Electrokinetic flows in a microdomain

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The discrete kinetic approach and diffuse-reflection type boundary conditions are adopted to solve the transport problem for many charged particles flowing along a microslab (or channel of a wide constriction within a confined slender microdomain). The preliminary results show that there are selected orientations related to the nontrivial velocity-slip fields for a range of Knudsen numbers if there is a nonboundary-driven forcing along the streamwise direction. As the Knudsen number increases, the value of this selected orientation decreases and the cross-stream velocity profile becomes relatively flat. Our results qualitatively resemble those reported by Burgreen and Nakache or Paul *et al.*

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I. INTRODUCTION

Investigation of electrokinetically driven flows could be dated back to early 1920s [1] (Debye and Hückel). In fact, Reuss discovered that, in 1808, flow through capillary elements can be induced by the application of an electric field. Later on, Wiedermann (say, 1852), Quinke (1859), Helmholtz (1879), Smoluchowski (1903), Freundlich (1909), and Gouy (1910) put forward the subsequent progresses in this field. The ionic distribution in solutions of low ionic energy was determined in Ref. [1] by means of a linear simplification of the exponential Boltzmann ion energy distribution. Later contributions could be traced in Ref. [2]. Interests are mostly focused on the macroscopic flow field.

Meanwhile, the one-dimensional long-time transport of dilute charges in a semiconductor had been investigated by the continuous kinetic theory [3], which excluded the shortrange interactions between charges. This problem was formulated in a classical picture of the electronic gas by particle collisions and any quantum effects (say, the Pauli exclusion principle) were not taken into account. They actually only considered the quasiparticles [3]. Meanwhile, similar (stationary state) problems for many neutral particles flowing in microdomains were successfully studied by the discrete kinetic theory [4]. To study the case of many charged particles where the body force or the action of the electric field is of paramount importance, we shall apply our verified approaches reported before [4] to this problem, especially in microscopic view. Considering a flow of a gas of interacting (charged) particles through a wide constriction in a onedimensional channel of which this sort is a common part of modern semiconductor devices, the quantum effects might be neglected (a complication, which is important for all realistic devices, is that when the wavelength of electrons is comparable with the width of constriction, then quantum mechanics should be used).

Note that, motion of two neutral molecules in a specularly reflecting box has been analyzed for two-dimensional (2D) case and the system of these two molecules were shown to be as chaotic [5]. Similar problems related to elastic reflection with certain boundaries had been raised by Sinai since early 1970s [6]. For a number of particles, if there are no interaction forces in between, the collisions (say, binary

only) between particles are complicated enough so that deterministic description of their motion is essentially difficult, boundary effects excluded. One problem is the determination of the stationary state (still away from equilibrium) once a well-defined entropy concept could be utilized. Recent attempts, for example, are to use dynamical ensembles for many particle systems [7].

Although some of the basic problems (many neutral or charged particles flowing hydrodynamically within confined simple geometry) could be *ad hoc* solved for the cases of hard-sphere gases by semianalytic ways (partly using numerical integration after asymptotic expansions), most of them were investigated by carrying out computer simulations, either the Monte Carlo or molecular dynamics methods. The difficulty lie in the mathematical treatments of the nonlinear Boltzmann equation (which treats the motion of dilute particles rather well and is in both partial-differential and integral forms) with the associated physical boundary conditions. Due to the mathematical complexity of the collision integral, it is a very hard task to obtain explicit results, especially for states far from equilibrium.

As far as the author knows, even the molecular dynamics or the Monte Carlo methods can obtain *ad hoc* satisfactory results for this problem with larger collision frequency or rarefaction parameter (which corresponds to larger Knudsen number K_n , defined as the mean-free path of the gases divided by the characteristic length of the physical problem). The computational cost is still too large. One of the reasons is that till now we only have the (limited) equilibrium state as the starting point or reference state for physical or mathematical problems [3–8]. But the clues given by the equilibrium state to the solving of the evolutional or nonequilibrium (even a little far from equilibrium) state, e.g., the stationary or steady flow (nonboundary-driven flow), which is reached when the external constant forcing is locally balanced by the dissipative wall shear, are very limited.

