Stationary 'V' States for Preferred Motions of Many Particles

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Received November 11, 2005; accepted March 13, 2006 Published Online: June 1, 2006

We use the discrete kinetic theory with the free-orientation parameter being fixed $(\pi/4)$ to derive the macroscopic velocity field for many particles flowing through a microdomain. Our results resemble qualitatively other hydrodynamical solutions. The V-shaped velocity field changes as the dominant physical parameter (Knudsen number) varies. We also briefly discuss the possible mechanism due to the entropy production along the boundaries.

KEY WORDS: Knudsen number; discrete kinetic model; dilute gases.

1. INTRODUCTION

Discrete kinetic theory (Chu, 2001, 2004; Godunov and Sultangazin, 1971) with the thermostat assumption or diffuse scattering boundary condition (Arkeryd and Maslova, 1994) have been adopted to *ad hoc* model the many-particle scattering situation along the gas-surface interacting interface in a plane channel (Chu, 2001). Specific orientations relevant to different rarefaction parameters were identified therein (Chu, 2001). Motivated by the recent interests in the quantum Boltzmann approach (Vedenyapin *et al.*, 1995) and the relevant studies (Platkowski and Illner, 1988; Cabannes *et al.*, 2002; Bellomo and Gustafsson, 1991; Bellomo and Gatignol, 2003), we continue our previous studies (Chu, 2001, 2004) by examining the related velocity and vorticity fields corresponding to those specific θ and Kn we obtained and checking the special case $\theta = \pi/4$.

Many interesting problems have been successfully solved (Carleman, 1957; Broadwell, 1964; Kawashima and Nishibata, 1999; Cornille, 1987; Bellomo and Kawashima, 1990; Cabannes, 1980; D'Almeida and Gatognol, 2003; Gatignol, 1975; Görsch, 2002) by using the discrete kinetic theory. Carleman (1957) developed 2-velocity models which are defined by abstract properties in order to

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produce only mathematical purposes. That model was not constructed on the basis of detailed analysis of the collision mechanics. Broadwell (1964) devised a 6velocity model to handle the simple shock wave problem. At first mathematicians have been interested in the discrete Boltzmann equation with the hope to provide, thanks to the relatively simpler structure of the equation as compared with that of the full Boltzmann equation, stronger results than those available for the Boltzmann equation or mathematical results suitable to be technically generalized to the full Boltzmann equation in the analysis of initial and initial-boundary value problems. However, the analysis over recent years has shown that this is not the case (Platkowski and Illner, 1988; Bellomo and Gustafsson, 1991; Bellomo and R. Gatignol, 2003). These have been reviewed considering mainly the mathematical aspects of the initial and initial-boundary value problems in order to provide a "more detailed" analysis in a "more specialized" field. In fact the consistency of the mathematical results depends on the structure of the mathematical problems: in some cases it is possible to obtain for the discrete Boltzmann equation "stronger" results than the corresponding ones for the Boltzmann equation, and in other case "weaker" results. Kawashima has proved the global existence of solutions to the initial-boundary value problems (I.-B.V.P.) for the discrete Boltzmann Equation in the 1D-region $0 < x < \infty$ or 0 < x < d (cf. Kawashima and Nishibata, 1999).

Cornille obtained some transient or stationary family of solutions for certain (fixed-orientation) discrete velocity models without considering the boundary conditions (Cornille, 1987). Recent advances or progresses using discrete velocity models could be traced in (Chu, 2001; Bellomo and Gatignol, 2003).

In this short paper, we plan to reconstruct the macroscopic velocity field of many dilute particles by the verified 4-velocity model (Chu, 2001) (the free orientation is fixed to be $\theta = \pi/4$) considering a simple test problem: many molecules or particles flowing along the bounded-plane channel and finally reaching a steady state. Our preliminary results might give clues to above problems or many-particles interaction problems. The verification of our approaches has been done in (Chu, 2001, 2004), the argues about the differences between different discrete velocity models included. For $\theta = \pi/4$ case, using a completely different solving procedure, we obtained velocity fields which have a V-shaped or chevron-structure.

