) method and the Monte Carlo (MC) methods. However, it is well known that the both the MD and MC approaches are computationally expensive. Therefore, it is still desired to develop more efficient and sophisticated hydrodynamics models that can be used for nanoscale fluid systems.

In this paper, we aim to propose an alternative generalized hydrodynamic model for fluid flows covering a wide scale range. This model is based on a recently developed kinetic model for inhomogeneous fluid systems.3 It is relatively new to apply the mesoscopic kinetic approach to fluid systems with strong inhomogeneity.4 It was in the late 1980s when Davis et al. proposed the first inhomogeneous kinetic theory.5-7 Later in the 1990s, Pozhar et al. proposed their kinetic theory for nanoscale fluids.8-10 However, these two kinetic models are rather complicated and their applications are difficult and computationally expensive. The recent kinetic model proposed by Guo et al. can be used for fluid systems with strong inhomogeneity is much simplified by invoking the single-relaxation time approximation, and thus becomes tractable. The generalized hydrodynamic model presented in this paper is derived from this simple kinetic model via some standard technique in kinetic theory.

The paper is organized as follows. Section II briefly presents the kinetic model in Ref. 3. In Sec. III we first present the derivation of the generalized hydrodynamic model from the kinetic model via the Chapman-Enskog technique, and then discuss the connections with other hydrodynamic equa-
tions in some special cases. This section also discusses the boundary condition for the generalized equations. Section IV gives the numerical results of the generalized model for several simple fluid systems. Section V provides a summary and concludes the paper.

II. KINETIC MODEL FOR INHOMOGENEOUS FLUID SYSTEMS

We consider an isothermal fluid near a solid wall, where the fluid molecules interact each other with a potential \( \phi(r) \), and the solid wall exerts on the fluid molecules a potential \( \phi_w(r) \). Usually, the intermolecular potential \( \phi \) can be decomposed into a short-range repulsive part \( \phi_0 \) and a long-range attractive part \( \phi_a \) (e.g., Refs. 11–14); i.e., \( \phi = \phi_0 + \phi_a \). For such a system, the motion of the fluid molecules can be described by the evolution of the singlet distribution function \( f(r, \xi, t) \) (\( r \) being the spatial position, \( t \) the time, and \( \xi \) the molecular velocity), which obeys the following kinetic equation:

\[
\frac{\partial f}{\partial t} + \xi \cdot \nabla f - \frac{1}{m} \nabla \left( \phi_0 + \phi_m \right) \cdot \nabla_{\xi} f = \Omega(f),
\]

where \( m \) is the molecule mass, and \( \phi_0 \) is the external force including that induced by the surrounding walls. \( \phi_m \) relates to the attractive part of the potential by \( \phi_m(r) = \int f(\mathbf{r} + \mathbf{r}') \phi_a(|\mathbf{r}'|) \, d\mathbf{r}' \), with \( n = \int f \, d\xi \) being the local number density; Here, \( \nabla \) and \( \nabla_{\xi} \) represent the gradient operators in terms of \( r \) and \( \xi \), respectively. \( \Omega(f) \) is the collision operator that models \( \phi_a \) as a hard-sphere potential with an effective diameter \( \sigma_c \). Usually, \( \sigma_c \) depends on the decomposition method of \( \phi \).

Following the projection method for the revised Enskog theory for homogeneous hard-sphere fluids,\(^5\) the collision operator \( \Omega(f) \) can be simplified by splitting it into a Boltzmann part and an excess part, \( \Omega = \Omega_B + \Omega_E \), where the former is further approximated by the Bhatnagar-Gross-Krook (BGK)-like model. The excess part \( \Omega_E \) is a function of the local density \( n \) for homogeneous fluids, and can be extended to inhomogeneous fluids by making use of the idea of the local average density model (LADM).\(^6\) As such, \( \Omega(f) \) for inhomogeneous fluids can be modeled as\(^3\)

\[
\Omega(f) = \frac{1}{\lambda} [f_M - f] - V_0 f_M (\xi - u) \cdot [2A \chi^{hs} (\eta) \eta + B \eta],
\]

where \( \lambda \) represents a velocity-independent relaxation time; \( f_M \) is the Maxwellian local equilibrium distribution function,

\[
f_M = n \frac{1}{(2\pi RT)^{3/2}} \exp \left[ -\frac{(\xi - u)^2}{2RT} \right],
\]

with \( R = k_b T / m \), and \( k_b \) is the Boltzmann constant; \( u = n^{-1} \int \xi f \, d\xi \) is the fluid velocity, and \( T \) is the constant temperature of the isothermal system. \( \chi^{hs}(\eta) \) in Eq. (2) is the radial distribution function (RDF) for a homogeneous hard-sphere fluid of density \( \eta \), with \( \eta = \int f w(n') (n + n') \, dr' \) being the average density of \( n \) with a weight function \( w(n') \). \( A \) and \( B \) are two vector functions defined by

\[
A(r) = \frac{1}{D} \int_{|\mathbf{r}'| < a r_2} r' \tilde{n}(r + r') \, dr',
\]

and

\[
B(r) = \frac{1}{D} \int_{|\mathbf{r}'| < a r_2} r' \chi^{hs} [\tilde{n}(r + r')] \, dr',
\]

respectively, with \( D = \pi a^2 \eta / 120 \).