In this paper, we plan to investigate the above-mentioned issues (which should be resolved, as the problems related to a number of charged particles that are driven by nonboundary forcing flowing in microdomains will be common in early 2000s [9]) by the verified discrete kinetic model [4,10–12]. This model was well developed and applied to many mathematical and physical problems since 1960s [10–12]. The main idea of this approach is to use a set of finite (or discrete) velocities (of particles) instead of continuous ones in the kinetic theory but to keep the space continuous without discretization. We thus can simplify the solving procedures for the test-case problems without touching the essential mathematical and physical difficulties. The boundary conditions we shall use are the discrete type of the diffuse reflection conditions [13]. The verifications of this model for many neutral particles have been done by comparison with previous experiments and/or other theoretical/numerical works [4,10-12]. We will focus on these results: preferred orientations selected from a set of limited admissible collisions for many charged particles driven by a nonboundary unit forcing finally reaching into a stationary state [4,14]. These kinds of Knudsen-number-dependent orientations for nonboundary-driven many-charged particles system have seldom been reported before [4,12]. Our preliminary results using a semiclassical approach show that as the mean-free path or Knudsen number increases, the value of this selected orientation decreases and the cross-stream velocity profile becomes relatively flat. Our results resemble qualitatively those electrokinetic flows reported by Paul, Garguilo, and Rakestraw, [2,15].

II. DISCRETE KINETIC FORMULATIONS

A. Discrete velocity models

Considering a simple monatomic gas of particles with mass *m* and cross-sectional area σ , the first step of the modeling procedures consists in discretizing the velocity directions in a finite number of unit vectors \mathbf{i}_k , $k=1,\ldots,p$. One or more moduli are then associated to each direction. The ratio of the moduli has, however, to be properly chosen, so that collisions between particles with different velocity moduli are possible. For one velocity moduli case, $\mathbf{u}_i = c \mathbf{i}_k$, $k=1,\ldots,p$; $c \equiv c(\mathbf{x},t)$, in general. Normally *c* is determined by the equilibrium distribution.

The charged particles (hard-sphere) move in the whole space and collide by simple elastic collisions locally in space. The mathematical model is an evolutional equation for the number densities $N_i(\mathbf{x},t)$ linked to the finite set of velocities \mathbf{u}_i . We write a balance equation for the number density of particles *i* in the form

$$\left[\frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla + \boldsymbol{\gamma} \cdot \frac{\partial}{\partial \mathbf{u}_i}\right] N_i = G_i - L_i, \quad \text{here } \nabla \equiv \frac{\partial}{\partial \mathbf{x}},$$

where $\gamma = e \mathbf{E}/m$ (a vector quantity), *e* is the electric charge of a carrier, *m* is its mass, **E** is a constant electric field here

[3]; L_i and G_i are the loss and the gain of the particles *i* due to collisions. In case of binary collisions an exact balance may be obtained, and is expressed with the transitional probabilities and the number densities. This model has the structure of a system of semilinear partial differential equations of hyperbolic type. The above equation could also be written as

$$\frac{\partial}{\partial t} N_i + \mathbf{u}_i \cdot \nabla N_i + \gamma \cdot \frac{\partial}{\partial \mathbf{u}_i} N_i$$
$$= \sum_{r=2}^R \sum_{I_r \in E_r} \sum_{J_r \in E_r} \delta(i, J_r, I_r) A_{I_r}^{J_r} N_{I_r}$$

where $i=1,\ldots,p$; here, by definition, an *r* collision ($r \ge 2$) involves *r* particles. $I_r = (i_1,\ldots,i_r)$, and $J_r = (j_1,\ldots,j_r)$ are two elements of E_r , which is the set of *r* not arranged numbers (considering the combinations instead of the order they appear) taken in the set $\{1,\ldots,p\}$.