This short paper is organized as follows. We introduce the general orientationfree 4-velocity model (Chu, 2001; Platkowski and Illner, 1988) in Section 2, and simplify it to a system of four equations for associated unknown functions. The general boundary conditions will be briefly introduced, too. Then, we define some macroscopic variables (like u, v) to suit our interest which is to find a class of steady (and parallel) non-boundary-driven solutions or flows for particles flowing along a microslab with bounded (flat-plane) walls. The orientation will be fixed as $\pi/4$ here when we solve the time-independent system of equations with relevant boundary conditions for the test case. As reported in (Chu, 2001), there will be no dispersion or absorption when we implement the model with this orientation so that we can resolve sharp velocity profiles. These kinds of solutions, u, which collect the main results of the present paper, are given in explicit form, and are functions of 1D coordinate: y or Y and are also dependent on certain integration constants or parameters due to the purely diffuse reflection boundary conditions. Finally, we analyze the solutions (V-shaped fields) and make some physical comments or discussions in comparison with the other flow-pattern selection due to the relative orientation effect upon binary encounter of many particles or unusual entropy production along the confined boundaries.

2. FORMULATIONS

Considering a simple fluid of particles with mass *m* and cross-sectional area σ , the first step of the modelling 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 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

$$\left[\frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla\right] N_i = G_i - L_i$$

where 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 semi-linear partial differential equations of hyperbolic type. Above equation could also be written as

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

where i = 1, ..., p; here, by definition, an *r*-collision ($r \ge 2$) involves *r* particles. $I_r = (i_1, ..., i_r)$, and $J_r = (j_1, ..., j_r)$ 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 $\{1, ..., p\}$.

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 $(\mathbf{u}_i, \mathbf{u}_j) \leftrightarrow (\mathbf{u}_k, \mathbf{u}_l), i, j, k, l = 1, ..., p$; and

the number of paired-outputs corresponding to a given paired-input is denoted by $q. N_{I_r}$ denotes the product $N_{i_1}N_{i_2} \dots N_{i_r}$.

 $\delta(i, J_r, I_r) = \delta(i, J_r) - \delta(i, I_r)$ 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 and considering the evolution of N_i , we have

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

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

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

with $i \in \Lambda = \{1, ..., p\}$, and the summation is taken over all $j, k, l \in \Lambda$, where A_{kl}^{ij} are nonnegative 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 collision, $A_{kl}^{ij} = A_{ij}^{kl}$: microreversibility condition. The conditions defined for the discrete velocity above requires that elastic, binary collisions, such that momentum and energy are preserved $\mathbf{u}_i + \mathbf{u}_j = \mathbf{u}_k + \mathbf{u}_l$, $|\mathbf{u}_i|^2 + |\mathbf{u}_j|^2 = |\mathbf{u}_k|^2 + |\mathbf{u}_l|^2$, 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 $A_{ij}^{kl} = S|\mathbf{u}_i - \mathbf{u}_j| a_{ij}^{kl}$, where,

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

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 collisions.

The discrete kinetic equations then (Chu, 2001, 2004; Bellomo and Gustafsson, 1991) assume the following form

$$\frac{\partial N_i}{\partial t} + c \left[\cos(\theta + (i-1) * \pi/q) \frac{\partial N_i}{\partial x} + \sin(\theta + (i-1) * \pi/q) \frac{\partial N_i}{\partial y} \right]$$
$$= \frac{2cS}{q} \sum_{j=1}^q (N_j N_{j+q} - N_i N_{i+q}) \text{ or } = \frac{2cS}{q} \sum_{l=1}^{q-1} (N_{i+l} N_{i+l+q} - N_i N_{i+q});$$



Fig. 1. Reference frame for the 4-velocity model with $\theta = \pi/4$ here.

$$i = 1, \dots, 2q,\tag{1}$$

where θ is the free orientation starting from the positive *x*-axis to the *u*₁ direction (Chu, 2001), $N_i = N_{i+2q}$ are unknown functions, and *c* is a reference velocity modulus.