The relaxation time \( \lambda \) in the collision operator is determined based on the LADM,\(^6\) i.e., \( \lambda = \mu(\eta) / n k_b T \), where \( \mu(n) \) is the viscosity for a homogeneous dense fluid with density \( n \),\(^7\) \( \mu(n) = \mu_0 n V_0 (1 + 0.8 + 0.7614) \) with \( \mu_0 = (5.0 / 16a^2) \sqrt{k_b T / \pi} \), \( Y = n V_0 \chi^{hs}(n), \) and \( V_0 = 2 \pi a^2 / 3 \).

The limitations of the kinetic model given by Eq. (1) together with Eq. (2) as a result of various approximations are as follows. First, like the kinetic model given by Davis,\(^5\) the present model is applicable to locally equilibrium inhomogeneous fluids only, and may become questionable in the confinements with at least one dimension on the order of one or two molecular diameters. Second, since the kinetic model is derived under isothermal conditions, it is inapplicable to the fluid systems involving heat transfer. Finally, the introduction of the BGK model in the collision operator implies that all of the physical modes decay with the same rate, resulting in an unphysical Prandtl number. Fortunately, this limitation is not a problem for the isothermal flows as considered in the present work.

III. THE GENERALIZED HYDRODYNAMIC MODEL

A. Hydrodynamic equations

We now follow the Chapman-Enskog procedure\(^7\) to derive the hydrodynamic equations from the kinetic equation (1). We first introduce the following expansions:

\[
f = \sum_{k=0}^{\infty} \epsilon^k f^{(k)} \rightarrow \sum_{k=0}^{\infty} \epsilon^k \frac{\partial^k f}{\partial t^k}, \lambda \rightarrow \lambda \epsilon, \quad (5)
\]

where \( \epsilon \) is a small parameter, which is on the order of the Knudsen number in homogeneous fluid. Consequently, the kinetic equation (1) is turned into an infinite hierarchy of equations according to the order of \( \epsilon \), of which the first several equations can be written as

\[
\epsilon^0: f^{(0)} = f_M, \quad (6)
\]

\[
\epsilon^1: D_0 f^{(0)} = -\frac{1}{\lambda} f^{(1)} + J, \quad (7)
\]

\[
\epsilon^2: \frac{\partial f^{(0)}}{\partial t} + D_0 f^{(1)} = -\frac{1}{\lambda} f^{(2)}, \quad (8)
\]

\[
\epsilon^3: \frac{\partial f^{(0)}}{\partial t} + D_0 f^{(1)} + D_0 f^{(2)} = -\frac{1}{\lambda} f^{(3)}, \quad (9)
\]

where \( D_0 = \partial_0 / \partial t + \nabla \cdot a \nabla + \nabla \cdot a \cdot \nabla \) with \( a = -\nabla (\phi_0 + \phi_m) / m \), and \( J = -V_0 f_M (\xi - u) \cdot [2A \chi^{hs}(\eta) \eta + B \eta] = -f_M (\xi - u) \cdot K \).

From Eq. (6) and the definitions of \( n \) and \( u \), we can obtain that...
\[ \int \psi_{d}^{(k)} d\xi = 0, \quad k > 0, \]  
where \( \psi_{d} \) and \( \xi \) are the summation invariants. Therefore, taking these moments of Eq. (7), we can obtain the following hydrodynamic equations at the order of \( \epsilon \):

\[ \frac{\partial n}{\partial t} + \nabla \cdot (nu) = 0, \]  
(11a)

\[ \frac{\partial (nu)}{\partial t} + \nabla \cdot \Pi = nG, \]  
(11b)

where \( \Pi = \int \xi \xi^{(0)} d\xi = nRTI + num, \) and \( G = a - RTK. \) In the above deduction, we have made use of the facts that

\[ \int Jd\xi = 0, \quad \int \xi d\xi = - nRTK. \]