A "transitional" probability denoted by $A_{I_r}^{J_r}$ is associated to each *r* collision $I_r \rightarrow J_r$. In the case of binary collisions, this term (also is called as the *transition rates*) is referred to the collisions $(\mathbf{u}_i, \mathbf{u}_j) \leftrightarrow (\mathbf{u}_k, \mathbf{u}_l)$, $i, j, k, l = 1, \ldots, p$; and the number of paired outputs corresponding to a given paired input is denoted by q. N_{I_r} denotes the product $N_{i_1}N_{i_2} \cdots N_{i_r}$. $\delta(i, J_r, I_r) = \delta(i, J_r) - \delta(i, I_r)$ is the algebraic number of particles *i* created through the collision $I_r \rightarrow J_r$. $\delta(i, I_r)$ is (positive or zero) the number of indices *i* present in the *r* set. If only nonlinear binary collisions are considered, considering the evolution of N_i , we have

$$\frac{\partial N_i}{\partial t} + \mathbf{u}_i \cdot \nabla N_i + \boldsymbol{\gamma} \cdot \frac{\partial}{\partial \mathbf{u}_i} N_i$$
$$= \sum_{j=1}^p \sum_{(k,l)} \left(A_{kl}^{ij} N_k N_l - A_{ij}^{kl} N_i N_j \right), \quad i = 1, \dots, p,$$

where (k,l) are admissible sets of collisions. We may then define the right-hand side of above equation as

$$Q_{i}(N) = \frac{1}{2} \sum_{j,k,l} (A_{kl}^{ij} N_{k} N_{l} - A_{ij}^{kl} N_{i} N_{j}),$$

with $i \in \Lambda = \{1, \dots, p\}$, and the summation is taken over all $j, k, l \in \Lambda$, where A_{kl}^{ij} are non-negative constants satisfying

 $A_{kl}^{ji} = A_{kl}^{ij} = A_{lk}^{ij}$, indistinguishability of the particles in collision,

 $A_{kl}^{ij}(\mathbf{u}_i + \mathbf{u}_j - \mathbf{u}_k - \mathbf{u}_l) = 0$, conservation of momentum in the collision,

$$A_{kl}^{ij} = A_{ij}^{kl}$$
, microreversibility condition.

The conditions defined for the discrete velocity above require that elastic, binary collisions, such that momentum and energy are preserved, $\mathbf{u}_i + \mathbf{u}_j = \mathbf{u}_k + \mathbf{u}_l$, $|\mathbf{u}_i|^2 + |\mathbf{u}_j|^2 = |\mathbf{u}_k|^2 + |\mathbf{u}_j|^2$, are possible for $1 \le i, j, k, l \le p$.

The collision operator is now simply obtained by joining A_{ij}^{kl} to the corresponding transition probability densities a_{ij}^{kl} through $A_{ii}^{kl} = S |\mathbf{u}_i - \mathbf{u}_i| a_{ii}^{kl}$, where,

$$a_{ij}^{kl} \ge 0, \sum_{k,l=1}^{p} a_{ij}^{kl} = 1, \forall i,j=1,\ldots,p,$$

with *S* being the effective collisional cross section. If all q (p=2q) outputs are assumed to be equally probable, then $a_{ij}^{kl} = 1/q$ for all *k* and *l*, otherwise $a_{ij}^{kl} = 0$.

The term $S|\mathbf{u}_i - \mathbf{u}_j|dt$ is the volume spanned by the particle with \mathbf{u}_i in the relative motion w.r.t. the particle with \mathbf{u}_j in the time interval dt. Therefore, $S|\mathbf{u}_i - \mathbf{u}_j|N_j$ is the number of j particles involved by the collision in unit time.

Collisions which satisfy the conservation and reversibility conditions which have been stated above are defined as *admissible collision*.