According to (Bellomo and Kawashima, 1990), for the 2q-velocity model that is $q \ge 3$, there are more *collision invariants* than the physical ones or conservation laws which are corresponding to the number of macroscopic variables (in 2D. there are only 4, i.e., one mass, two momenta, one energy). That's to say, there are unphysical or *spurious* invariants or macroscopic variables for $q \ge 3$ models (which could be, however, well handled by adding multiple collisions (Bellomo and Kawashima, 1990)). Thus, we plan to use only the orientation-free 4-velocity model for our test-case problem below.

2.1. Boundary Conditions

We use purely diffuse reflection boundary condition (Chu, 2001; Arkeryd and Maslova, 1994) here, which means properties of the reflected particles are independent of their properties before the impact. In other words, the re-emitted 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 particles are in Maxwellian equilibrium with the wall ("the wall locally behaves as a thermostat," i.e., the particles 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 particles to the wall quantities, and N_{wi} is the discrete Maxwellian densities for the 'i'-direction set of particles. That is, we have

$$|\mathbf{u}_j \cdot \mathbf{n}| N_{wj} = \sum_{i \in I} B_{ij} |\mathbf{u}_i \cdot \mathbf{n}| N_{wi}, \quad j \in R, \quad B_{ij} \ge 0, \quad \sum_{j \in R} B_{ij} = 1; \quad (2)$$

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.

2.2. Flows in a Plane Channel

We firstly define the related macroscopic variables $n = N_1 + N_2 + N_3 + N_4$, $nU = c(\alpha N_1 - \beta N_2 - \alpha N_3 + \beta N_4)$, $nV = c(\beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4)$, (the latter two are the momentum flux along *x*- and *y*-directions) with $\rho = n m$, *m* is the mass of the molecule, ρ is the macroscopic density of the gas. Then, set $n_i = N_i/n$, i = 1, 2, 3, 4; and then use non-dimensional u = U/c, v = V/c, Y = y/d, where *c* may be related to the external forcing (Chu, 2001, 2005; Courant and Friedriches, 1948). *d* is the full channel width. y = 0 is along the center-line.

The geometry of a 2D problem we shall consider is a kind of microchannels with bounded flat-plane walls which are separated apart by a width *d*. Particles (driven by an external constant forcing initially) flowing along this channel will finally reach a fully developed state (steady state and $\partial u / \partial x = 0$, v = 0).

We derive the solutions with $\alpha \equiv \cos \theta = \beta \equiv \sin \theta = \sqrt{2}/2$ case here. The algorithm is different from those previously reported, we must solve the independent number density respectively then combine them into macroscopic ones since the original macroscopic equation is singular (cf. equations in (Chu, 2001)). Meanwhile, from the preliminary results reported in (Chu, 2001, 2004), it seems, for the case of $\theta = \pi/4$, 4-velocity model will give completely different dispersion relations for the thermodynamic checking of the perturbed Maxwellian equilibrium state. There will be no dispersion or absorption for this particular case.

The governing Equation (1), for the assumptions prescribed above, now become

$$\frac{dn_1}{dY} = -\frac{dn_2}{dY} = -\frac{dn_3}{dY} = \frac{dn_4}{dY} = \frac{\sqrt{2}}{4\mathrm{Kn}}(1-2a) = \frac{\sqrt{2}}{\mathrm{Kn}}(n_2n_4 - n_1n_3), \quad (3)$$

here, $n_3 = a - n_1$, $n_2 = 1/2 - n_1$, $n_4 = 1/2 - a + n_1$; Kn= 1/(dSn) is the Knudsen number. The diffuse reflection boundary conditions become:

$$N_{w2}N_1 = N_{w1}N_2, \qquad \beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4 = 0,$$
 (4)

it means (i) the Maxwellian equilibrium at the walls dominates, (ii) no penetration occurs across the wall. The discrete Maxwellian densities N_{wi} at the wall, as derived before (please see the detailed references in (Cabannes, 1980), are

$$N_{wi} = \left(\frac{n}{4}\right) \left\{ 1 + \left(\frac{2}{c^2}\right) \mathbf{u}_w \cdot \mathbf{u}_i + (-1)^i [(\mathbf{u}_w \cdot \mathbf{u}_2)^2 - (\mathbf{u}_w \cdot \mathbf{u}_1)^2] \left(\frac{1}{c^4}\right) \right\}.$$
 (5)

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Here, boundary conditions are, as $\mathbf{u}_w = 0$ (the walls are static and fixed) and by assuming the symmetry,

$$n_1 = B_{31}n_3 + B_{41}n_4$$
, at $Y = -1/2$, $n_3 = B_{13}n_1 + B_{23}n_2$, at $Y = 1/2$,
(6)

with the discrete Maxwellians $N_{wi}|_{\pm} = 1/4$. Integration of Equation (3) gives

$$n_1 = \frac{\sqrt{2(1-2a)}}{4\mathrm{Kn}}Y + b.$$

Now, set $A = 1/(4\sqrt{2} \text{ Kn})$, so we get from above equations to solve for a, b:

$$[2A(1 + B_{31} - B_{41}) - B_{31} + B_{41}]a + (1 + B_{31} - B_{41})b$$

= $\frac{B_{41}}{2} + (1 + B_{31} - B_{41})A,$ (7)

$$[1 + 2A(1 + B_{13} - B_{23})]a + (B_{23} - B_{13} - 1)b = \frac{B_{23}}{2} + A(1 + B_{13} - B_{23}), \text{ or}$$
(8)

$$C a + D b = G, \qquad E a + F b = H.$$
(9)

After manipulations, we have

$$a = \frac{FG - DH}{CF - DE}, \qquad b = \frac{CH - EG}{CF - DE}; \tag{10}$$

where $CF - DE = 4A(B_{23} - B_{13} - 1) + (B_{23} - B_{13})(B_{41} - B_{31}) - 1$, and $FG - DH = (B_{23} - B_{13} - 1)[A(1 + B_{31} - B_{41}) + B_{41}/2] + (1 + B_{31} - B_{41})$ $[A(B_{23} - B_{13} - 1) - B_{23}/2]$, $CH - EG = A[(B_{23} - 1)(1 - B_{41}) - B_{31}(2 + B_{13} - 2B_{31})] + [(B_{23} - 1)B_{41} - B_{23}B_{31}]/2$.

Since $nU/c = \sqrt{2}/2(N_1 - N_2 - N_3 + N_4)$, so we have a family of (particular) flow field in terms of the macroscopic velocity

$$u = \sqrt{2}(2n_1 - a) = \frac{1 - 2a}{\mathrm{Kn}}Y + \sqrt{2}(2b - a).$$
(11)

3. RESULTS AND DISCUSSIONS

This class of solution *u* obtained by fixing the orientation to be $\pi/4$ is in general different from those reported in (Chu, 2001). Note that, for one extreme case of boundary conditions as mentioned in Equation (2): $B_{31} = B_{41}$, and $B_{13} = B_{23}$; we have

$$a = \frac{2A + (B_{41} + B_{23})/2}{1 + 4A}, \quad b = \frac{A(1 + B_{41} - B_{23}) + B_{41}/2}{1 + 4A}.$$
 (12)



Fig. 2. (a), (b) Rarefaction effects (Kn) on the velocity field u or the V-shaped or chevron-like structure. Kn= 1/(d S n) is the Knudsen number. *S* is the effective collision cross-section. *n* is the number density of particles.

