Generalized hydrodynamics and microflows

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In this paper, a mathematical model within the framework of generalized hydrodynamics is developed for the description of flows in microsystems where the Knudsen number is large and the aspect ratio [(width)/(length)] is not so small. The model is based on a set of empirical generalized hydrodynamic equations, which are fashioned from the steady-state generalized hydrodynamic equations derived from the Boltzmann equation in a manner consistent with the laws of thermodynamics. The constitutive equations used for the model are highly nonlinear, unlike the Newtonian law of viscosity and the Fourier law of heat conduction, but they are thermodynamically consistent. In the absence of heat conduction, the model yields exact solutions for the velocity components and a nonlinear differential equation for the pressure distribution in the rectangular microchannel. The Langmuir adsorption model for surface-gas interaction is used for boundary conditions for the velocity. The calculated flow rate exhibits a Knudsen minimum with respect to the Knudsen number. The longitudinal velocity profile is also non-Poiseuille. The differential equation for pressure distribution is also solved approximately in order to obtain an analytic formula for the flow rate, which exhibits a Knudsen minimum. The formula, although approximate, provides considerable insights into the Knudsen flow phenomena in microchannels.

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I. INTRODUCTION

Because of the technological applications, flows in systems of micro- and nanoscales are of considerable current interest [1–6]. However, the problems are also of great significance from the fundamental theoretical viewpoint because physical phenomena, including flow phenomena in systems of the aforementioned spatial scales, reveal new aspects not amenable to the classical hydrodynamical treatments, and call for approaches to understanding them. For this reason, there has been considerable attention paid to the subject in recent years within the framework of the Navier-Stokes theory with slip boundary conditions, but there are still many areas of study on the subject that should be carried out in order to put the theory into a form comparable to that for macroscopic scale flows. The present work is a contribution toward that end.

It is generally known that classical hydrodynamics is not capable of satisfactorily treating flows in microsystems. The important questions are to what extent and in which direction should the classical hydrodynamics, namely, the Navier–Stokes–Fourier (NSF) theory, as a continuum mechanics theory, be modified if a continuum mechanics approach is to be taken for the flow phenomena of interest. These questions are all very worthy and challenging from the fundamental theoretical and practical viewpoints. As a way to improve the situation beyond the NSF theory approach, the direct simulation Monte Carlo (DSMC) method [7] has been increasingly used for study of microflows [8,9]. The DSMC method facilitates the understanding of microflow phenomena from a purely computational standpoint, but it is also known that it has its own limitations [8] when applied to phenomena in the large Knudsen number regime in the case of two- or three-dimensional flows. In any case, it is desirable to have a continuum hydrodynamical approach, which gives a different perspective to the understanding of the subject matter and even gives semianalytical results for some flow problems. The present work is aimed at such a goal.

As the size of the flow system gets smaller, the relative size of the boundaries of the flow system becomes increasingly large compared with the fluid volume flowing through the system, and thus the boundary conditions evidently begin to play an important role in determining flow characteristics. In other words, the surface-fluid interactions can have major effects in determining the physical properties of flow characteristics. Microflow phenomena, however, is not the first subject that requires the recognition of the importance of surface-fluid interaction effects, since surface-fluid interaction effects, in fact, have been well recognized and studied extensively in surface and colloid sciences for a long time since the pioneering work of Langmuir [10]. Therefore, study of flows in micro- or nanostructures should have much to benefit from the concepts, notions, and theories developed in surface science and, in particular, in the field of surface-gas scattering [11–13]. It, however, should be remarked that the surface-fluid molecule interactions are actively present, regardless of the sizes of the systems and the density of the fluid in hand, but their effects do not become manifestly observable, and they play a significant role in determining flow characteristics unless the Knudsen number of the flow becomes sufficiently large.

In this work we would like to combine the surface-gas interactions with the ideas of continuum mechanics theory to see how far the combination mentioned can be pushed for-

ward and where the limitations of such a combination lie. What we report in this work represents an elaboration of the generalized hydrodynamics formulation for microflows sketched out in a recent work [14]. In the present work, not only is the formulation reworked, but also numerical analysis is made to see if the theory has practical utility in microflow studies. We show that it is capable of describing the Knudsen flow, which is known to be one of the prominent features of microflows.

This paper is organized as follows: In Sec. II the generalized hydrodynamic equations [14–16] are presented for gas flows in a rectangular microchannel. They can be derived [17] from the Boltzmann equation in conformity with the laws of thermodynamics, but may be treated as phenomenological equations if the transport coefficients are accepted as phenomenological parameters. In the case of the latter approach, they may be regarded as a thermodynamically consistent phenomenological model for the hydrodynamic description of microflows. Since the surface-gas interactions become increasingly important as the ratio of the surface area to the characteristic gas volume in the flow system increases, and the boundary conditions are thereby modified, it is necessary to examine and take into account such interaction effects in the formulation of flow problems. This aspect of the flow problem is also considered in Sec. II. Then, a solvable model for the steady-state generalized hydrodynamic equations for the rectangular channel flow in the microscale is developed and solved with the boundary conditions that take into account the surface-gas interactions in Sec. III. Such boundary conditions will be given the term Langmuir boundary conditions. The flow characteristics thus obtained are described in Sec. IV. The numerically computed flow rate exhibits a Knudsen minimum, as observed experimentally [18–20]. Approximate analytic expressions for pressure distribution and flow rate are also presented for the insights they provide with regard to microflows. The approximate, but analytic, flow rate formula thus obtained also exhibits a minimum. Discussions and concluding remarks are given in Sec. V.

II. GENERALIZED HYDRODYNAMIC EQUATIONS

If the fluid is far removed from equilibrium because the Knudsen or Mach number is large, then the conventional hydrodynamic equations, such as the NSF equations, lose their effectiveness in the description of flow in such a condition. This is well recognized in rarefied gas dynamics [23]. It has been shown in the literature [14–16,24–27] that the classical hydrodynamics equations, namely, the NSF equations, can be generalized for the flow regimes, where the aforementioned fluid dynamic numbers are large, in such a manner that they fully obey the laws of thermodynamics. When the laws of thermodynamics are strictly satisfied by a set of hydrodynamic evolution equations, the set is said to be thermodynamically consistent, and the aformentioned generalized hydrodynamic equations are examples for such thermodynamically consistent evolution equations for macroscopic flow variables. Although the generalized hydrodynamic equations are continuum theory equations, they are still applicable to large Knudsen number flows because the nonlinear transport processes are appropriately taken into consideration in them, so that the flows are properly described despite the large Knudsen number. The breakdown in the large Knudsen number regime of the classical hydrodynamics, and the first-order Chapman-Enskog kinetic theory that underlies the classical hydrodynamics, have given rise to the unfortunate belief that the continuum mechanics loses its power in the large Knudsen number regime. Such a belief appears to be unjustified on the basis of the evidence [14–16,24–27] accumulated so far by means of the generalized hydrodynamics and the results presented in the following in this work, since they indicate that if the crucial nonlinear transport processes are properly taken into consideration, the continuum mechanics concept produces sensible results and thus is still applicable to large Knudsen number flows.

The thermodynamic consistency constraint used for deriving the generalized hydrodynamic equations is very useful for acquiring hydrodynamic equations that are not only in conformity with the laws of thermodynamics but also very effective in describing nonlinear processes occurring far removed from equilibrium. Such generalized hydrodynamic equations have been formulated for the purpose just mentioned and applied to various large scale flow problems. In this work we apply them to microflow phenomena involving large Knudsen numbers. Since the generalized hydrodynamic equations are sufficiently well reviewed in the literature, it is not warranted to go over their derivation, and the reader is referred to Refs. [14–16] and the references quoted therein for their derivation and details, especially, with regards to their relation to the classical hydrodynamics equations and also their validity. In this work we will simply cast them into the appropriate forms necessary for the flow problem at hand.

The notation used in this work is kept the same as in Refs. [14–16] so as to make the reading of this article as easy as possible in reference to the body of the previous work on the subject matter. We simply note that $\mathbf{u}=(u_x,u_y,u_z)$ is the fluid velocity and ρ is the mass density. The stress tensor will be denoted by $\mathbf{P}$ and its traceless symmetric part by $\mathbf{\Pi}$, that is,

$$\mathbf{\Pi} = \rho\hat{\mathbf{\Pi}} = \frac{1}{2}(\mathbf{P} + \mathbf{P}^t) - \frac{1}{3}\boldsymbol{\delta}\,\mathrm{Tr}\,\mathbf{P}, \tag{1}$$

where $\boldsymbol{\delta}$ stands for the unit second rank tensor. The excess normal stress will be denoted by

$$\Delta = \rho\hat{\Delta} = \frac{1}{3}\mathrm{Tr}\,\mathbf{P} - \rho \tag{2}$$

with p standing for the hydrostatic pressure.

Under the assumption of uniform temperature, we consider the channel flow in which the axial direction of the flow is assumed to be parallel with the x axis of the coordinate system whose origin is suitably fixed at a point. This means that heat flow is absent, and hence the heat flux evolution equation is not taken into consideration. The channel is assumed to have a width D in the y direction, whereas the z direction is neutral and has no flow in that direction. There-

fore there is no flow velocity in the z direction, that is, $u_z = 0$. In this case, the flow becomes two dimensional. Since the length L of the channel is necessarily finite in the case of microflows, the translational invariance of flow variables along the channel axis is broken. This broken translational invariance means that the flow variables depend on the axial position x, and it thus gives rise to a coupled system of partial differential equations for flow variables varying with respect to x and y. Under the assumptions made, the generalized hydrodynamic equations consist of the equation of continuity, momentum balance equation, and the shear stress evolution equation, because for a dilute gas, the excess normal stress identically vanishes [15,16]; that is, $\Delta = 0$. For the flow problem at hand, the generalized hydrodynamic equations become those of a steady-state two-dimensional flow.