Similarly, the corresponding equations at the order of \( \epsilon^2 \) can be obtained by taking the moments of Eq. (8),

\[ \frac{\partial n}{\partial t} = 0, \]  
(12a)

\[ \frac{\partial (nu)}{\partial t} + \nabla \cdot \Pi = 0, \]  
(12b)

where \( \Pi = \int \xi \xi^{(1)} d\xi. \) By making use of Eq. (7) and the equations at the order of \( \epsilon, \) (11), we obtain that

\[ - \frac{1}{\lambda} \Pi^{(1)} = \frac{\partial \Pi^{(0)}}{\partial t} + \nabla \cdot \int \xi \xi^{(0)} d\xi + a \int \xi \xi \nabla \xi^{(0)} d\xi \]

\[- \int \xi \xi d\xi = \left[ n \nabla u - \nabla \cdot (nuu) - u \nabla nRT \right] + \left[ RT \nabla (nu) \right] \]

\[ + \nabla \cdot (nuu) \]  
\[ - n \nabla \nabla \nabla u, \]  
(13)

where the tilde of a dyadic means the summation of itself and its transpose, i.e., \( \tilde{\nabla}u = [\nabla u + (\nabla u)^T]. \)

Summing up the hydrodynamic equations (11) and (12), we finally obtain the following hydrodynamic equations for the isothermal fluid systems:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \]  
(14a)

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) + RT \nabla \rho + \frac{\rho}{m} \nabla (\rho u + \rho n) \]

\[ = \nabla \cdot (\mu \nabla u) - \rho \nabla \left[ 2A \chi^{\alpha} (\tilde{n}) + B \tilde{n} \right] V_0, \]  
(14b)

where \( \rho = mn \) is the mass density of the fluid.

**B. Connections with other hydrodynamic equations**

In some special cases, the generalized hydrodynamic model can be simplified. For example, in a weak inhomogeneous fluid system,

\[ \bar{n} = n, \quad \tilde{A} = \nabla n, \quad \tilde{B} = \nabla \chi^{\alpha}(n), \]

\[ \phi_m = \int n(r + r') \phi_\alpha(|r'|) dr' = -2an - \kappa \nabla \tilde{n}. \]

where \( a \) and \( \kappa \) are two constants given by

\[ a = -\frac{1}{2} \int \phi_\alpha(|r|) dr, \quad \kappa = -\frac{1}{6} \int r^2 \phi_\alpha(|r|) dr. \]

Therefore, under such a circumstance, the hydrodynamic equation (14) becomes

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = - \nabla \rho + \nabla \cdot (\mu \tilde{n} u) + \nabla \cdot C + \rho F, \]

(15)

which is just the conventional Navier-Stokes equation with a zero bulk viscosity. Therefore, the present generalized hydrodynamic model can be viewed as an extension of the conventional hydrodynamic models, and thus it is expected that this model is applicable to fluid systems ranging from nanoscale to macroscale.

It is interesting to make a comparison between the generalized hydrodynamic equations (14) and the conventional Navier-Stokes equations. It is first noticed that in the generalized model, the fluid-wall and fluid-fluid interactions are explicitly included through the last gradient term on the left hand side of Eq. (14b), and the induced inhomogeneity in the fluid takes effects implicitly through the averaging process of evaluating \( \tilde{n} \) and the two functions \( A \) and \( B. \) Therefore, the generalized hydrodynamic model Eq. (14) has the potential to capture the unusual behaviors of nanoscale fluids. While in the conventional Navier-Stokes equations, these interfacial effects and the inhomogeneity are usually neglected. Therefore, it is not surprising that the Navier-Stokes equations work well for macroscopic fluid systems in which the interfacial effects and the inhomogeneity are negligible, but become invalid for nanoscale fluid systems with strong inhomogeneity.

**C. Boundary condition**

In solving the generalized hydrodynamic equations (14), we need to specify boundary conditions. As sketched in Fig. 1, as a fluid flows over a solid surface, there exists a near-wall region in which the fluid molecules are strongly affected by the solid wall, beyond which (i.e., in the bulk region) the fluid molecules are almost unaffected by the wall.
Usually, in the continuum limit, the collective dynamics of the molecules in the bulk region can be described by the conventional Navier-Stokes equations. However, in the near-wall region, the induced inhomogeneity is so strong that the Navier-Stokes equations become inadequate to describe the collective dynamics of the fluid molecules. In the usual macroscale fluid systems, the near-wall region is so small that can be neglected in comparison with the bulk region, and the whole flow field can be described by the Navier-Stokes equations with a no-slip boundary condition for the whole flow field. Such a treatment has been shown to be good enough for macroscale fluid systems.

However, with the shrinkage of the flow field down to the micro- or nanometer scale, the near-wall region will influence the overall flow more and more and cannot be neglected. Therefore, it is not surprising that under such cases the Navier-Stokes equations with the no-slip boundary condition would fail to describe the fluid flow in the whole domain.

