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Enhanced stationary flow due to grazing collisions

W Kwang-Hua Chu†

24, Lane 260, Section 1, Muja Road, Taipei, Taiwan 11646, Republic of China

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Abstract. Grazing collisions occurring along the gas–solid interacting region are considered together with the discrete velocity model in order to obtain the enhanced volume flow rate (of a quasi-2D flow) for many molecules subjected to a non-boundary-driven force in a confined slender channel. This presents the first test of this effect on a many-particle system not far from equilibrium.

1. Introduction

Many molecules subjected to mutual collisions occurring in a molecular gas flow may approach a stationary state [1] under certain constraints. The relevant (simple hydrodynamic) quasi-2D solutions in a confined domain, e.g. a rather long (slender) channel, will strongly depend on the (dynamical) ensemble we can propose [2] or the related near-equilibrium distribution function of molecular velocities, e.g. Maxwellian, a kind of *thermostat*. Solutions of simple stationary (molecular) flows could also be dependent on boundary conditions for cases driven by boundaries or others which are driven by non-boundary forces.

Starting from a simple approach, such as taking only binary collisions into consideration, many results for simple quasi-2D molecular gas flows have been obtained *ad hoc* [3]. Most of them are based on continuous and discrete Boltzmann and/or Enskog equations [4] together with diffuse-reflection boundary conditions along the gas–solid boundaries [5]. Effects of *grazing collisions* (contacts with zero momentum transfer), however, were seldom considered or included since there are intrinsic mathematical difficulties or singularities when they are adopted or implemented [4, 6–8]. With the hard-sphere potential (considered in collision kernel), the positions and momenta of outgoing particles or molecules after grazing collision do not depend smoothly—sometimes not even continuously—on incoming data.

For such collisions, the deflection is small and there is practically no difference between the post- and pre-collisional velocities. Thus, the collision kernel presents a strong singularity for *grazing collisions* [8] and the integrability of the collision kernel can only be guaranteed when grazing collisions are neglected. The latter is the so-called ‘cutoff assumption’. This kind of collision, however, does lead to the existence of partial flows [4, 6] and produces non-negligible effects for long time [8]. Besides, it is usual that distant collisions (in plasma) involve small momentum transfers. This resembles the effect of grazing collisions.

In this paper we present consequences of grazing collisions that might enhance the volume flow rate for the stationary flow of many molecules subjected to a non-boundary-driven unit force in a confined slender channel by adopting the discrete velocity model [9, 10] without using the continuous Boltzmann approach. We noticed that 1D test case had been considered before [4, 12]. The test case here will be a quasi-2D one.

† Address for correspondence: PO Box 30-15, Shanghai 200030, People’s Republic of China.

2. Mathematical formulations

The governing equations we use had been well developed in the 1980s [9–13], depending on the discrete velocity models [14–16] that will be used,

$$\frac{\partial N_i}{\partial t} + \boldsymbol{u}_i \cdot \nabla N_i = \frac{1}{2} \sum_{j,k,l} (A_{kl}^{ij} N_k N_l - A_{ij}^{kl} N_i N_j) \qquad i = 1, \ldots, p \tag{1}$$

where N_i is the discrete number density and $\boldsymbol{u}_i$ is the associated velocity. $A_{kl}^{i,j}$ is the transitional measure related to the collisions from $\{i, j\}$ to $\{k, l\}$. The stationary solutions for simple geometry problems were also reported recently [4]. We can transform this system of partial differential equations [12] into a nonlinear ordinary differential equation for the 2D velocity field after we introduce the macroscopic density and mean velocity field (in the present study, we shall choose $p = 2q$, q being a positive integer 2 [11]). This is a four-velocity coplanar model. The above equations (1) can thus be simplified by adjusting the appropriate $A_{kl}^{i,j}$ and following the assumptions of this model.

A_{kl}^{ij} are nonnegative constants satisfying (i) *indistinguishability of the molecules in collision*, (ii) *conservation of momentum in the collision* and (iii) *the microreversibility condition*. Here they are related to the product of the effective collision cross-section S and the molecular velocity modulus with the admissible collision probability, i.e. collisions: $\{1, 3\}$ to $\{2, 4\}$.

To demonstrate our approach, but to retain simplicity, we shall consider a simple-geometry test case: many particles flowing along a slender long channel from an inlet to an outlet (the length in between is L, both walls being confined and separated by a distance d ($d \ll L$). Now, $u_1 = c(\alpha, \beta)$, $u_2 = c(-\beta, \alpha)$, $u_3 = -c(\alpha, \beta)$, $u_4 = c(\beta, -\alpha)$, $\alpha = \cos(\theta)$, $\beta = \sin(\theta)$; θ is the angle between the ξ-axis and the u_1-direction and c is the reference velocity modulus [9–17]; here the ξ-axis is in the streamwise direction. The grazing collisions arise from the very small angle between the incoming velocity and the flat-wall plane or almost-null incoming (and/or thus reflecting) velocity of the particles.