Since $\mathbf{\Pi}$ is traceless and symmetric it follows that in the case of the two-dimensional flow,

$$\Pi_{xx} + \Pi_{yy} = 0. \tag{3}$$

Since ρ and T are in the set of local conserved variables, which relax much more slowly than the nonconserved variables such as the stress tensor and heat flux, the ideal gas equation of state can be shown [15,16] to be valid even if the flow is far removed from equilibrium. If the gas is ideal and the temperature is spatially uniform, then the ideal gas equation of state

$$p = \rho k_B T \tag{4}$$

can be used to eliminate the density in the equation of continuity and other evolution equations given earlier. With the definition of the primary normal stress difference

$$N_1 = \Pi_{xx} - \Pi_{yy} = 2\Pi_{xx} = -2\Pi_{yy}, \tag{5}$$

the steady-state generalized hydrodynamic equations in the adiabatic approximation [14–16] can be put into the forms

$$\frac{\partial p u_x}{\partial x} + \frac{\partial p u_y}{\partial y} = 0, \tag{6}$$

$$\frac{p}{k_B T}\left(u_x \frac{\partial}{\partial x} + u_y \frac{\partial}{\partial y}\right) u_x = -\frac{\partial p}{\partial x} - \left(\frac{1}{2}\frac{\partial}{\partial x} N_1 + \frac{\partial}{\partial y}\Pi_{xy}\right), \tag{7}$$

$$\frac{p}{k_B T}\left(u_x \frac{\partial}{\partial x} + u_y \frac{\partial}{\partial y}\right) u_y = -\frac{\partial p}{\partial y} - \left(\frac{\partial}{\partial x}\Pi_{xy} - \frac{1}{2}\frac{\partial}{\partial y} N_1\right), \tag{8}$$

$$\frac{p}{\eta_0} q(\kappa) N_1 = -2p\left(\frac{\partial u_x}{\partial x} - \frac{\partial u_y}{\partial y}\right) + \frac{1}{2} N_1 \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) + \Pi_{xy}\left(\frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x}\right), \tag{9}$$

$$\frac{p}{\eta_0} q(\kappa)\Pi_{xy} = -p\left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}\right) - \Pi_{xy}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) + \frac{1}{2} N_1 \left(\frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x}\right). \tag{10}$$

In these equations, $q(\kappa)$ is the nonlinear factor defined by

$$q(\kappa) = \frac{\sinh \kappa}{\kappa},$$

where κ is the dissipation function, which, when expressed in terms of the shear stress Π_{xy} and the primary normal stress N_1 is given by

$$\kappa = \frac{\tau}{2\eta_0}\left(\Pi_{xy}^2 + \frac{1}{2} N_1^2\right)^{1/2}, \tag{11}$$

with τ denoting the relaxation time defined by

$$\tau = (\eta_0 \sqrt{2 m_r k_B T})^{1/2} (n k_B T \sigma)^{-1}. \tag{12}$$

Here m_r is the reduced mass, σ is the size parameter (i.e., diameter) of the molecule, n is the number density, k_B is the Boltzmann constant, and η_0 is the viscosity of the gas—the Chapman-Enskog viscosity.

If the evolution equations for the stress tensor $\mathbf{\Pi}$ and the heat flux are derived from the Boltzmann equation, the nonlinear factor $q(\kappa)$ arises if the Boltzmann collision term is expanded in cumulants, which are basically resummations of an expansion of the Boltzmann collision integral in an infinite series of the Knudsen number. The nonlinear factor, therefore, enables us to describe rather effectively transport processes to infinite order in the Knudsen number, and as a consequence, the transport processes described by the evolution equations, such as Eqs. (9) and (10), are highly nonlinear. Moreover, because the nonlinear factor is intimately connected to the local form of the second law of thermodynamics and satisfies the inequality $\kappa \sinh \geqslant 0$ demanded by the latter, the generalized hydrodynamics equations satisfy the second law of thermodynamics. Therefore they are thermodynamically consistent.

Equations (9) and (10) are the steady-state constitutive equations for the primary normal stress difference and the shear stress, respectively. Equation (10), in particular, reduces to the Newtonian law of viscosity if the equation is linearized with respect to the Π and N_1 dependence. Therefore, the model generalizes the NSF equations with respect to the constitutive equations for stress tensor components. The generalized hydrodynamic equations (6)–(10) are applicable to monatomic gases that flow in a steady state far removed from equilibrium. The size of the system, and hence the Knudsen number, is not as yet manifest in the equations presented. To make them apparent it is necessary to cast the generalized hydrodynamic equations into dimensionless forms.

A. Nondimensionalization of the generalized hydrodynamic equations

The evolution equations presented are made nondimensional by suitably scaling the variables involved. Let us de-

note by L the channel length, by D the channel width, by u_e the entrance velocity, and by p_e the pressure at the entrance of the channel. The exit pressure will be denoted by p_0. We also define the nondimensional fluid dynamic parameters

$$\varepsilon = \frac{D}{L}, \quad N_{\mathrm{Re}} = \frac{\rho_e u_e D}{\eta_0}, \quad N_M = \frac{u_e}{\sqrt{\gamma k_B T}}, \tag{13}$$

where γ is the polytropic ratio (ratio of specific heats) of the gas. The parameter ε is the aspect ratio, N_{Re} is the Reynolds number, and N_M is the Mach number at the channel entrance. The mean-free path l of the gas entering the channel is defined by the relation

$$\eta_0 = \frac{1}{2} m \rho_e u_e l. \tag{14}$$

This is the mean-free free path theory expression [28] for the shear viscosity of the gas. The mean-free path l must be estimated in terms of molecular parameters if it is to be made use of in fluid dynamic investigations. We use the following method:

If the Chapman–Enskog shear viscosity [28–30] for hard spheres,

$$\eta_0 = \frac{5}{16} \frac{\sqrt{m k_B T}}{\sqrt{\pi}\sigma^2},$$

is used for η_0 then the mean-free path is more explicitly given by the formula

$$l = \frac{5}{8} \frac{\sqrt{m k_B T}}{\sqrt{\pi}\sigma^2 m \rho_e u_e} = \frac{5}{16\sqrt{2}} \frac{1}{\sigma^2 \rho_e}. \tag{15}$$

This is good enough for our purpose here, but if an expression for a nonhard sphere potential model is desired for l—e.g., for the Lennard-Jones potential model—then l may be expressed in terms of the collision bracket integral for η_0 of the Lennard-Jones gas. This will require a numerical computation of the collision bracket integral involved, which in turn requires the collision cross section as a function of scattering angles and the relative kinetic energy of collision. We would like to avoid the need for computing collision bracket integrals because we are principally interested in the hydrodynamic aspects of the flow phenomenon of interest, which can be examined without such complications mentioned.

With the mean-free path so given in terms of density as in Eq. (15), the transversal Knudsen number is defined by

$$N_{Kn} = \frac{l}{D}. \tag{16}$$

This implies that there are some relations among nondimensional fluid dynamic parameters N_{Re}, N_M, and N_{Kn} in the case of l for hard spheres we obtain

$$N_M = \sqrt{\frac{2}{\gamma\pi}} N_{\mathrm{Re}} N_{K_n}. \tag{17}$$

For this relation, u_e is taken as the root mean square speed of the gas

$$u_e = \sqrt{\frac{8 k_B T}{\pi m}}.$$

The fluid dynamic number associated with the dissipation function κ is the nonuniformity number N_δ defined by [14–16]

$$N_\delta = \sqrt{\frac{2\gamma}{\pi}} N_M N_{Kn}. \tag{18}$$

This nonuniformity number plays an important role in the generalized hydrodynamic equations since it is the parameter determining the measure of energy dissipation in the flow process, since κ in the nonlinear factor $q(\kappa)$ is proportional to N_δ. If the nonconserved variables in Eqs. (9) and (10) are expanded in a series of N_δ then the leading order equations are those of the classical hydrodynamics, namely, the Navier–Stokes theory. For the discussion of this aspect, see Refs. [14–16].

With various nondimensional numbers so introduced, if various variables involved in the evolution equations are nondimensionalized as follows:

$$\xi = x L^{-1}, \quad \zeta = y D^{-1},$$

$$u = u_x/u_e, \quad v = u_y/\varepsilon u_e, \quad \phi = p/p_e,$$

$$\psi = N_\delta \Pi_{xy}(\eta_0 u_e/D), \quad \varphi = N_\delta N_1(\eta_0 u_e/D), \tag{19}$$

the generalized hydrodynamic equations then can be given the nondimensionalized forms

$$\varepsilon \frac{\partial \phi u}{\partial \xi} + \varepsilon \frac{\partial \phi v}{\partial \zeta} = 0, \tag{20}$$

$$\frac{\partial \psi}{\partial \zeta} + \varepsilon \frac{\partial}{\partial \xi}\left(\phi + \frac{1}{2}\varphi\right) + \gamma \varepsilon N_M^2 \phi \left(u \frac{\partial u}{\partial \xi} + v \frac{\partial u}{\partial \zeta}\right) = 0, \tag{21}$$

$$\varepsilon \frac{\partial}{\partial \zeta} + \left(\phi - \frac{1}{2}\varphi\right) + \varepsilon^2 \frac{\partial \psi}{\partial \xi} + \gamma \varepsilon^3 N_M^2 \phi \left(u \frac{\partial v}{\partial \xi} + v \frac{\partial v}{\partial \zeta}\right) = 0, \tag{22}$$

$$q(\kappa)\psi = -\left(N_\delta - \frac{2}{\pi} N_{Kn} \frac{\varphi}{\phi}\right) \frac{\partial u}{\partial \zeta} - \frac{4}{\pi} \varepsilon N_{Kn} \frac{\psi}{\phi} \left(\frac{\partial u}{\partial \xi} + \frac{\partial v}{\partial \zeta}\right) - \varepsilon^2 \left(N_\delta + \frac{2}{\pi} N_{Kn} \frac{\varphi}{\phi}\right) \frac{\partial v}{\partial \xi}, \tag{23}$$

$$q(\kappa)\varphi = \frac{4}{\pi} N_{Kn} \frac{\psi}{\phi} \frac{\partial u}{\partial \zeta} - 2\varepsilon N_\delta \left(\frac{\partial u}{\partial \xi} - \frac{\partial v}{\partial \zeta}\right) + \frac{2}{\pi} \varepsilon N_{Kn} \frac{\varphi}{\phi} \left(\frac{\partial u}{\partial \xi} + \frac{\partial v}{\partial \zeta}\right) = \varepsilon^2 \frac{4}{\pi} N_{Kn} \frac{\psi}{\phi} \frac{\partial v}{\partial \xi}. \tag{24}$$