It is noted that in some studies of micro- and nanoscale fluid flows, the conventional Navier-Stokes equations are still used to describe the fluid motion in the bulk region, but with a certain “slip” boundary condition specified at the fluid-wall interface:

\[ u_s = u - u_w = L_s \dot{\gamma}, \tag{19} \]

where \( u_w \) is the wall velocity, \( \dot{\gamma} \) is the local shear rate evaluated at the interface between the near-wall region and bulk region (see Fig. 1). \( u_s \) is the slip velocity, and \( L_s \) is the so-called slip length, which is defined as the distance from the wall where the linearly extrapolated tangential velocity matches that of the wall. Clearly, in this approach, the flow information in the near-wall region is completely lost. The fluid velocity \( u \) at the wall determined by the slip boundary condition (19) is meaningless and nothing but a parameter for the bulk flow. The reliability of such a “Navier-Stokes plus slip boundary condition (NS+SBC)” approach depends greatly on the choice of the slip length \( L_s \). In general, \( L_s \) depends on a number of factors, such as the fluid-fluid and fluid-wall interactions, \(^{19,20}\) the shear-rate, \(^{21}\) and the system temperature.\(^ {22-24}\) Therefore, in this approach, the fluid-wall interaction and the induced inhomogeneity are in fact effectively incorporated into the slip boundary condition.

In the present generalized hydrodynamic model, however, the fluid-wall and fluid-fluid interactions and the induced inhomogeneity are explicitly included and are irrelevant to the boundary condition. Therefore, in theory the present generalized hydrodynamic model can be applied to the flow in the whole domain, provided that a boundary condition is specified at the interface between the near-wall region and the solid wall.

In this paper, we assume the no-slip boundary condition at the fluid-wall interface for the proposed generalized hydrodynamic equations, which means that the collective velocity of the fluid molecules in contact with the wall is the same as the wall velocity \( u_w \). We noted that in some previous studies, the no-slip boundary condition has also been employed in the study of inhomogeneous fluid systems.\(^ {7}\) Unlike the NS+SBC approach, the flow information in the near-wall region can still be captured by the present generalized model with the no-slip boundary. It should be pointed out that the no-slip condition for the generalized hydrodynamic equations does not mean a no-slip boundary condition for the Navier-Stokes equations. Of course, the no-slip boundary condition is just one of the choices, and it does not preclude us from using other more sophisticated boundary conditions.

IV. APPLICATIONS

In this section, we apply the generalized hydrodynamic model to study the static and dynamic behaviors of a fluid system confined between two infinite parallel plates. As sketched in Fig. 2, the two plates are infinite in the \( x-y \) plane, and locate at \( z=0 \) and \( z=H \), respectively. The fluid molecules interacted with one another through a potential \( \phi(r) \), and each wall exerts a potential \( \phi_s(z) \) on the fluid molecules. Therefore, the two walls induce an external potential in the fluid:

\[ \phi_s(z) = \phi_s(z) + \phi_s(H-z), \quad 0 \leq x \leq H. \tag{20} \]

In the solution of the general hydrodynamic equations, the average density \( \bar{n} \) is determined using the Tarazona average method\(^ {25,26}\) and the RDF \( \chi^{(n)} \) used in this study is that proposed by Carnahan and Sterling:\(^ {27}\)

\[ \chi^{(n)}(n) = \frac{1 - 0.5 \eta}{(1 - \eta)^3}, \quad \eta = \frac{nV_0}{4}. \tag{21} \]

A. Static fluid structure

We first study the static structure of the confined fluids with different fluid-fluid and fluid-wall potentials. It is noted that at equilibrium, i.e., \( \mathbf{u} = (u, v, w) = 0 \), where \( u, v, \) and \( w \) are the velocity components in the \( x, y, \) and \( z \) directions,
respectively. Furthermore, at equilibrium, the fluid is uniform in both x and y directions, and the inhomogeneity only appears in the z direction. Therefore, under such a circumstance, the momentum equation (14b) for component w reduces to a Yvon-Born-Green (YBG)-like equation

\[ \frac{d}{dz} \left[ \ln n + \frac{\phi_r + \phi_m}{k_B T} \right] = -\left[ 2A(n) \chi(n) + B(n) n \right] V_0. \]  \hspace{1cm} (22)

Equation (22) is then solved numerically to obtain the equilibrium density distribution in the slit with the given external and the intermolecular potentials. In the following computations, we use an integration step \( \Delta z = 0.01 \sigma \).

We first consider a 12-6 Lennard-Jones (LJ) fluid confined between two 10-4-3 LJ walls, in which

\[ \phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right], \]  \hspace{1cm} (23)

\[ \phi_n(z) = 2\pi \varepsilon_n \left[ \frac{2}{3} \left( \frac{\sigma}{z} \right)^{10} - \left( \frac{\sigma}{z} \right)^{4} - \frac{\sigma^4}{3\Delta(z+0.61\Delta)^3} \right], \]  \hspace{1cm} (24)

where \( \Delta = \sigma / \sqrt{2} \). In our computation, the fluid-fluid potential \( \phi \) is decomposed following the Barker-Henderson method,\(^{12}\) \( \phi = \phi_r + \phi_m \), in which

\[ \phi_r(r) = \begin{cases} \phi(r), & r < \sigma, \\ 0, & r > \sigma, \end{cases} \quad \phi_m(r) = \begin{cases} 0, & r < \sigma, \\ \phi(r), & r > \sigma. \end{cases} \]  \hspace{1cm} (25)

The repulsive part of the fluid-fluid potential \( \phi_r \) can be modeled by a hard-sphere potential with an effective diameter \( \sigma_r \).