The discrete kinetic equations [4,10-12] then assume the following form:

$$\frac{\partial N_i}{\partial t} + u_{i_x} \frac{\partial N_i}{\partial x} + u_{i_y} \frac{\partial N_i}{\partial y} + \gamma_x \frac{\partial N_i}{\partial u_{i_x}} + \gamma_y \frac{\partial N_i}{\partial u_{i_y}}$$

$$= \frac{2cS}{q} \sum_{\substack{j=1\\j \neq i}}^{q} (N_j N_{j+q} - N_i N_{i+q}) \quad \text{or}$$

$$= \frac{2cS}{q} \sum_{l=1}^{q-1} (N_{i+l} N_{i+l+q} - N_i N_{i+q}), \quad i = 1, \dots, 2q,$$
(1)

where $u_{i_x} = c \cos[\theta + (i-1)\pi/q]$, $u_{i_y} = c \sin[\theta + (i-1)\pi/q]$, θ is the orientation starting from the positive *x* axis to the u_1 direction, where $N_i = N_{i+2q}$ are unknown functions, and *c* is a reference velocity modulus.

According to Refs. [10–12], for the 2*q*-velocity model, that is, $q \ge 3$, there are more *collision invariants* than the physical ones or conservation laws, which correspond to the number of macroscopic variables (in 2D, they are only four, i.e., one mass, two momenta, one energy). That is to say, there are *spurious* invariants or macroscopic variables for $q \ge 3$ models. These models have been verified in Refs. [4,10–12] by checking the thermodynamics or equilibrium state of q=2,3,4 models.

B. Boundary conditions

People normally use purely diffuse-reflection boundary conditions [3,4,11-13], which means properties of the reflected particles are independent of their properties before the impact, for this problem. In other words, the reemitted stream has completely lost its memory of the incoming stream, except for the conservation of the number of particles. Moreover, we impose the following conditions: The

gases are in equilibrium with the wall ("the wall locally behaves as a thermostat," i.e., the gases reflect after they have been in thermodynamic equilibrium with the wall temperature) satisfies $N_i(\mathbf{r},t) = \gamma_i(\mathbf{r},t)N_{wi}(\mathbf{r},t)$, where γ_i expresses the accomodation of the discrete gas to the wall quantities, and N_{wi} is the discrete equilibrium densities for the *i*-direction set of particles; that is, we have

$$|\mathbf{u}_{j} \cdot \mathbf{n}| N_{wj} = \sum_{i \in I} B_{ij} |\mathbf{u}_{i} \cdot \mathbf{n}| N_{wi}, \quad j \in R, \quad B_{ij} \ge 0,$$
$$\sum_{j \in R} B_{ij} = 1, \tag{2}$$

with $I = \{i, (\mathbf{u}_j - \mathbf{u}_w) \cdot \mathbf{n} < 0\}$ related to the impinging set of particles, $R = \{j, (\mathbf{u}_j - \mathbf{u}_w) \cdot \mathbf{n} > 0\}$ related to the emerging set of particles, **n** is the outer normal, \mathbf{u}_w is the wall velocity.

C. Derivation of the governing equation

Now, for the four-velocity model we use here, $u_1 = c(\alpha, \beta)$, $u_2 = c(-\beta, \alpha)$, $u_3 = -c(\alpha, \beta)$, $u_4 = c(\beta, -\alpha)$, $\alpha = \cos(\theta)$, $\beta = \sin(\theta)$; θ is the angle between the *x* axis and the u_1 direction, *c* is the reference velocity modulus [4,10–12]. To obtain the macroscopically hydrodynamical field, which is useful for comparison with previous experimental data, we let $n = N_1 + N_2 + N_3 + N_4$, $nu = c(\alpha N_1 - \beta N_2 - \alpha N_3 + \beta N_4)$, $nv = c(\beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4)$, which are the total number density, the *x*- and *y*-direction momentum flux (per unit mass), respectively. *u* and *v* are then the *x*- and *y*-direction mean velocities; $\rho = n m$ is the macroscopic density, where *m* is the mass of the particle.