The dissipation function κ is now given by the formula

$$\kappa = \frac{1}{2}\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{\phi}\left(\psi + \frac{1}{2}\varphi^2\right)^{1/2}. \tag{25}$$

The dissipation function in the present reduced form superficially appears to be independent of N_δ. However, it should be remembered that it is a consequence of the particular manner of scaling made for Π_{xy} and N_1 in Eq. (19). Nevertheless, κ in effect depends implicitly on N_δ through its appearance in the other parts of the equations. The present manner of scaling the variables is convenient for developing approximations for the nonlinear flow problem under consideration, especially if nonlinear dissipative effects are desired to be taken into account.

If the axial flow velocity is known, the volume flow rate may be calculated with it. Since the temperature is uniform, by using the reduced equation of state, the volume flow rate can be cast into the form

$$\int_0^1 d\zeta \phi(\xi,\zeta)u(\xi,\zeta)|_{\xi=0} = \int_0^1 d\zeta \phi(\xi,\zeta)u(\xi,\zeta)|_{\xi=1}. \tag{26}$$

With the definition

$$f(\xi) = \int_0^1 d\zeta \phi(\xi,\zeta)u(\xi,\zeta), \tag{27}$$

this particular form of the mass conservation law represented by Eq. (26), therefore, may be written as a differential equation

$$\frac{df(\xi)}{d\xi} = 0. \tag{28}$$

Equation (26) and (28), when explicitly worked out, can be found to be a differential equation for pressure distribution along the axial direction. This equation can be equivalently replaced by the boundary conditions for the transversal component v at the walls of the channel, which produces a differential equation for the pressure distribution, as will be discussed and used later. The differential equations (20)–(24) and Eq. (28) complete the evolution equations with which to determine flow variables for the microchannel flow under consideration.

B. Langmuir boundary conditions

We have seen in previous studies [14–16,26,31] of macroflows in the large Knudsen and Mach number regimes that with just stick boundary conditions, the generalized hydrodynamic equations still can adequately account for flow characteristics in the flow regimes mentioned, because the nonlinear energy dissipation mechanism, which is properly built into them, is adequate for giving rise to nonlinear transport processes. However, as the size of flow systems is diminished to the level of microflows or nanoflows, the ratio of the boundary layers of the flow system to the fluid volume, which is roughly of the order of the Knudsen number, becomes increasingly large, and consequently the effects of the boundaries on the flow characteristics are no longer negligible. As a matter of fact, they even become dominant effects. This is well recognized in rarefied gas dynamics, and there are numerous works devoted to this aspect in the literature [32,33]. Therefore, surface-fluid interactions [34] must be properly taken into account if one desires to comprehend various flow characteristics in microflows from the hydrodynamical viewpoint.

In the approach to this problem in the field of microflows, various authors [1,4] have employed the Navier-Stokes theory and have implemented it with the conventional slip boundary conditions in the same manner as originally developed by Maxwell [32] and, for example, often used in rarefied gas dynamics [23]. This approach not only limits the hydrodynamic description to that of the classical theory, but also requires an expansion of the flow velocity in a series of mean-free paths and the determination of the expansion coefficients in terms of accommodation coefficients. [13] Such an approach does not make evident the connection between the accommodation coefficients and the interaction of the surface and fluid molecules. The desired connection cannot be achieved unless the molecular nature of surface is explicitly taken into account by means of a suitable molecular model.

On the other hand, it was shown by Eu *et al.* [26] that if the generalized hydrodynamic equations are combined with the Langmuir adsorption theory [10], which adequately takes into account the surface-fluid interactions, flow characteristics of rarefied gases can be adequately accounted for. This Langmuir adsorption model was applied to a microflow problem by Myong [35] within the framework of the classical NSF hydrodynamic theory. However, it is desirable to improve upon the classical NSF theory in order to capture more satisfactorily the basic feature of the Knudsen flow. We will show in this work that the generalized hydrodynamics equations can be employed with the Langmuir adsorption theory [15,26,35]. There still is room for improving the Langmuir boundary conditions in their application to microflow problems, but we will defer a further study of them to the future.

Equations (20)–(24) will be solved subject to the boundary conditions

$$u(\zeta = 0,\xi) = u_a, \quad u(\zeta = 1,\xi) = u_a',$$

$$u(\zeta = 0,\xi) = v(\zeta = 1,\xi) = 0,$$

$$\phi(\xi = 0,\zeta) = \phi_0, \quad \phi(\xi = 1,\zeta) = \phi_1 (0\zeta \leqslant 1), \tag{29}$$

where u_a and u_a' are the boundary values of the velocity, which will be elaborated later, and ϕ_0 and ϕ_1 are reduced pressures at the entrance and exit of the channel. It should be noted that u_a and u_a' are equal to zero in the case of stick boundary conditions, but, as already mentioned, such boundary conditions are generally unsuitable in the case of flows in microchannels, because despite that the surface-fluid molecule interactions play important roles in small systems, the stick boundary conditions do not take them into account. The stick boundary conditions are appropriate if the density of the gas is such that gas molecules fully cover the surface of the channel.

In order to take the wall-gas interaction into account so that the physicochemical properties of the fluid and the walls of the flow system are well reflected in the flow behavior of the fluid, we modify the boundary conditions in a manner similar to the method used by Eu *et al.* [26] and Bhattacharya *et al.* [27]. According to the aforementioned theory of boundary conditions based on the Langmuir adsorption model, the velocity boundary conditions can be modified to the form [14]

$$u_a = \theta(T)u_w + [1 - \theta(T)]u_g. \tag{30}$$

In this expression, u_w is the wall velocity, u_g is the streamwise velocity of the fluid one or a fraction of a mean-free path away from the wall; and in the case of a long mean-free path comparable with the channel width D, the streamwise velocity u_g may be taken for the midstream velocity. A similar equation holds for the boundary condition on u at $\zeta=1$:

$$u_a' = \theta(T)u_w + [1 - \theta(T)]u_g', \tag{31}$$

where the meaning of u_g' is similar to that of u_g.

Since the velocity profile should be symmetric in the present flow problem, we may take u_g as u at position $\zeta_l = l/(1+\chi N_{Kn})D = N_{Kn}/(1+\chi N_{Kn})(\chi > 2)$, or u_g' as u at position $\zeta_l = 1 - N_{Kn}/(1+\chi N_{Kn})$:

$$u_g = u\left(\frac{N_{Kn}}{1+\chi N_{Kn}}\right),$$

$$u_g' = u\left(1 - \frac{N_{Kn}}{1+\chi N_{Kn}}\right), \tag{32}$$

where χ is a constant. The precise ζ dependence of u_g and u_g' is not determined yet: it must be determined self-consistently for the flow problem of interest by using the flow profile for u with respect to ζ

C. A model for the surface coverage θ

For the original Langmuir adsorption isotherm in the simplest form, it is generally assumed that the surface is covered by monolayers of fluid molecules. In this case, the fraction $\theta(T)$ of the surface covered is given by the formula [10,14,26]

$$\theta(T) = \frac{bp}{1+bp}, \tag{33}$$

where the parameter b is closely related to the surface-gas interaction characteristics and p is the pressure of gas that is assumed to be in equilibrium with the adsorbed layer. The parameter b may be expressed by the formula [26,27]

$$b = \frac{K}{k_B T} \tag{34}$$

(where K is the equilibrium constant), which permits evaluation by means of statistical mechanics since the equilibrium constant K can be calculated with the surface-gas interaction model that treats adsorption of the fluid molecules on the surface as a kind of chemical reaction. Here, T is the wall temperature. The equilibrium constant K depends on the wall temperature and the wall-gas interaction parameters. We remark that in the derivation of the formula for $\theta(T)$ in Eq. (33), there is no condition whatsoever on the magnitude of p. Furthermore, because the collisions of fluid molecules with the surface occur on the time scale of 10^{-14}–10^{-12}s, which is much shorter than the hydrodynamic relaxation times, and on the scale of hydrodynamic processes the fluid molecules may be regarded as being in equilibrium with the surface in the interface, the assumption of equilibrium between the surface and the fluid is not at all inconsistent with the flow problem under consideration and is justifiable.