In Fig. 3, we present the density distribution of the fluid system at \( T = 1.2 \) with some different pore-averaged number densities defined by \( n_0 = H^{-1} \int_0^H n(z) dz \). For comparison, the Monte Carlo results\(^{29}\) are also shown in Fig. 3. It is seen that the fluid structure predicted by the generalized hydrodynamic model agrees well with the MC results quantitatively.

If the distance between the walls is large enough, the fluid will be homogeneous near the central region of the system, and the density profile can thus be regarded as that of a fluid in contact with a single wall. In Fig. 4, the density profiles of a hard-sphere fluid and a LJ fluid near a hard wall are shown and compared with the Monte Carlo results.\(^{30,31}\)

Here, the width of the channel is set to be \( H = 60 \sigma \). It is again observed that the fluid structures predicted by the generalized hydrodynamic model are in good agreement with the MC results.

B. Planar Couette and Poiseuille flows

1. Analysis

We now study the dynamic behavior of a dense LJ fluid in a nanochannel, where the fluid-fluid potential is given by Eq. (23), and each wall exerts a 10-4 LJ potential,

\[ \phi_n(z) = 1.6\pi \varepsilon_n \left[ \frac{2}{3} \left( \frac{\sigma}{z} \right)^{10} - \left( \frac{\sigma}{z} \right)^{4} \right]. \]  \hspace{1cm} (27)
For the Couette flow, the top and bottom walls move with constant velocities $U$ and $-U$, respectively. At steady state, the momentum equation (14b) of the generalized hydrodynamic model reduces to

$$\frac{d}{dz} \left[ \ln n + \frac{\phi_x + \phi_m}{k_B T} \right] = -\left[ 2A(\tilde{n}) \chi(\tilde{n}) + B(\tilde{n}) \tilde{n} \right] V_0$$

(28)

for velocity component $w$, and

$$\frac{d}{dz} \left( \mu(\tilde{n}) \frac{du}{dz} \right) = 0$$

(29)

for the velocity component $u$. For the Poiseuille flow, the flow is driven by a constant external force $G$ applied in the $x$ direction, which makes it a one-dimensional problem. The equation for the velocity component $w$ is the same as Eq. (28), and the equation for the streamwise velocity $u$ is

$$\frac{d}{dz} \left( \mu(\tilde{n}) \frac{du}{dz} \right) + mnG = 0.$$  

(30)

It is noted that Eq. (28) is the same as the YBG-like equation (22) for an equilibrium system, which means that the density distribution is not influenced by the flow. This fact has also been observed in previous numerical studies.16

From Eq. (28), we can see that the term $(\phi_x + \phi_m)/k_B T$ plays a central role for the system. For the present fluid system, the overall effect of this term on the fluid system can be estimated by the parameter

$$\Phi = \frac{1}{H - 2\delta} \int_{\delta}^{H-\delta} \frac{\phi_x + \phi_m}{k_B T} dz = \frac{\epsilon}{k_B T} \left( \alpha_c \sigma \epsilon_w / \epsilon + \alpha_m n_0 \sigma^3 \right),$$

(31)

where $\delta$ is the distance from some point in the fluid to the wall. For instance, for a small $H$, this point can be chosen to be the one where the first density peak occurs; for a larger $H$, it can be taken to be the one where the second density peak occurs. $\alpha_c$ is a constant derived from $\phi_x$ and depends on $\delta$ and $H$ only, $\alpha_m$ is a parameter related to $\phi_m$ and can be estimated through $a$ and $x$ given by Eq. (17). From Eq. (31), we can see that the system is characterized by four dimensionless parameters: the reduced temperature $T' = k_B T / \epsilon$, which measures the ratio of the kinetic energy to the internal potential energy of the fluid; the reduced channel width $H' = H / \sigma$; the reduced fluid-wall potential energy strength $\epsilon_w = \epsilon_u / \epsilon$, which measures the ratio of the fluid-wall potential energy to fluid-fluid energy; and the reduced fluid density $n_0' = n_0 \sigma^3$. It is noted that similar argument can also be made for the general hydrodynamic equations (14). Therefore, these four parameters are the characteristic parameters for an inhomogeneous fluid system modeled by the present generalized hydrodynamic model.