We can easily observe that, from Equation (11), that u = 0 everywhere for all Knudsen numbers (Kn). There is no macroscopic flow (Landau and Lifshitz, 1987) for many particles once the boundary conditions are selected above.

Otherwise, the velocity field (from Equation (11)) as shown in Fig. 2 is qualitatively similar to the V-shaped (Deem and Zabusky, 1978) or *chevron*-like structure or pattern (Rossberg and Kramer, 1998) reported before in other physical systems. The velocity field is tuned mainly by the Kn and weakly by *a* and *b* with the latter due to the boundary conditions. We note that *a* might depend on the physical properties of fluids and the geometry of the solid-wall as it comes from the gas-solid interaction or reflection. The flow-pattern selection mechanism is yet open to the best knowledge of the authors but might be partially linked to that reported in (Chu, 2001) since there will be an essential singularity when integrating Equation (1) for $\theta = \pi/4$ case. In short, as Kn increases, the chevron front becomes more flat.

The macroscopic vorticity ω (or the mean shear) could be obtained by noting

$$\omega = \frac{du}{dY} = \frac{1 - 2a}{Kn} + \frac{d[\sqrt{2(2b - a)}]}{dY},$$
(13)

with

$$a = \frac{2A(1+B_{31}-B_{41})(B_{23}-B_{13}-1) + [2B_{41}B_{23}-B_{41}(B_{13}+1)-B_{23}(1+B_{31})]/2}{4A(B_{23}-B_{13}-1) + (B_{23}-B_{13})(B_{41}-B_{31}) - 1},$$
 (14)

where the last term of Equation (13) is generally zero. Once the Knudsen number (Kn; a kind of rarefaction measure for many-particles interactions or collisions) is fixed, the vorticity is a constant with the related B_{ij} subjected to the constraint in Equation (2). In fact, B_{ij} should depend on the detailed interactions of the gas-solid interface, like a kind of (known) molecules colliding with specific walls made of (already) specified material. It is bounded above but difficult to be fixed even for specific model and boundary value problem (Kawashima and Nishibata, 1999).

Our results for the vorticity field, at least, qualitatively matches with the hydrodynamic two-dimensional solution (Landau and Lifshitz, 1987) when the weakly compressible (incompressible) particles flow along a static flat-plane channel and finally reach a fully developed state even though the particles are initially driven by a constant pressure-gradient or unit forcing. How the transition forms from a class of *soliton-like* solutions (Chu, 2001) to uniform V-shaped or *chevron-like* states as reported here, however, is yet open to our best knowledge. Interestingly, similar sharp flow fields of solitary wave profiles (the highest one, cf. Figs. 9 and 10 by (Wu *et al.*, 2005) and constant-V vortex was reported recently (Faller, 2001) in other physical system dealing with confined flow transports.

To further interpret the mechanism, we propose that the complicated rate of entropy production along the boundaries (e.g., cf. Schnute, 1975; Andrey, 1985) might favor the smearing of viscous diffusion (toward the away-from-wall regions) so that the sharp and strange pattern could form and then there is no significant smoothing of the profiles along the cross-section.

Note that, the approach here: firstly tracing or obtaining (solving the corresponding equation in (3)) each individual discrete number density (n_i) then by summing up the corresponding projection to obtain u, is different from that in (Chu, 2001): directly construct the macroscopic solutions from the relevant governing equation for macroscopic variables (u). The boundary treatment which is relevant to the entropy production there is thus entirely different. The corresponding non-equilibrium states (due to different rates of entropy production and their decay) approaching to the final equilibrium states which are used as our boundary conditions might then be different. In fact, as we noticed, the argument raised in (Andrey, 1985) could be applicable to present approach as evidenced in the boundary operator as expressed in Equation (2) (could be represented as similar divergence form). Otherwise, if our interpretations don't work, there might exist other unknown mechanism which need our further works.

ACKNOWLEDGMENTS

The author is partially supported by the China Post-Dr. Science Foundation under Grant No. 1999-17.

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