However, in practice the surface is not smooth, but rough [36]. Furthermore, it can be covered by not only monolayers but also by multiayers of adsorbed molecules as rough edges in the surface can attract many molecules at a site. Phrased in more appropriate terms, more than a molecule can get adsorbed (i.e., physically, but not chemically bound) at a site on the surface, which is rather rough in the scale of microflows. The average number of molecules adsorbed at a site may be in principle found by applying a statistical mechanics method, but it constitutes a full-fledged question of its own right, and it is not a problem we would like to devote ourselves to in this work because it will take us far afield from the question of fluid dynamics. We would rather like to treat it empirically and answer the fluid dynamics question of interest here. In this spirit, we assume that $\nu = 1+\delta (\delta > 0)$ particles on the average are adsorbed at a site on the surface. If we further assume that the adsorption processes may be regarded as a kind of chemical reaction between the ν gas molecules (M) and the adsorption site (S) on the surface according to the reaction model

$$S + \nu M = SM_\nu,$$

then it is possible to calculate the coverage θ explicitly in terms of molecular parameters by means of a statistical mechanics method in a way similar to the case of monolayer adsorption. If $\delta=0$, this model reduces to the original Langmuir model in which the surface is covered by monolayers. By using the same method as for the derivation of Eq. (33), it is possible to show that the fraction θ of coverage of the surface by the gas molecules is given by the formula

$$\theta(T) = \frac{b' p^\nu}{1 + b' p^\nu}, \tag{35}$$

where b' is a parameter depending on T and molecular parameters characteristic of the surface and gas molecules; it is comparable to the parameter b. It will be empirically found that δ is less than unity. The temperature and molecular parameter dependences of b' may be calculated by means of statistical mechanics under some simplifying assumptions, but it is not essential at this point to know its temperature and molecular parameter dependence for the purpose of calculating flow variables, especially with respect to the Knudsen and other fluid dynamics numbers. Since $\theta(T)$ generally depends on pressure, and hence on the density of the gas, it varies with the Knudsen number. Formula (35) modifies the

coverage formula exmployed in the discussion given for the Langmuir boundary conditions in Ref. [14].

III. SOLVABLE MODEL EQUATIONS FOR MICROCHANNEL FLOW

Microchannel flow problems that we have in mind usually deal with flows with a rather low Mach number, although the Knudsen number may not be small because of a small channel width and length. On the other hand, although the aspect ratio ε is small, it is not vanishingly small. Therefore, we are interested in creeping flows in a microchannel with a moderately small aspect ratio. Consequently, it is reasonable to retain only the terms of first order with respect to N_M and ε in the generalized hydrodynamic equations. Examining the evolution equations (20)–(24), we see that the inertia terms are multiplied by N_M^2. Therefore, in the small Mach number limit, the intertia terms are of second-order importance. In any case, we take the set of equations as a proposition for a model for nonlinear constitutive relations—a non-Newtonian approximation. We will see that they are capable of accounting for the important features of flow behavior in microflows, notably, the velocity profiles and the Knudsen minimum in the flow rate. Thus, on retaining only such terms as mentioned, the following equations arise for the flow problem of interest:

$$\varepsilon\phi\frac{\partial u}{\partial \xi}+\varepsilon u\frac{\partial \phi}{\partial \xi}+\varepsilon\phi\frac{\partial v}{\partial \zeta}+\varepsilon\phi\frac{\partial \phi}{\partial \zeta}=0, \tag{36}$$

$$\frac{\partial \psi}{\partial \zeta}+\varepsilon\frac{\partial \phi}{\partial \xi}=0, \tag{37}$$

$$\varepsilon\frac{\partial \phi}{\partial \zeta}=0, \tag{38}$$

$$q(\kappa)\psi=-N_\delta\frac{\partial u}{\partial \zeta}, \tag{39}$$

$$\int_0^1 d\zeta\ \phi(\xi,\zeta)u(\xi,\zeta)|_{\xi=0}=\int_0^1 d\zeta\ \phi(\xi,\zeta)u(\xi,\zeta)|_{\xi=1}, \tag{40}$$

or

$$\frac{\partial}{\partial \xi}f(\xi)=0, \tag{41}$$

for which we have used $\varphi=0$ that arises from the equation

$$q(\kappa)\varphi=0, \tag{42}$$

holding to the lowest order in ε. Equation (41) yields a differential equation for pressure variation in the axial direction, but the vanishing transversal velocities at the boundaries $\zeta=0$ and 1 may be used equivalently for the purpose of obtaining the differential equation mentioned. In order to remind us of the order of ε taken, we have kept ε in Eqs. (36) and (38) even though it may be factored out. Equation (41) implies that the primary normal stress difference φ does not exist in the present model.

On close examination of these equations, we find that they are almost the same as the one-dimensional channel flow equations for a channel of infinite length [14–16] except for the equation of continuity and the condition on mass flux, Eq. (40). We solve these equations and examine their predictions for flow characteristics. This set of equations can be, in fact, reduced to a single nonlinear differential equation for the reduced pressure ϕ. Therefore, when the differential equation for ϕ is solved, the flow properties of the gas in the microchannel are fully determined.

Equation (38) implies that pressure is a function of ξ only:

$$\phi=\phi(\xi). \tag{43}$$

Therefore, the pressure is transversally uniform. It also follows that the equation of continuity takes the form

$$\phi\frac{\partial u}{\partial \xi}+u\frac{\partial \phi}{\partial \xi}+\phi\frac{\partial v}{\partial \zeta}=0. \tag{44}$$

This equation may be used for determining the pressure distribution along the channel axis, but it is not directly involved in the determination of u. It will be considered later to determine the transversal velocity v after the remaining equations are solved for the longitudinal velocity u.

A. Longitudinal velocity profile

Since $\varphi=0$, the dissipation function is given by the formula

$$\kappa=\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi}(\psi^2)^{1/2}=\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi}|\psi|. \tag{45}$$

The constitutive equation (39), therefore, can be written as

$$\sinh\left(\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi}|\psi|\right)=-N_\delta\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi}\frac{\partial u}{\partial \zeta}.$$

By inverting this relation, we find the reduced shear stress

$$\psi=2\sqrt{\frac{\gamma}{\pi^{3/2}}}\phi\sinh^{-1}\left(-N_\delta\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi}\frac{\partial u}{\partial \zeta}\right). \tag{46}$$

At this point, it is convenient to define some abbreviations:

$$\alpha\equiv\frac{\omega}{\phi}=N_\delta\sqrt{\frac{\pi^{3/2}}{\gamma}}\frac{1}{2\phi},\quad \omega=\frac{1}{2}N_\delta\sqrt{\frac{\pi^{3/2}}{\gamma}}, \tag{47}$$

$$\beta=-\mu^{-1}\frac{\partial \ln\phi}{\partial \xi},\quad \mu^{-1}=\frac{\varepsilon}{2}\sqrt{\frac{\pi^{3/2}}{\gamma}}. \tag{48}$$

On taking the derivative of ψ with respect to ζ and using Eq. (37), we then obtain the differential equation for u

$$\frac{\partial}{\partial \zeta}\sinh^{-1}\left(-\alpha\frac{\partial u}{\partial \zeta}\right)=\beta. \tag{49}$$

Integrating it with respect to ζ yields the equation

$$\alpha\frac{\partial u}{\partial \zeta}=-\sinh(\beta\zeta+C), \tag{50}$$

where C is a constant. The integration of Eq. (50) once more gives the solution for u:

$$\alpha u = -\frac{1}{\beta}\cosh(\beta\zeta + C) + C_1, \tag{51}$$

where C_1 is an integration constant. This form of solution for u was also known [15,16] for the infinite channel flow problem obeying the same constitutive equation for ψ, as considered here. The difference in the two cases lies in the fact that α and β now depend on the longitudinal position ξ. Therefore, u presented in Eq. (51) is not a complete solution for the flow problem until α and β are determined with regard to their longitudinal position (ξ) dependence. The constants of integration C and C_1 can be determined by the boundary conditions on u.

The modified boundary conditions alter the velocity profile. Using the boundary conditions (30) and (31) in the velocity formula (51) we find at $\zeta=0$,

$$\alpha\beta[1-\theta(T)]u_g = -\cosh C + \beta C_1, \tag{52}$$

where u_g is the fluid velocity at a fraction of a mean-free path away from the wall at $\zeta=0$. At the wall at $\zeta=1$, there holds a similar equation

$$\alpha\beta[1-\theta(T)]u_g' = -\cosh(\beta + C) + \beta C_1, \tag{53}$$

where u_g' is the fluid velocity at a fraction of a mean-free free path away from the wall at $\zeta=1$. Since the flow profile must be symmetric around the axis of the channel, if the distances away from the walls are taken equal, then $u_g=u_g'\equiv u_0$. Solving the Eqs. (52) and (53) for C and C_1 we obtain

$$C = -\frac{\beta}{2},$$

$$\beta C_1 = \alpha\beta[1-\theta(T)]u_0 + \cosh\frac{\beta}{2}. \tag{54}$$

Hence, the streamwise velocity profile is given by the formula

$$u = \frac{1}{\alpha\beta}\left[\cosh\frac{\beta}{2} - \cosh\beta\left(\zeta - \frac{1}{2}\right) + \alpha\beta[1-\theta(T)]u_0\right], \tag{55}$$

which, as will be shown, reduces to the stick boundary condition result [14–16] if $\theta=1$, that is, if the surface is completely covered or, put in another way, if the fluid fully sticks at the walls.

It is necessary to determine u_0. Taking the velocity value at position $\zeta=N_{Kn}/(1+\chi N_{Kn})$ near $\zeta=0$ and position $\zeta=1-N_{Kn}/(1+\chi N_{Kn})$ near $\zeta=1$, respectively, we find

$$u_0 = \frac{u_l}{\theta\alpha\beta}, \tag{56}$$

where

$$u_l = \cosh\frac{\beta}{2} - \cosh\left[\frac{\beta}{2}\left(\frac{1+(\chi-2)N_{Kn}}{1+\chi N_{Kn}}\right)\right]. \tag{57}$$

The velocity profile under the Langmuir boundary conditions is finally given by the formula

$$u = \frac{1}{\alpha\beta}\left[\cosh\frac{\beta}{2} - \cosh\beta\left(\zeta - \frac{1}{2}\right) + (\theta^{-1}-1)u_l\right]. \tag{58}$$

This means that as $p\to\infty$, that is, as $\theta\to 1$, the velocity profile becomes that of the usual macroscopic channel flow, whereas it begins to progressively exhibit the effects of surface on the flow in the channel as $p\to 0$, that is, as $\theta\to 0$.