For the Couette and Poiseuille flows, the local density is obtained by solving Eq. (28) numerically, just as the solution of Eq. (22). After obtaining $n$, we integrate Eq. (29) numerically to find the streamwise velocity $u$ for the Couette flow, and Eq. (30) for the Poiseuille flow. In the computations, the no-slip boundary condition is employed.

FIG. 5. Density (top panel) and velocity (bottom panel) profiles of the Couette flow for a LJ fluid with density $n_0 = 0.692 \sigma^{-3}$ at $T = 1.1 \epsilon/k_B$. Solid lines: Present prediction. Symbols: MD results (see Ref. 16).

2. Validation

In Fig. 5, we compared the predicted density and velocity profiles with the MD results16 for the Couette flow with a pore-averaged density $n_0 = 0.692 \sigma^{-3}$ at $T = 1.1 \epsilon/k_B$. The channel width is $H = 7.178 \sigma$. It is seen that both the density and velocity profiles of the present hydrodynamic model and those of the MD simulations are in good agreement.

It can be clearly seen from Fig. 5 that the competition between the fluid-wall and fluid-fluid interactions results in a strong inhomogeneity in the fluid. The fluid density shows a significant oscillation across the channel, and there exists a vacancy between the first fluid layer and the wall due to the repulsive force exerted by the wall. Owing to this inhomogeneity, the velocity profile deviates significantly from the linear distribution, which should be for a bulk system.

3. Effects of channel width

As indicated in Eq. (31), the reduced channel width $H'$ is one of the key parameters for the flow system. We show in Fig. 6 the density and velocity distributions for channels with different width. As seen, for a channel with $H' = 10$, the density profile oscillates across the whole channel; As $H'$ increases to 20, the density is almost constant in the region $0.3 \leq z/H \leq 0.7$, which can be identified as the bulk region; As $H'$ reaches 40, the density becomes flat in the region $0.15 \leq z/H \leq 0.85$. It is also observed that the magnitude of the first density peak near the wall decreases with increasing $H'$.

Accordingly, the velocity profile for the Couette flow approaches the linear distribution across the channel with the increase in $H'$ [Fig. 6(b)]. In Fig. 6(c), we present the velocity profiles for the Poiseuille flow with different channel widths as $G = 0.02 \epsilon / m \sigma$. It is seen that for a small $H'$, the velocity profiles are different dramatically from those predicted by the conventional Navier-Stokes equations, which should be a parabola. However, as $H'$ becomes large enough, the profile recovers the parabolic distribution. These
observations support our previous assessment that the inhomogeneity of a fluid system will become weaker for large scale systems.

4. Effects of fluid-wall potential

From Eq. (31), we can see that the reduced wall potential $\epsilon_w^*$ is also a key factor that affects the fluid system. To investigate its effect, we calculated the density and velocity profiles for both the Couette flow and Poiseuille flow as $\epsilon_w^*$ varies from 0.1 to 10.0, with $H^*=10$, $n_0^*=0.692$, and $T^*=1.1$.

The predicted density and velocity are presented in Fig. 7. We can see that both the Couette flow and the Poiseuille flow in the nanoscale are significantly influenced by the wall property. For a wall with a weak energy, the induced density oscillation in the fluid is also relatively weak. With the increase in wall energy, the induced inhomogeneity becomes larger and larger, and more fluid molecules accumulate near the wall. The first density peak near the wall also climbs with increasing wall energy [Fig. 7(a)]. Accordingly, the velocity profiles [Figs. 7(b) and 7(c)] also demonstrate different patterns as the fluid-wall potential changes. As the $\epsilon_w^* < 1$, the motion of the fluid is less influenced by the wall motion. In such a case, the bulk flow demonstrates a normal slip, i.e., the slip length $L_s$ is positive, or the point where the linearly extrapolated tangential velocity matches that of the wall is outside the fluid domain. On the other hand, with the increase of wall energy, more and more fluid molecules are attracted by the wall. Finally, as $\epsilon_w^*$ becomes larger enough, the so-called stick-slip occurs; i.e., $L_s < 0$. These observations are qualitatively consistent with previous MD studies.19,20,32

From Figs. 7(b) and 7(c), we see that the flow information in near-wall region can indeed be captured by the generalized hydrodynamic model, although the no-slip boundary condition is employed. It is also seen that the velocity profiles in the bulk region are still linear for the Couette flow and parabolic for the Poiseuille flow in the case considered. Therefore, it is expected that the bulk flow can also be described by the Navier-Stokes equations given some slip-boundary conditions are appropriately prescribed, but with the sacrifice of the near-wall information.

5. Effects of fluid density

The reduced pore-averaged density $n_0^*$ is another key parameter for nanoscale fluid flows. The density and velocity profiles for the Couette and Poiseuille flows with different $n_0^*$ are presented in Figs. 8 and 9 for $\epsilon_w^* =0.01$ and 4, respectively.