Based on the system of four equations obtained from Eq. (1) and these macroscopic variables, we can use linear combinations of these equations, purely algebraic manipulations, to derive the final governing equations we want to solve. First, let $R = S(N_2N_4 - N_1N_3)$, or $\overline{R} = (n_2n_4 - n_1n_3)$, where $n_i = N_i/n_0$, and then use nondimensional variables

$$U = u/c_0, V = v/c_0, Y = y/d,$$

where *d* is the channel width, n_0 is related to the total discrete number density and will be defined below, c_0 could be related to a referenced nonboundary-driven forcing speed [4,14]. We can obtain

$$\left(\sin\theta \pm \frac{\cos\theta}{m^2}\right)\frac{\partial N_1}{\partial y} = R, \quad \left(\cos\theta \mp \frac{\sin\theta}{m^2}\right)\frac{\partial N_2}{\partial y} = R,$$
(3)

$$-\left(\sin\theta\pm\frac{\cos\theta}{m^2}\right)\frac{\partial N_3}{\partial y}=R, \quad -\left(\cos\theta\pm\frac{\sin\theta}{m^2}\right)\frac{\partial N_4}{\partial y}=R,$$
(4)

by adopting the change of variables technique reported in Ref. [3] (by Baranger and Wilkins). Here, the first sign is selected for the positive-charge carrier in the second term of the left-hand side of Eqs. (3) and (4). Note that the derivation of the second term in above equations is based on the assumption that γ_x is not a constant (cf. [3] for the 14th reference set by Baranger and Wilkins).

We look for a solution depending on y (the cross-stream direction) only, i.e., the case of many charged particles flowing hydrodynamically only along x direction (confined in a slender channel) with $\gamma_y=0$, and γ_x equals to constant γ_0 . The system of equations above can thus be simplified to

$$\frac{\partial N_1}{\partial y} = \frac{R}{\beta}, \quad \frac{\partial N_2}{\partial y} = -\frac{R}{\alpha}, \quad \frac{\partial N_3}{\partial y} = -\frac{R}{\beta}, \quad \frac{\partial N_4}{\partial y} = \frac{R}{\alpha}, \quad (5)$$

or

$$\frac{\partial n_1}{\partial Y} = \frac{\bar{R}}{\beta K_n}, \quad \frac{\partial n_2}{\partial Y} = -\frac{\bar{R}}{\alpha K_n}, \quad \frac{\partial n_3}{\partial Y} = -\frac{\bar{R}}{\beta K_n},$$
$$\frac{\partial n_4}{\partial Y} = \frac{\bar{R}}{\alpha K_n}, \tag{6}$$

where the Knudsen number $K_n = 1/(dSn_0)$. After using linear combinations, we have

$$\frac{\partial n/n_0}{\partial Y} = 0$$
 and $\frac{\partial (nu/c)}{\partial y} = \frac{2}{\alpha\beta}R.$ (7)

As $U = cn_0(\alpha n_1 - \beta n_2 - \alpha n_3 + \beta n_4)/(nc_0)$, so we also have

$$\frac{nc_0}{cn_0}\frac{\partial U}{\partial Y} = \frac{2}{K_n \alpha \beta} \overline{R} = \frac{2}{\alpha}\frac{\partial n_1}{\partial Y} = \frac{2}{\beta}\frac{\partial n_4}{\partial Y}$$
$$= -\frac{2}{\beta}\frac{\partial n_2}{\partial Y} = -\frac{2}{\alpha}\frac{\partial n_3}{\partial Y}.$$
(8)

Integrating the above equation we obtain

$$2n_1 = AU + K_1, \quad 2n_4 = BU + K_4,$$

$$2n_2 = -BU + K_2, \quad 2n_3 = -AU + K_3, \quad (9)$$

where $A = \alpha (nc_0)/(cn_0)$ and $B = \beta (nc_0)/(cn_0)$. When the reference state is selected as the fully developed state (a stationary state with balancing between externally nonboundary-driven unit forcing and dissipations due to confined boundaries [4]), or $n = n_0$, $c = c_0$, then we obtain $A = \alpha$, $B = \beta$.

As for the general boundary conditions [13], we use the idea that the number density $N_i = N_{wall}|_i$ (the equilibrium-state density) at the wall for i = 1,2,3,4, which means molecules are in equilibrium with the boundary just before they reemit from the confined boundary, e.g., the wall. The derivations of these kinds of equilibrium density can be found in Refs. [11,12].