The fraction of coverage of the surface θ given in Eq. (35) is expressible in terms of the Knudsen number as follows:

$$\theta(T) = \frac{b''/N_{Kn}^{\nu}}{1+b''/N_{Kn}^{\nu}} \equiv \frac{1}{1+c^{*}N_{Kn}^{\nu}} \quad (\nu = 1+\delta), \tag{59}$$

where b'' is related to b' through the transformation $p\to N_{Kn}$. Thus, as the Knudsen number increases, the gas density or pressure is reduced and the surface coverage accordingly diminishes. This, in turn, implies that the flow tends to be more and more rectangular, since $\alpha=\alpha_0 N_{Kn}$, where α_0 is independent of N_{Kn} and hence

$$\lim_{N_{Kn}\to\infty} u = \frac{c^{*}}{\alpha_0\beta_\infty}\left[\cosh\frac{\beta_\infty}{2} - \cosh\frac{\beta_\infty}{2}\left(\frac{\chi-2}{\chi}\right)\right], \tag{60}$$

where $\beta_\infty=\lim_{N_{Kn}\to\infty}\beta$ and, as a consequence, the right-hand side of Eq. (60) is independent of N_{Kn} and also of ζ. An approximate formula for β_∞ will be given later for the insight it provides. Because the large N_{Kn} limit of u is independent of ζ, the axial flow profile is rectangular—a plug flow, which may be regarded as being axially ballistic in motion. In such a regime of N_{Kn} we practically have a beam of molecules. This limiting behavior of u is consistent with the DSMC velocity profiles [4] and velocity profiles [37] obtained by the solution of a linearized Boltzmann equation [i.e., Bhantnagar-Gross-Krook (BGK) equation], which becomes increasingly flat as the Knudsen number increases. Such limiting behavior of u indeed can be verified numerically, as is evident in Fig. 2 presented in Sec. IV below. The plug flow behavior is also reminiscent of the beaming effect considered by Clausing [38] and later by others [39,40] in connection with vacuum technology. However, it should be noted that the aforementioned authors examined the beaming effect by using the Knudsen cosine law of reflection [19]. This mechanism is different from that of the Langmuir boundary condition used here.

If the parameters α and β are determined and, in fact, if ϕ is determined together with its derivative $\phi_\xi=\partial\phi/\partial\xi$, velocity profile is fully determined. The determination of ϕ is achieved by imposing the mass conservation in the flow through the channel or deriving a differential equation for ϕ from the equation of continuity with the help of the boundary conditions on the transversal velocity component v at $\zeta=0$ and 1. We will use the latter approach.

B. Shear stress profile

The profile for the shear stress is readily obtained by using the streamwise velocity formula. Since

$$\alpha\frac{\partial u}{\partial\zeta} = -\sinh\beta\left(\frac{1}{2} - \zeta\right), \tag{61}$$

ψ is given by

$$\psi = -\varepsilon \frac{\partial \phi}{\partial \xi}\left(\zeta - \frac{1}{2}\right), \tag{62}$$

which satisfies Eq. (37). Despite the flow velocity nonlinear with respect to ζ, the shear stress is linear with respect to ζ in the present flow configuration. It is a peculiarity of the rectangular channel flow considered here; in the case of other configurations, such as, a circular tube flow, this ζ dependence of ψ is not expected to hold true, as has been shown for flows in an infinite tube [15,21].

C. Transversal velocity profile

The transversal velocity v can be readily calculated by using the streamwise velocity u calculated earlier. By using the formula (55) for u and the equation of continuity (44), the differential equation for v is obtained. For the purpose of making the symmetry property of v and its equation more transparent, it is convenient to transform the independent variable

$$z = \zeta - \frac{1}{2},$$

so that the range of the variable z becomes $\left[-\frac{1}{2}, \frac{1}{2}\right]$. Then the differential equation for the transversal velocity v is given by

$$\frac{\partial v(z)}{\partial z} = v_t^0 - \frac{1}{(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\cosh\,\beta z + \frac{1}{\alpha\beta}\frac{\partial \beta}{\partial \xi} z\,\sinh\,\beta z - \frac{\mu}{\alpha}\cosh\,\beta z, \tag{63}$$

where

$$v_t^0 = \left[\cosh\frac{\beta}{2} + (\theta^{-1}-1)u_1\right](\alpha\beta)^{-2}\frac{\partial \alpha\beta}{\partial \xi} - \frac{1}{2\alpha\beta}\left[\sinh\frac{\beta}{2} + 2(\theta^{-1}-1)\frac{\partial u_l}{\partial \beta}\right]\frac{\partial \beta}{\partial \xi} + \frac{\mu}{\alpha}\cosh\frac{\beta}{2}. \tag{64}$$

This equation clearly indicates that $\partial v(z)/\partial z$ is even with respect to transformation $z \to -z$, and v is odd.

Integrating Eq. (63) yields the transversal velocity

$$v(z) = V_0 + v_t^0 z - \frac{1}{\beta(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\sinh\,\beta z + \frac{1}{\alpha\beta^3}\frac{\partial \beta}{\partial \xi}(\beta z\,\cosh\,\beta z - \sinh\,\beta z) - \frac{\mu}{\beta\alpha}\sinh\,\beta z. \tag{65}$$

Imposing the boundary conditions $v\left(-\frac{1}{2}\right) = v\left(\frac{1}{2}\right) = 0$, we obtain

$$0 = V_0 + \frac{1}{2}v_t^0 - \frac{1}{\beta(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\sinh\frac{\beta}{2} + \frac{1}{\alpha\beta^3}\frac{\partial \beta}{\partial \xi}\left(\frac{\beta}{2}\cosh\frac{\beta}{2} - \sinh\frac{\beta}{2}\right) - \frac{\mu}{\beta\alpha}\sinh\frac{\beta}{2},$$

$$0 = V_0 - \frac{1}{2}v_t^0 + \frac{1}{\beta(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\sinh\frac{\beta}{2} - \frac{1}{\alpha\beta^3}\frac{\partial \beta}{\partial \xi}\left(\frac{\beta}{2}\cosh\frac{\beta}{2} - \sinh\frac{\beta}{2}\right) + \frac{\mu}{\beta\alpha}\sinh\frac{\beta}{2}.$$

For these boundary conditions to be consistent with each other, the constant V_0 must be equal to zero identically: $V_0 = 0$. Therefore, we obtain the equation for β

$$v_t^0 - \frac{2}{\beta(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\sinh\frac{\beta}{2} + \frac{2}{\alpha\beta^3}\frac{\partial \beta}{\partial \xi}\left(\frac{\beta}{2}\cosh\frac{\beta}{2} - \sinh\frac{\beta}{2}\right) - \frac{2\mu}{\beta\alpha}\sinh\frac{\beta}{2} = 0. \tag{66}$$

This gives rise to Eq. (69) for β more explicitly given in the following. The transversal velocity is now given by

$$v(z) = v_t^0 z - \frac{1}{\beta(\alpha\beta)^2}\frac{\partial \alpha\beta}{\partial \xi}\sinh\,\beta z + \frac{1}{\alpha\beta^3}\frac{\partial \beta}{\partial \xi}(\beta z\,\cosh\,\beta z - \sinh\,\beta z) - \frac{\mu}{\beta\alpha}\sinh\,\beta z. \tag{67}$$

This solution is indeed odd with respect to z. Note that $v(z)$ is equal to zero at $z \pm \frac{1}{2}$ and at $z = 0$. Therefore, its shape should be something like an inverted S, as will be evident from Fig. 4, presented in the following section. It should be also recalled that since the actual transversal velocity is proportional to the aspect ration, it vanishes as the channel length becomes infinite.

D. Differential equation for β

We will use the transversal velocity v to derive the differential equation for β. This equation is, in fact, the solvability condition for the model generalized hydrodynamic equations. Using Eq. (67), evaluated at $z = \frac{1}{2}$ or $-\frac{1}{2}$ and the identity

$$\frac{1}{\alpha\beta}\frac{d\alpha\beta}{d\xi} = \mu\beta + \frac{1}{\beta}\frac{d\beta}{d\xi}, \tag{68}$$

we obtain the differential equation for β or $\ln\,\phi$

$$L_1(\beta)\frac{d\beta}{d\xi} + \mu\beta^2 L_2(\beta) = 0, \tag{69}$$

where

$$L_1(\beta) = \frac{4}{\beta}\sinh\frac{\beta}{2} - 2\,\cosh\frac{\beta}{2} + \frac{\beta}{2}\sinh\frac{\beta}{2} - (\theta^{-1}-1)u_l + \beta(\theta^{-1}-1)\frac{\partial u_l}{\partial \beta},$$

$$L_2(\beta) = \frac{4}{\beta}\sinh\frac{\beta}{2} - 2\,\cosh\frac{\beta}{2} - (\theta^{-1}-1)u_l. \tag{70}$$

Solution of this nonlinear ordinary differential equation provides β, and thus α, which can be used in the expressions for u and f for the flow rate.

This differential equation (69) can be cast into the form

$$\frac{d^2\phi^2}{d\xi^2} - 4\phi\frac{d^2\phi}{d\xi^2} + 2\left[1 - \frac{\frac{\beta}{2\theta}\sinh\frac{\beta}{2} + \beta(\theta^{-1}-1)\frac{\partial u_l}{\partial \beta}}{L_1(\beta)}\right]\left(\frac{d\phi}{d\xi}\right)^2 = 0. \tag{71}$$

By using the identities

$$\frac{d^2\phi^2}{d\xi^2} - 4\phi\frac{d^2\phi}{d\xi^2} = 2\left(\frac{d\phi}{d\xi}\right)^2 - 2\phi\frac{d^2\phi}{d\xi^2},$$

$$\frac{d}{d\xi}\frac{\phi}{\left(\frac{d\phi}{d\xi}\right)} = 1 - \left(\frac{d\phi}{d\xi}\right)^{-2}\phi\frac{d^2\phi}{d\xi^2}, \tag{72}$$

the differential equation may be put in a more convenient form

$$\frac{d}{d\xi}\frac{1}{\beta} = \mu - \frac{\mu}{2\theta}\beta\frac{\left[\sinh\frac{\beta}{2} + 2(1-\theta)\frac{\partial u_l}{\partial \beta}\right]}{L_1}, \tag{73}$$

which seems to be more readily amenable to approximate treatments.