From Fig. 8, it is seen that for a weak fluid-wall potential, as the fluid density is relatively low ($n_0^* =0.5$), the oscillation in the density field is rather weak. The density profile is nearly flat in the central region, and the first density peak is almost the same as the bulk density. As $n_0^*$ increases to 0.7, density oscillation also appears in the central region, and the first density peak becomes obvious. As $n_0^*$ reaches to 0.9, the
density oscillates significantly, meaning that the inhomogeneity in the fluid becomes very strong. The velocity field also varies with $n_0^*$. It is seen from Figs. 8(b) and 8(c) that for both the Couette and Poiseuille flows, the velocity profiles deviate from their corresponding Navier-Stokes predictions, and the bulk flow demonstrates a normal slippage, which tends to become weaker with the increase in $n_0^*$.

For a wall with strong potential, the fluid behavior also demonstrated a strong dependence on the fluid density. As shown in Fig. 9, the fluid density in the central region is still flat in the case of $n_0^*=0.5$, but the first density peak is more obvious than it is in the cases of weak fluid-wall interactions. The inhomogeneity in the fluid also increases with $n_0^*$, just as in the weak wall case. However, owing to the strong fluid-wall interaction, more fluid molecules accumulate in the near-wall region in this case. As a result, the bulk flow demonstrates a stick-slip [Figs. 9(b) and 9(c)], which is different from that in the former case. The common in the two cases is that the degree of slip, either normal or stick, decreases with increasing $n_0^*$.

6. Effects of system temperature

We now investigate the effect of the reduced system temperature $T^*$. The density and velocity profiles for the Couette and Poiseuille flows at different $T^*$ are presented in Figs. 10 and 11 for weak and strong fluid-wall interactions, respectively. From the density profiles, it is first observed that in both cases the inhomogeneity at a lower $T^*$ is usually stronger than that at a higher $T^*$. However, the first density peak near the wall tends to increase with a increasing $T^*$ as the fluid-wall interaction is weak, but tends to decrease as the fluid-wall potential is strong. The velocity profiles in Figs. 10 and 11 for both the Couette and Poiseuille flows show that the degree of slip in both cases for the bulk flow tends to decrease as $T^*$ increases.
C. Mechanical properties of the Poiseuille flow

For the planar Poiseuille flow driven by an external force, the classical Navier-Stokes theory predicts a constant pressure, a linear strain rate, and a linear stress. These results are reasonable as the wall separation is sufficient large. If the separation is shrunk down to several to ten diameters of the fluid molecule, however, these mechanical properties may be quite different. In this subsection we shall study these mechanical properties for the planar Poiseuille flow using the generalized hydrodynamic model.

In what follows, we consider the 12-6 LJ fluid system given by Eq. (23), and assume that the wall potential $\phi_w$ is given by Eq. (24).

1. Pressure force at the wall

As shown earlier, in the planar Poiseuille flow the fluid density is not affected by the flow. Therefore, the normal pressure $P_N$ at the wall exerted by the fluid molecules equals to the static normal pressure, and can be given by

$$P_N = -\int_0^H mn(z) \frac{d\phi_w}{dz} dz.$$  \hspace{1cm} (32)

$P_N$ is closely related to the solvation pressure or disjoining pressure $P_s$ through $P_s = P_N - P_b$, where $P_b$ is the bulk pressure. Previous computer simulations indicate that $P_N$ oscillates with the separation $H$, and decays to $P_b$ as $H \to \infty$.

In order to obtain $P_N$ from Eq. (32), the local density distribution $n(z)$ must be found first, which can be achieved by solving the YBG-like equation (28). In Fig. 12, we present our calculation results of the normal pressure $P_N$ versus the pore width $H$ and compare them to the MC results of Snook and van Megen, where the fluid-wall potential energy is set to be $\epsilon_w = \epsilon$, and the fluid between the solid walls is characterized by its temperature $T = 1.2$ and a bulk density $n_b^* = 0.5925$. We can see that the agreement is excellent, and the oscillation behavior of $P_N$ against $L$ is successfully captured by the present hydrodynamic model.

2. Strain rate and shear stress

The strain rate of the planar Poiseuille flow can be calculated from the velocity as

$$\dot{\gamma}(z) = \frac{du}{dz},$$  \hspace{1cm} (33)

from which it follows that the Navier-Stokes strain rate profile will be a linear function of the coordinate $z$. However, from the results presented in earlier subsections, we can observe that the velocity profiles deviate from the classical behavior as the pore width is comparable to the fluid molecule diameter. Therefore, we can expect that the shear rate will also be a nonlinear function in such a case.