The diffuse-reflection boundary condition [3,4,12,13] along one boundary becomes

$$N_{w2}N_1 = N_{w1}N_2, \quad \beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4 = 0, \quad (10)$$

which means (i) the equilibrium state at the wall dominates, (ii) no penetration occurs across the wall. The equilibrium densities N_{wi} at the wall, as derived in Ref. [11], are

$$N_{wi} = (n/4) \{ 1 + (2/c^2) \mathbf{u}_{\mathbf{w}} \cdot \mathbf{u}_i + (-1)^i \\ \times [(\mathbf{u}_w \cdot \mathbf{u}_2)^2 - (\mathbf{u}_w \cdot \mathbf{u}_1)^2] (1/c^4) \}.$$
(11)

From these boundary conditions, with V=0, i.e., $\beta(n_1 - n_3) = \alpha(n_4 - n_2)$, and $n=n_1+n_2+n_3+n_4=1$, we thus get $K_1=K_3$, $K_2=K_4$, $K_1+K_2=1$ and

$$\frac{dU}{dY} = \frac{\alpha^2 - \beta^2}{2K_n \alpha \beta} \left(u^2 - \frac{K_1 - K_2}{\alpha^2 - \beta^2} \right), \quad \alpha \neq \beta, \quad \alpha \beta \neq 0.$$
(12)

D. Semianalytic solutions

Assuming the symmetry principle holds for this kind of nonboundary-driven flow, the remaining boundary conditions are

$$\frac{dU(0)}{dY} = 0, \quad U(Y = 1/2) = U_s = \frac{2K_2 - 1}{\alpha + \beta},$$

where U_s is the velocity slip at the wall, the latter comes from Eqs. (2) and (10) [4]. U_{wall} equals to zero here.

After direct integration of ordinary differential equation (10), we obtain one family of solutions for certain α , β , K_n ; α , β being strongly linked to maximum admissible orientations (θ), (whereas the minimum θ corresponds to $U_s = 0$, which is a trivial solution)

$$U = G \tanh(C - G KY), \tag{13}$$

where

$$G = \left(\frac{2K_1 - 1}{\alpha^2 - \beta^2}\right)^{1/2}, \quad K = \frac{\alpha^2 - \beta^2}{2\alpha\beta K_n}$$

where C depends on the specific gas-surface interface.

The principle to fix θ from a nonlinear ordinary differential equation subjected to implicit boundary conditions [3,4,13] is similar to that adopted in Ref. [16]. Because of the universality of $C(\theta, \text{ too})$ for general gas-solid interactions, specific and physical test case should be adopted here. Once we have the test case of a nonboundary-driven flow, for instance, we take those data (trend of current density vs K_n) in Ref. [3] into consideration since their continuous kinetic approaches considering a kind of nonboundary-driven electrongas flows could be a guideline for our macroscopic velocity field. For example, C could be fixed once the specific gas and the solid boundary (walls) are known.

III. RESULTS AND DISCUSSION

Equation (13) gives us nontrivial macroscopic velocity fields corresponding to a range of admissible orientations (θ) based on the four-velocity model for admissible collisions: {1,3} to {2,4} and confined (slab-wall) boundary conditions. But, we still have no clear idea how many charged particles



FIG. 1. Velocity fields U for different Knudsen numbers K_n in full-width (d) channel. U, Y, and K_n are dimensionless. Y = y/d. $K_n = 1/(dSn)$, n is the number density, S is the effective collision cross section. (Please cf. Ref. [2] for qualitative comparison with our smaller K_n cases.)

can be organized and flow into a stationary state [5,6] within a slender confined channel since there are no quantitative measurements up to now, to the best of knowledge of the authors. In essence, there should be field effects in between for the many-body problem of charged particles during their encounters. We adopt the hard-sphere gas assumption here and neglect the potential (force) contribution in the collision sum (or integral) in Eq. (1) [8,11,12]. It seems the field effect (repulsive forces between like-charge particles) will enlarge the mean-free path compared to that of many neutral particles during collisions. However, there will be screening effects even they are possibly minor.