IV. FLOW PROFILES

Since the differential equation for β is not analytically solvable in closed form, it must be treated numerically or in an approximation. Before resorting to a numerical treatment of the differential equation, we examine an approximation method for it. We will consider only the differential equation holding for the Langmuir boundary conditions, which is more general than the differential equation in the stick boundary conditions.

A. Approximate treatment of β

Before presenting flow characteristics computed with the numerical solutions of Eq. (69) or, equivalently, Eq. (73), we will consider an approximate solution of Eq. (73) and an approximate flow rate calculated therewith. We thereby gain considerable insights into the Knudsen number dependence of the flow rate and the physical and mathematical causes underlying the emergence of Knudsen minimum.

Since β is $O(\varepsilon)$ and ε is usually less than unity, it is reasonable to expand the numerator and the denominator on the right-hand side of the differential equation (73) in a series of β to obtain

$$\frac{\partial}{\partial \xi}\frac{1}{\beta} = \mu - 6\frac{\mu}{(3-\theta)}\frac{\left(1 + \frac{1}{24}\beta^2 + \cdots\right)}{\left[1 - \frac{3}{80}\left(\frac{5-\theta}{3-\theta}\right)\beta^2 + \cdots\right]}. \tag{74}$$

To the lowest order, this equation is approximated by

$$\frac{\partial}{\partial \xi}\frac{1}{\beta} = \mu - 6\frac{\mu}{(3-\theta)}. \tag{75}$$

This equation is easily integrated to the form

$$\frac{1}{\beta} = -\mu\left(\frac{3+\theta}{3-\theta}\right)\xi + C. \tag{76}$$

Therefore, the differential equation for the reduced pressure in this approximation is

$$\frac{d\ln\phi}{d\xi} = \frac{-\mu}{d - \mu\left(\frac{3+\theta}{3-\theta}\right)\xi}. \tag{77}$$

By integrating it again, we obtain

$$\phi = d_1\left[d - \mu\left(\frac{3+\theta}{3-\theta}\right)\xi\right]^{(3-\theta)/(3+\theta)}, \tag{78}$$

where d and d_1 are integration constants. They are determined by the boundary conditions on pressure at the entrance and exit of the channel:

$$d = \mu\left(\frac{3+\theta}{3-\theta}\right)\left[1 - \left(\frac{\phi_1}{\phi_0}\right)^{(3+\theta)/(3-\theta)}\right]^{-1},$$

$$d_1 = \phi_0\left[\mu\left(\frac{3+\theta}{3-\theta}\right)\right]^{-(3-\theta)/(3+\theta)}\left[1 - \left(\frac{\phi_1}{\phi_0}\right)^{(3+\theta)/(3-\theta)}\right]^{(3-\theta)/(3+\theta)}. \tag{79}$$

Finally, on substitution of d and d_1, the pressure distribution in the lowest order approximation is given by the formula

$$\phi = \phi_0\left\{1 - \left[1 - \left(\frac{\phi_1}{\phi_0}\right)^{(3+\theta)/(3-\theta)}\right]\xi\right\}^{(3-\theta)/(3+\theta)}. \tag{80}$$

From this result follows the expression for β in the same approximation:

$$\beta = \frac{1}{\mu}\left(\frac{3-\theta}{3+\theta}\right)\frac{\left[1 - \left(\frac{\phi_1}{\phi_0}\right)^{(3+\theta)/(3-\theta)}\right]}{1 - \left[1 - \left(\frac{\phi_1}{\phi_0}\right)^{(3+\theta)/(3-\theta)}\right]\xi},$$

which yields the value of β at the exit of the channel, namely, at $\xi=1$

$$\beta_1 = \frac{1}{\mu}\left(\frac{3-\theta}{3+\theta}\right)\left[\left(\frac{\phi_0}{\phi_1}\right)^{(3+\theta)/(3-\theta)} - 1\right]. \tag{81}$$

In this approximation we find

$$\beta_\infty = \frac{1}{\mu}\left(\frac{\phi_0}{\phi_1} - 1\right), \tag{82}$$

which verifies that β_∞ is independent of N_{Kn}. On use of the formula for θ given in Eq. (59), this form of β_1 may be written as

$$\beta_1 \equiv 2\beta_0\left[1 + \lambda\frac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}} + O(\lambda^2)\right], \tag{83}$$

where

$$\beta_0 = \frac{1}{2\mu}\ln\left(\frac{\phi_0}{\phi_1}\right), \quad \lambda = \frac{1}{2}\ln\left(\frac{\phi_0}{\phi_1}\right).$$

On substituting the formula for u (58) and performing an integration over ζ, we obtain the flow rate [41,42]

$$f = \frac{\phi_1}{\alpha\beta}\left[\cosh\frac{\beta}{2} - \frac{2}{\beta}\sinh\frac{\beta}{2} + c^* N_{Kn}^{\nu} u_l\right]. \tag{84}$$

By using the solution for β obtained from Eq. (69) this formula can be readily calculated at different values of N_{Kn}.

To gain an insight into the behavior of $f_1 = f(\beta_1)$ with respect to N_{Kn} we use the approximate formula β_1 for β. On setting

$$\alpha_1 \equiv \alpha(\xi = 1) \equiv \hat{\omega} N_{Kn} \tag{85}$$

and scaling the flow rate f_1 with constant factors independent of N_{Kn},

$$M_f = \frac{2\hat{\omega}\beta_0 f_1}{\phi_1}, \tag{86}$$

we find the scaled flow rate in the form

$$\begin{aligned} M_f = \frac{1}{N_{Kn}\left(1 + \lambda\dfrac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right)} \Bigg\{ & \cosh\ \beta_0\left(1 + \lambda\frac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right) \\ & - \frac{\sinh\ \beta_0\left(1 + \lambda\dfrac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right)}{\beta_0\left(1 + \lambda\dfrac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right)} \\ & + c^* N_{Kn}^{\nu}\cosh\ \beta_0\left(1 + \lambda\frac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right) \\ & - c^* N_{Kn}^{\upsilon}\cosh\left[\beta_0\left(1 + \lambda\frac{4 + 3c^* N_{Kn}^{\nu}}{2 + 3c^* N_{Kn}^{\nu}}\right)\right. \\ & \left.\times\left(\frac{1 + (\chi - 2)N_{Kn}}{1 + \chi N_{Kn}}\right)\right]\Bigg\}. \end{aligned} \tag{87}$$

If λ is small, it is possible to approximate this formula as follows:

$$\begin{aligned} M_f = \frac{1}{N_{Kn}}\Bigg\{ & \cosh\ \beta_0 - \frac{\sinh\ \beta_0}{\beta_0} + c^* N_{Kn}^{\nu}\cosh\ \beta_0 \\ & - c^* N_{Kn}^{\nu}\ \cosh\left[\beta_0\left(\frac{1 + (\chi - 2)N_{Kn}}{1 + \chi N_{Kn}}\right)\right]\Bigg\}. \end{aligned} \tag{88}$$

As $N_{Kn} \to 0$,

$$M_f \sim \frac{1}{N_{Kn}},$$

whereas as $N_{Kn} \to \infty$

$$M_f \sim c^{*2}\left[\cosh\ \beta_0 - \cosh\frac{(\chi - 2)}{\chi}\beta_0\right] N_{Kn}^{\delta}.$$

Since

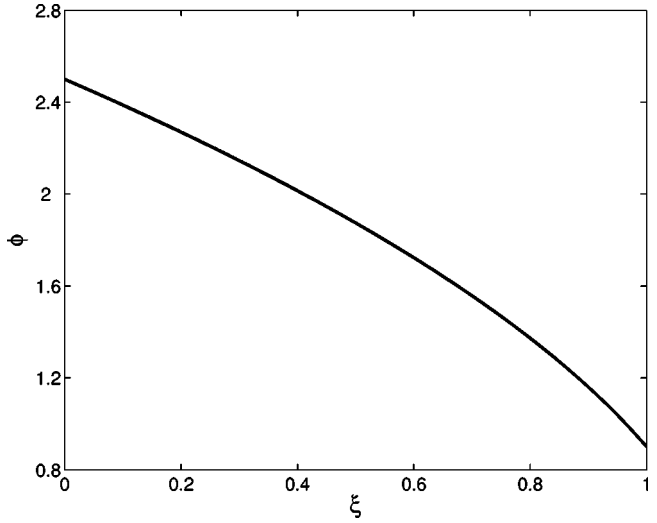

FIG. 1. Pressure distribution in the axial direction in the case of $\phi_0 = 2.5$, $\phi_e = 0.9$, $N_M = 0.1$, $N_{Kn} = 0.1$. Other parameters are: $\gamma = 5/3$, $\chi = 3$, $c^* = 2.0$, $\epsilon = 1/20$, $\delta = 0.25$.

$$\left(\frac{\chi - 2}{\chi}\right) < 1$$

we find the coefficient is positive and, therefore, M_f exhibits a minimum. This feature captures the experimentally observed [18] Knudsen number dependence of flow rate in an infinitely long circular tube. The Knudsen minimum was shown to follow from a generalized hydrodynamic theory [21] and to be responsible for laser-induced drift [22] of gas in a long thin tube observed experimentally [43]. The minimum occurs approximately at $N_{Kn} = 1$ for a suitably chosen set of parameters.