The shear stress $-\Pi_{xz}$ can be obtained in two ways. One way is to integrate the equation

$$\frac{d\Pi_{xz}}{dz} = mnG,$$  \hspace{1cm} (34)

which gives

$$\Pi_{xz} = \int_0^z mn(z) G dz + C,$$ \hspace{1cm} (35)

where $C$ is an integration constant which ensures the stress is zero at the center of the pore. Another way to calculate the stress is by making use of the linear constitutive relation

$$\Pi_{xz} = -\mu \langle \ddot{u} \rangle \gamma.$$  \hspace{1cm} (36)

From Eqs. (30) and (34), we can see that the two approaches should be identical.

Using the present hydrodynamic model, we simulated a LJ fluid system with $n_0^* = 0.65$ and $T^* = 0.722$, and the energy of the 10-4-3 fluid-wall potential is set to be $\epsilon_w = 0.615 \epsilon$. The flow is driven by a constant force $G = 0.02 \epsilon / \sigma$. These parameters are chosen according to the MD system, where the wall is composed of a three-layer fcc lattice.
In Fig. 13, the strain rate profiles calculated by the present hydrodynamic model are presented, and the corresponding velocity profiles are also shown for reference. Deviations from linearity in the strain rate are clearly shown, which indicates the departure from the Navier-Stokes predictions of the present hydrodynamic model. As expected, these derivations are particularly pronounced for the narrowest pore \( H^* =5.1 \); As \( H^* \) increases to 10.2, linearity appears in the central region of the strain rate profile, although strong nonlinearity is still observed in the near-wall regions. As \( H^* \) further increases up to 15.3, the linearity in the central region becomes more apparent, and the portion of nonlinearity near the two walls decreases. Accordingly, the shear stress calculated from Eq. (34) or (36) (the results from these two equations are indistinguishable) are presented as a function of \( z \) in Fig. 14, and similar trends observed in Fig. 14 are demonstrated again. These observations are consistent with previous MD results.\(^34\)

3. Mass flow rate

The mass flow rate for the Poiseuille flow is defined as

\[
Q = \int_0^H mn(z)u(z)dz. \tag{37}
\]

The normalized mass flow rate, \( Q^* = Q/Q_0 \) with \( Q_0 = H^2 p_0 G/\sqrt{2RT} \), is a linear function of \( H \) if the classical Navier-Stokes equation is employed. Due to the highly nonuniform density distribution and the nonparabolic velocity profile of the Poiseuille flow in very narrow pores, the normalized mass flow rate is expected to deviate from the linear dependency of the pore width in such circumstances.

In Fig. 15, we presented \( Q^* \) as \( H^* \) changes from 4 to 40 and \( n_0^* \) varies from 0.1 to 0.7 at \( T^*=0.772 \) and 1.2, respectively. As expected, the normalized flow rate demonstrated as a highly nonlinear function of the pore width. It is seen that for the same fluid density, the flow rates at higher temperatures are greater than those at lower temperatures, and the derivation is more prominent for small fluid densities.

![Fig. 13. Strain rate (solid line, in unit of \((\varepsilon/m\sigma)^{1/2}\)](image1)

![Fig. 14. Shear stress (in units of \(\varepsilon/\sigma^3\)) profiles.](image2)

![Fig. 15. Normalized mass flow rate profiles as a function of pore width.](image3)
It is also seen from Fig. 15 that at low temperature ($T^* = 0.722$), the flow rate profile exhibits a “minimum” as $n_p \leq 0.5$. It is interesting to compare this phenomenon with the “Knudsen-minimum paradox” in rarefied gas dynamics but here the fluid system is still rather “dense.” It would be interesting to verify such a phenomenon in nanoscale fluid systems using other experimental and/or simulation methods. However, for a denser fluid ($n_p = 0.7$), this “minimum” phenomenon disappears. At a higher temperature, $T^* = 1.2$, however, the flow rate profiles with the densities considered demonstrate no such minimum at all; instead, the profiles indicate that the normalized flow rate is a nonlinear increasing function of the pore width. It is further observed that the linear dependence on $H$ of $Q^*$ is recovered for large values of $H^*$, which means as expected that the Navier-Stokes theory is still applicable if the pore is wide enough.

V. SUMMARY

In a fluid system at a small scale, the interaction between the fluid and the solid walls usually becomes significant, and may create some peculiar static and dynamic flow behaviors that are different from those occurring in a large-scale fluid system. The conventional hydrodynamic model may encounter difficulties in modeling such small scale fluid systems. In this work, we have proposed a generalized hydrodynamic model for modeling fluid systems in a wide scale range. Several typical fluid systems have been studied via the generalized model. The results indicate that the dynamic behavior of a fluid at the nanoscale may be rather different from that at the macroscale, and the flow behaviors depend on a number of factors. Although preliminary, these results indicate that the present generalized hydrodynamic model may serve as a practical hydrodynamic model for fluid flows ranging from nanoscale to macroscale.

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