To fit our interests here, we present velocity fields for smaller and larger mean-free path or K_n relevant to the range of those nontrivial or maximum admissible orientations (θ) that can produce physically verified velocity fields. Maxima of K_i are set to one and C is fixed for all results presented here. Results show that the maximum admissible θ will decrease once K_n increases. For instance, the maximum admissible θ equals to 0.1768, 0.0996, and 0.0562 for K_n = 0.5,1.0,2.0, respectively. This observation resembles that of many neutral particles [4]. These selected orientations for many charged particles subjected to hard-sphere collisions may also be due to the nonlinear coupling between the nonboundary-driven forcing and the confined boundary once the entropy selected favors for the final stationary state [7,13,16].

We plot the velocity profile U vs Y for different Knudsen numbers (K_n =0.05, 0.1, 0.15, 0.2, 0.25, 0.5, 1.0, 1.35, 2.0, 3.0) in full-width channel in Figs. 1 and 2. Each curve in Fig. 2 shows a plug-like scalar flow or implies a plug-like velocity profile (the cross-stream profiles remain relatively flat, especially for larger K_n) and is qualitatively the same as that of electrokinetically driven flows reported in Ref. [15] (cf. those images of Figs. 5 and 6 therein). Other views of these velocity fields (U) w.r.t. Y and K_n are presented in Fig. 3.



FIG. 2. Velocity fields U for different Knudsen numbers K_n in full-width (d) channel. U, Y, and K_n are dimensionless. Y = y/d. $K_n = 1/(dsn)$, n is the number density, s is the effective collision cross section. (Please cf. Ref. [2] for qualitative comparison with our smaller K_n cases.)

For smaller K_n cases, our velocity results qualitatively resemble those reported in Ref. [2]. (Note that, in Ref. [2], as reported by Burgreen and Nakache, electrokinetic flow in ultrafine capillary slits were considered. Their results, however, were not presented in terms of the Knudsen number so that we cannot directly compare ours with them; cf. Figs. 2 and 3 of Burgreen and Nakache or Fig. 1 of Rice and Whitehead [2].) But, we can verify our results especially for cases of $K_n \sim O(1)$ by comparison with the apparent velocity obtained from images of electrokinetically driven flows using a technique that employs an ultraviolet laser pulse to write a pattern into the flow by uncaging a fluorescent dye by Paul, Garguilo, and Rakestraw [15]. We only take the 99-ms image (considering the upstream part) presented in Fig. 5 of Ref. [15] into account. Those data were obtained for a electrokinetically driven flow through a 75- μ m capillary [15]. This rather-fit comparison shown in Fig. 4 confirms our approach.



FIG. 3. The overall view of U w.r.t. Y and K_n in half channel.



FIG. 4. Comparison with the apparent velocity (taken in the 99-ms image) reported by Paul, Garguilo and Rakestraw [15] (cf. Fig. 5 therein). We only compare the upstream-part data (image), which is a electrokinetically driven flow through a 75- μ m capillary.

In our illustrations, as K_n is large enough, there will be significant microscopic effects: nonzero slip velocities occurring along the boundaries [17,18], which are due to the unbalanced momentum or energy transfer microscopically