Such a minimum indeed occurs when Eq. (69) is solved numerically and the flow rate

$$f = \frac{2\hat{\omega}\beta_0 f(\beta(1))}{\phi_1} \tag{89}$$

is calculated with β so calculated, as will be shown presently.

B. Numerical solution for β and flow profiles

The longitudinal and transversal velocities, shear stress tensor, pressure distribution, and flow rate are calculated with the values numerically obtained for β from Eq. (73). In Fig. 1, the pressure distribution along the longitudinal direction is plotted in the case of parameters $N_{Kn} = 0.1$, $N_M = 0.5$, $\varepsilon = 1/20$, $\chi = 3$, $\delta = 0.25$, and $c^* = 2.0$. It is concave in qualitative agreement with experiment [44]. In Fig. 2, the reduced streamwise velocity profiles ($u_s = u/u^*$) are plotted for $N_{Kn} = 0.1$, 1.0, and 10 in the case of the same values taken for other parameters as for Fig. 1. The velocity is scaled by u^*, which is the integral of $u(\zeta)$ over $0 \leqslant \zeta \leqslant 1$, that is, the mean velocity with respect to ζ. The streamwise velocity exhibits a slip phenomenon developing from the entrance of the channel. As the Knudsen number increases, the profiles clearly get flatter, exhibiting the plug flow behavior in accordance

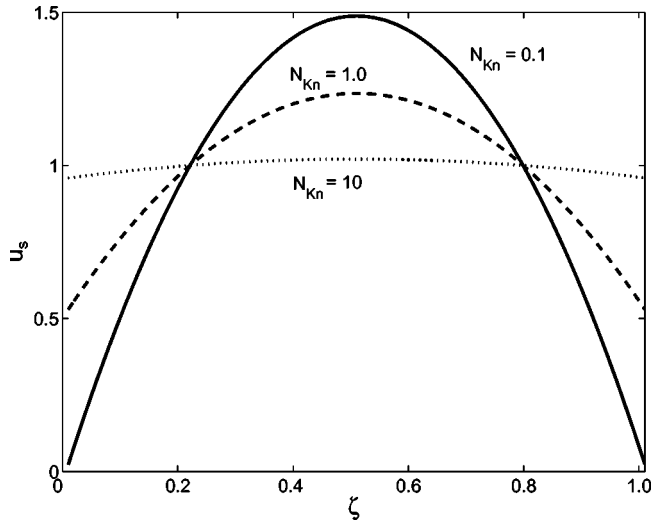

FIG. 2. Reduced streamwise velocity profile ($u_s = u/u^*$). The parameters except for N_{Kn} and c^* are the same as for Fig. 1. The solid curve is for $N_{Kn}=0.1$, $c^*=20$; the broken curve is for $N_{Kn}=1$, $c^*=2.5$; and the line with dots is for $N_{Kn}=10$, $c^*=0.25$. The velocities slip at the boundaries.

with the limiting behavior established in Eq. (60), and the velocity slip also increases with increasing N_{Kn}. The increasing velocity slip arises from the combination of the Langmuir boundary conditions and the nonlinear effect arising from the nonlinear constitutive equation for the stress tensor—or, alternatively put, the non-Newtonian viscosity, depending on density. The non-Newtonian viscosity arises because of the nonlinear factor $q(\kappa)$ in the stress evolution equation. We remark that the sliplike effect [24,25,45] in the velocity profile can occur because of the non-Newtonian viscosity even if the stick boundary conditions are used. The Langmuir boundary conditions simply contribute further to the slip already present in the velocity because of the nonlinear transport coefficient. Such a tendency is in agreement with the DSMC results [4] and the results by the numerical solutions of a linearized Boltzmann equation [37].

In Fig. 3 we show that the streamwise velocity profile (shown by the solid curve) u, calculated for $N_{Kn}=1$ with formula (58) and the numerical solutions of Eq. (73) are indeed in agreement with the results (open circles) by the empirical formula (Eq. (5.3) of Ref. [4]) devised by Karniadakis and Beskok (KB). Since Karniadakis and Beskok [4] have shown that when the parameter b_{KB} (b in their notation) in the KB formula for the slip boundary conditions is suitably chosen, the KB empirical formula for slip boundary conditions yields results in excellent agreement with the DSMC results and the profiles obtained with the BKG linearized kinetic equation [37], we compare our results with only those of Karniadakis and Beskok to avoid the clutter of data in the figure. Therefore, the predictions of the present theory are also seen to be in good agreement with the DSMC results, provided the parameter c^* is varied with N_{Kn}, indicated in Fig. 3. This suggests that this parameter c^* plays a role similar to the Karniadakis-Beskok parameter b_{KB} in Eq. (5.3) of Ref. [4] It should be noted that whereas the Karniadakis-Beskok velocity profile is an empirical formula, the velocity profile formula (58) is a solution of the generalized hydrodynamic equations subject to the Langmuir boundary conditions. Thus, the comparison made in Fig. 3 provides support for the utility of generalized hydrodynamic equations for the description of microflows.

In Figs. 4 and 5, the transversal velocity profile and the shear stress profile are presented in the case of parameters that are the same as for Fig. 1. The transversal velocity is odd

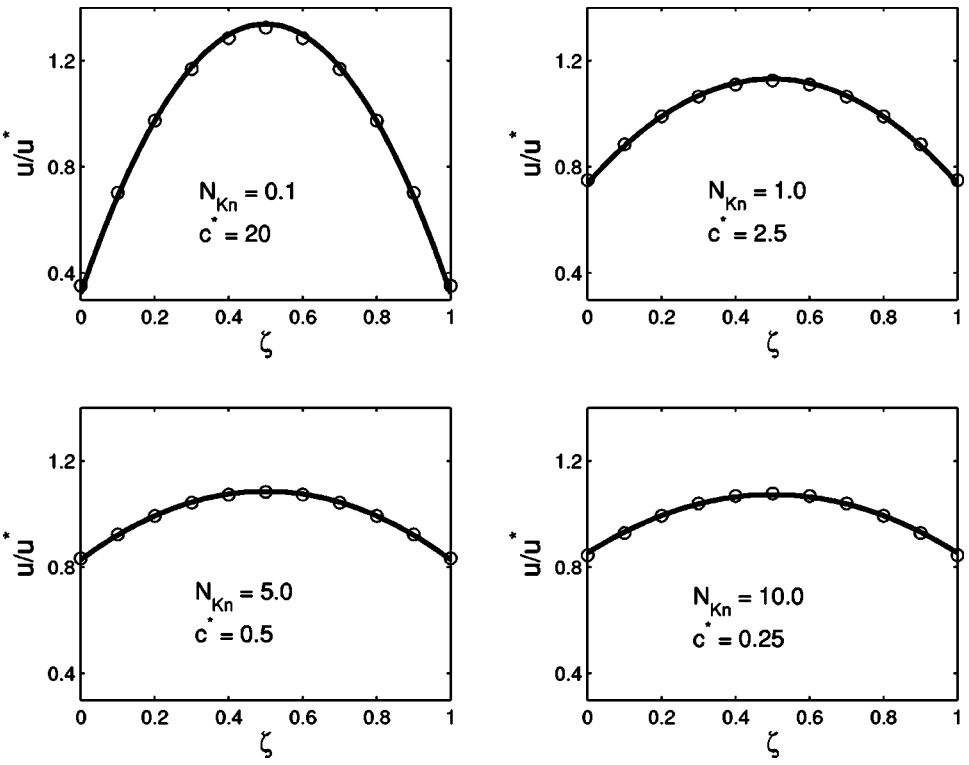

FIG. 3. Comparison of the streamwise velocity profile of the present theory and the prediction by the empirical formula by Karniadakis and Beskok {Eq. (5.3) of Ref. [4]} in the case of $N_{Kn}=0.1, 1.0, 5.0, 10.0$. The solid curve is the present theory predictions. The open circles representing the predictions by the Karniadakis-Beskok empirical formula with the Karniadakis–Beskok parameter $b_{KB}=-1$ is not distinguishable from the present theory results.

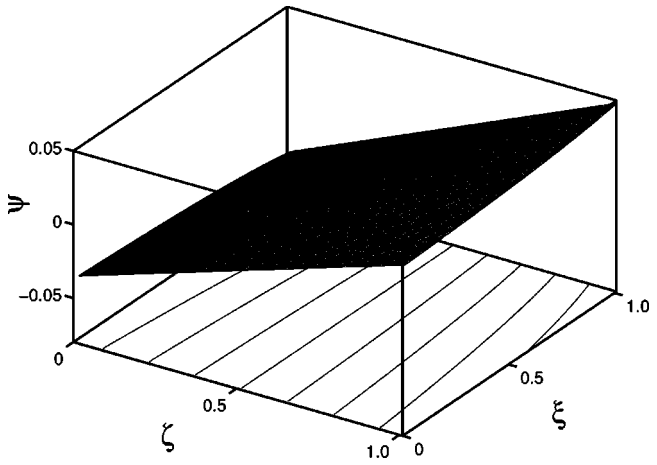

FIG. 4. The transversal velocity profile, with the same parameters as for Fig. 1.

with respect to the transversal coordinate $z=\zeta-1/2$ as predicted by the equation for v. The shear stress profiles shown in Fig. 5 clearly change linearly. It is interesting to see that the shear stress is linear with respect to ζ in the present flow configuration even if the viscosity is non-Newtonian. We remark that this is a peculiar feature of the rectangular flow configuration in the absence of the normal stress differences. If the normal stress differences are nonvanishing, the shear stress is not expected to be a linear function of ζ according to the studies [24,25] on macroflows.