- [1] P. Debye and H. Hückel, Phys. Z. 24, 185 (1923).
- [2] D. Burgreen and F.R. Nakache, J. Phys. Chem. 68, 1084 (1964); C.L. Rice and R. Whitehead, *ibid.* 69, 4017 (1965).
- [3] H.U. Baranger and J.W. Wilkins, Phys. Rev. B 30, 7349 (1984); S.A. Trugman and A.J. Taylor, *ibid.* 33, 5575 (1986);
 C. Cercignani, J. Stat. Phys. 77, 1039 (1994); J.J. Harris, J.A. Pals, and R. Woltjer, Rep. Prog. Phys. 52, 1217 (1989).
- [4] W.K.-H. Chu, Phys. Scr. 62, 453 (2000); W.K.-H. Chu, J. Phys. A 33, 7103 (2000).
- [5] M. Hasegawa, K. Nanbu, and K. Iwata, Math. Methods Appl. Sci. 3, 693 (1993).
- [6] Ya.G. Sinai, Russ. Math. Surveys 25, 137 (1970).
- [7] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. 74, 2694 (1995).
- [8] T. Carleman, Acta Math. 60, 91 (1932).
- [9] D.J. Nagel and M.E. Zaghloul, IEEE Circuits Devices Mag. 17, 14 (2001); D. Bishop, P. Gammel, and R. Giles, Phys. Today 54, 38 (2001); R.B.M. Schasfoort, S. Schlautmann, J. Hendrikse, and A. van den Berg, Science 286, 942 (1999); R.E. Howard and A.B. Lidiard, Rep. Prog. Phys. 27, 162 (1964); M. Esashi, K. Minami, and T. Ono, Condens. Matter News 6, 31 (1998).
- [10] M. Slemrod, A. Qi, M. Grinfeld, and I. Stewart, Math. Methods Appl. Sci. 18, 959 (1995); N.A. Nurlybaev, Transp. Theory Stat. Phys. 22, 109 (1993).
- [11] H. Cabannes, The Discrete Boltzmann Equation. Theory and

when particles interacting or colliding with the solid walls. This observation, even though for cases of smaller K_n there exist nonzero velocities for our results, however, is difficult to be found in Figs. 2 and 3 of Burgreen and Nakache [2] (especially for smaller α , the ionic energy parameter therein). The reason could be due to the macroscopic approach they adopted in Ref. [2], which cannot resolve the near-wall microscopic effects [17,18].

As this model had been verified previously [4,10–12] and the qualitative or quantitative comparison illustrated here shows minor differences in between, we have confidence about these results: There are preferred motions for many charged particles flowing in a slender confined channel over a range of collision frequencies or Knudsen numbers when these charged particles are driven by a uniform (constant) nonboundary-driven forcing. At least, our results of velocity fields resemble those of electrokinetic flows reported in Refs. [2,15] qualitatively or quantitatively for certain range of Knudsen numbers. We hope in the future we can address other complicated problems [19–22] by modifying our present approach.

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Applications (University of California, Berkeley, 1980).

- [12] N. Bellomo and T. Gustafsson, Rev. Math. Phys. 3, 137 (1991).
- [13] L. Arkeryd and N. Maslova, J. Stat. Phys. 77, 1051 (1994).
- [14] R. Courant and K.O. Friedriches, Supersonic Flow and Shock Waves (Interscience, New York, 1948), p. 15.
- [15] P.H. Paul, M.G. Garguilo, and D.J. Rakestraw, Anal. Chem. 70, 2459 (1998).
- [16] H. Struchtrup and W. Weiss, Phys. Rev. Lett. 80, 5048 (1998).
- [17] D.C. Tretheway and C.D. Meinhart, Phys. Fluids 14, L9 (2002); Y.X. Zhu and S. Granick, Phys. Rev. Lett. 87, 096105 (2001); V.S.J. Craig, C. Neto, and D.R.M. Williams, *ibid.* 87, 054504 (2001).
- [18] Y.X. Zhu and S. Granick, Phys. Rev. Lett. 88, 106102 (2002);
 J.-T. Jeong, Phys. Fluids 13, 1884 (2002).
- [19] L.L. Bonilla, J. Phys.: Condens. Matter 14, R341 (2002); V.V. Larkin *et al.*, Nanotechnology 13, 487 (2002).
- [20] A. Einstein, Ann. Phys. Chem. (IV. Folge) 17, 891 (1905).
- [21] A.P. Long, P.H. Beton, and M.J. Kelly, Semicond. Sci. Technol. 1, 63 (1986); M.C. Barbosa, J. Phys.: Condens. Matter 14, 2461 (2002).
- [22] A.M. Anile and G. Mascali, Appl. Math. Lett. 14, 245 (2001);
 V.K. Arora, Phys. Rev. B 30, 7297 (1984); M.Ya. Azbel and D.P. DiVincenzo, *ibid.* 30, 6877 (1984); I.O. Kulik, R.I. Shekhter, and A.N. Omel'yanchuk, Solid State Commun. 23, 301 (1977).