In microflows, the Knudsen effect manifests itself in the flow rate, and it is known empirically that there exists a minimum in flow rate plotted against N_{Kn}. As we have shown by means of an approximate but analytic solution, there is indeed a minimum in the flow rate versus N_{Kn}. It is shown in Fig. 6 where the flow rates f for values of $\delta=0.25$ and 0.5 and for $c^*=10$ are plotted against N_{Kn} for the same values of the other parameters as used for Fig. 1. The N_{Kn} dependence of f clearly indicates the limiting behaviors exhibited by M_f calculated with the approximate solution for β as shown earlier, and the flow rate f for the parameter values chosen has

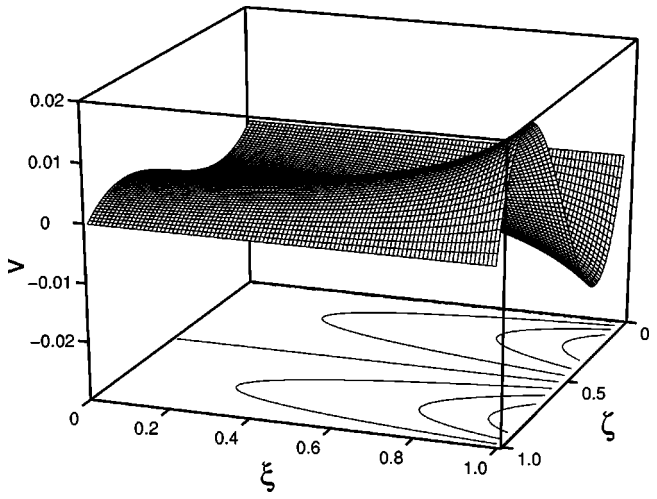

FIG. 5. The shear stress profile, with the same parameters as for Fig. 1.

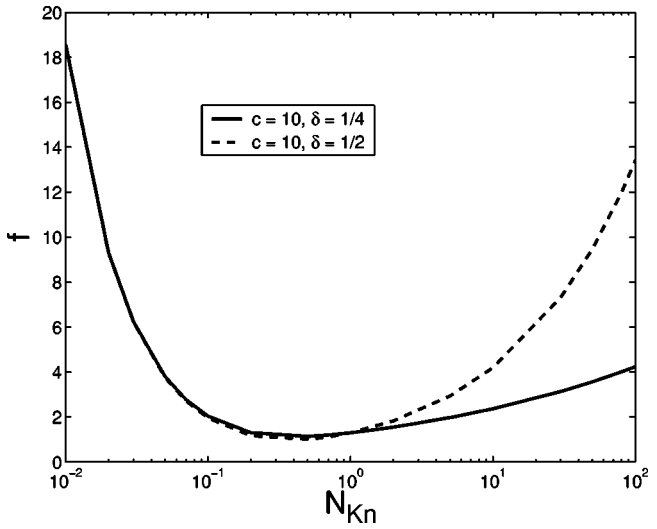

FIG. 6. The Knudsen number dependence of flow rate f. The parameters are the same as for Fig. 1, except for the Knudsen number treated as an independent variable. The exponent δ is treated as an empirical parameter for this figure. The values of δ are: $\delta=0.25, 0.5$. If $d>0$ there appears a minimum in the flow rate around $N_{Kn}\simeq 1$. The asymptotic behavior of the flow rate is fairly sensitive to the coverage exponent δ, which reflects the surface roughness and interactions between the surface and the gas.

a minimum around $N_{Kn}\simeq 1$, as shown by DSMC simulations [7–9]. The appearance of a minimum in the flow rate as pressure or the Knudsen number changes is a hallmark of rarefied gas flows, which were originally discovered by Knudsen [18,19] in the case of an infinite tube flow. The flow rate increases in the high Knudsen number regime past the minimum because the flow tends to be ballistic as the gas rarefies and the mean-free path becomes comparable with, or larger than, the channel width. We have had a glimpse of how this situation arises when we have examined the limiting behavior of the streamwise velocity in Eq. (60), which shows a plug flow profile indicating that the flow is axially ballistic. The Langmuir boundary conditions resulting in a slip behavior of the flow play an important role in producing such a ballistic flow behavior. The flow rate shown in Fig. 6 indicates that the generalized hydrodynamics model, with Langmuir boundary conditions presented in this work, captures the most important of the features of microflows observed experimentally or in the DSMC simulations. This feature is a product of interplay between the nonlinear transport process, namely, non-Newtonian viscosity, and the Langmuir boundary conditions. The curve depends on the value of the exponent δ, which we consider to be an empirical measure of the multiplicity of layer covering the surface. Thus, the parameter is an indication that the sites are covered by more than one layer of gas molecules. Nevertheless, the Langmuir boundary conditions and the gas-surface interactions in the context of microflows need further study in depth, but the present model indicates such study should be useful and worthwhile for a better understanding of microflows. The point we would like to make here is that the flow profiles in microchannels are products of a combination of the nonlinear constitutive equation—a non-Newtonian law of

viscosity—and Langmuir boundary conditions, which are an effect of the surface on the flow.

Equation (38) for ϕ and its solution (43) indicate that ϕ is independent of the transversal position ζ. Therefore, since the temperature is uniform in the channel, the transversal density distribution is uniform by virtue of the ideal gas equation of state, perhaps, except in the Langmuir boundary layers. The thickness of the Langmuir boundary layers consistent with the velocity profile is

$$\Delta\zeta = N_{Kn}/(1 + \chi N_{Kn}).$$

This means that in the midportion of the channel, excluding $\Delta\zeta$ near the walls, the density distribution is uniform as predicted by $\rho = p/k_B T$. In the Langmuir layers the density is given by the equilibrium value, determined by the bulk density minus the adsorbed portion of the gas as determined by the Langmuir isotherm at the given temperature.

It is interesting that even a gas exhibits a non-Newtonian behavior as it rarefies sufficiently, so that the Knudsen number becomes large. The present model suggests that the non-Newtonian viscosity η depends on density in the manner

$$\eta \sim n \ln n^{-1} \sim N_{Kn}^{-1} \ln N_{Kn}, \tag{90}$$

as n decreases to the rarefied regime or N_{Kn} increases beyond unity.

V. CONCLUDING REMARKS

In this paper, we have presented a generalized hydrodynamics model for microchannel flows, which captures the important features of microflows experimentally observed. The model combines the generalized hydrodynamics and the Langmuir boundary conditions. In the case of macroflows, the former is known to be capable of describing flows far removed from equilibrium. For example, the generalized hydrodynamic equations have been shown to account for macroscopic flows of rarefied gases [24,25,46], shock wave structures of monatomic [47] and diatomic [48] gases, and ultrasonic dispersion and absorption of di-atomic gases [49]. Since the generalized hydrodynamics reduce to the classical NSF theory in the limit of very small N_δ, the model is inclusive of the NSF theory, which has usually been employed for the description of microflows [1,5] in the transient regime of flow with the help of slip boundary conditions. The Langmuir boundary conditions take into account the important surface-fluid interactions by using a model closely resembling the original adsorption theory of Langmuir [10]. Therefore, the present model improves the NSF-Langmuir boundary condition model of Myong [35] in the two aspects that the generalized hydrodynamics equations are used and the Langmuir boundary conditions proposed in Refs. [14,26,35] are modified, so as to account for multiple adsorption of molecules at an adsorption site on the surface. Such a multiple adsorption model does not appear to be farfetched considering the roughness of boundary surfaces in a micrometer scale as observed by Harley *et al.* [36]. In surface science, such rough surfaces are known to provide sites for multiple adsorption of molecules. The accommodation coefficients in the NSF theory approach, taken by various authors in microflows [1,4], remain as adjustable parameters until they are calculated by means of a suitable surface-gas molecule interaction model, whereas the coverage parameter θ used in this work is explicitly computable by means of statistical mechanics. This is an important theoretical difference between the two approaches with regard to the boundary conditions.

The necessity of taking the surface-fluid molecule interactions into account in the description of microflows calls for broadening the scope of purely fluid dynamic modes of thinking into the realm of the surface-molecule scattering theory, which is also a many-body problem, but not in the sense of the molecular theory description required of fluid dynamic flows of matter. The surface-molecule scattering phenomena are what may be justifiably called few-body dynamics problems at the molecular level of description, which require the quantum mechanics of a few particles involved. Therefore, in this work it is suggested that microflows may be described by combining two divergent viewpoints toward flows of matter into a single harmonized theory, namely, a combination of a continuum mechanics theory in the form of generalized hydrodynamics appropriate for fluids far removed from equilibrium and the Langmuir boundary conditions that can describe the surface-molecule interactions on the basis of few-body dynamics using quantum-mechanical methods. The same remark probably applies to nanoflows in systems of nanoscales. We believe that the present approach of separating the two basic aspects is simpler than the Maxwell slip boundary condition approach where two aspects are inextricably meshed up in a continuum theory of flows. It is also easier in the present approach to implement the quantum-mechanical calculation required for boundary conditions on the basis of surface-gas molecule interactions. The present theory is aimed at contributing toward a fuller theoretical understanding of the fascinating subjects of flows in small scales. A great deal of work remains to be done in connection with the boundary conditions, taking into account the surface-fluid molecule interactions and their effects on flows in microsystems and nanosystems, as well as applications of the present generalized hydrodynamic theory.

For lack of experimental data on flow profiles in microchannels, we have been able to compare the results of the present theory with either DSMC results or the results predicted by the Boltzmann equation. Recent developments [50,51] in particle image velocimetry will hopefully be able to provide the desired experimental data that will enable us to make a comparison of the prediction by the theory with laboratory experiments.

The present theory can be applied to nonhard sphere gases. Since there are some simulation results [52] for density and velocity profiles available for a large Knudsen number flow in the Lennard-Jones gas, it would be useful to investigate such a case, but it is not done here for lack of the

viscosity data for the Lennard-Jones fluids that are necessary for the present line of theory.

ACKNOWLEDGMENTS

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