To obtain the macroscopically hydrodynamical field, which is useful for comparison with previous experimental data, we let $n = N_1 + N_2 + N_3 + N_4$, $nu = c(\alpha N_1 - \beta N_2 - \alpha N_3 + \beta N_4)$ and $nv = c(\beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4)$; these are the total number density and the ξ- and η-direction momentum flux (per unit mass), respectively. u and v are then the ξ- and η-direction mean velocity; $\rho = nm$ is the macroscopic density, where m is the mass of the gas molecule.

Based on the system of four equations obtained from (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.

The general simplified equations are now

$$\frac{\partial N_1}{\partial t} + c\left(\alpha \frac{\partial N_1}{\partial \xi} + \beta \frac{\partial N_1}{\partial \eta}\right) = cS(N_2 N_4 - N_1 N_3) \tag{2}$$

$$\frac{\partial N_2}{\partial t} + c\left(-\beta \frac{\partial N_2}{\partial \xi} + \alpha \frac{\partial N_2}{\partial \eta}\right) = -cS(N_2 N_4 - N_1 N_3) \tag{3}$$

$$\frac{\partial N_3}{\partial t} + c\left(-\alpha \frac{\partial N_3}{\partial \xi} - \beta \frac{\partial N_3}{\partial \eta}\right) = cS(N_2 N_4 - N_1 N_3) \tag{4}$$

$$\frac{\partial N_4}{\partial t} + c\left(\beta \frac{\partial N_4}{\partial \xi} - \alpha \frac{\partial N_4}{\partial \eta}\right) = -cS(N_2 N_4 - N_1 N_3) \tag{5}$$

where S is the effective collision cross-section [9–16].

2.1. Boundary conditions

We use purely diffuse reflection boundary conditions [3–5, 10, 11, 13] here, i.e. the properties of the reflected molecules 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 molecules (see [4, 5] for the continuous mathematical form). Moreover, we impose the following conditions: the gases are in Maxwellian 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), satisfying $N_i(\boldsymbol{r}, t) = \gamma_i(\boldsymbol{r}, t)N_{wi}(\boldsymbol{r}, t)$, where γ_i express the accomodation of the discrete gas to the wall quantities, and N_{wi} is the discrete Maxwellian densities for the 'i'-direction set of molecules. That is, we have

$$|\boldsymbol{u}_j \cdot \boldsymbol{n}|N_{wj} = \sum_{i\in I} B_j|\boldsymbol{u}_i \cdot \boldsymbol{n}|N_{wi} \qquad j \in R \qquad B_j \geqslant 0 \qquad \sum_{j\in R} B_j = 1 \tag{6}$$

with $I = \{i, (\boldsymbol{u}_j - \boldsymbol{u}_w) \cdot \boldsymbol{n} < 0\}$ related to the impinging set of molecules and $R = \{j, (\boldsymbol{u}_j - \boldsymbol{u}_w) \cdot \boldsymbol{n} > 0\}$ related to the emerging set of molecules; $\boldsymbol{u}_w$ is zero here.

Then, from the above relations, with the velocities of the model being symmetric w.r.t. the wall, we can see that γ_j ($j \in R$) does not depend on j, thus at the wall we have $N_j = nN_{wj}$, $\forall j \in R$ by the definition of n, and considering $\boldsymbol{u} \cdot \boldsymbol{n} = 0$, $|\boldsymbol{u}_i \cdot \boldsymbol{n}| = |\boldsymbol{u}_j \cdot \boldsymbol{n}|\forall i, j, \boldsymbol{u}_w = 0$.

The diffuse reflection boundary conditions become

$$N_{w2}N_1 = N_{w1}N_2 \qquad \beta N_1 + \alpha N_2 - \beta N_3 - \alpha N_4 = 0. \tag{7}$$

This means (i) the Maxwellian at the walls dominates and (ii) no penetration occurs across the wall.

The Maxwellian densities N_{wi} at the wall, as derived in [4, 11], are

$$N_{wi} = (n/4)\{1 + (2/c^2)\boldsymbol{u}_w \cdot \boldsymbol{u}_i + (-1)^i[(\boldsymbol{u}_w \cdot \boldsymbol{u}_2)^2 - (\boldsymbol{u}_w \cdot \boldsymbol{u}_1)^2](1/c^4)\}. \tag{8}$$

2.2. Stationary non-boundary-driven quasi-2D flow

We look for a solution depending on η (the cross-stream direction) only, i.e. the case of many molecules flowing (with macroscopical $u(\eta)$) hydrodynamically only along the ξ-direction (confined in a slender channel) between an inlet and outlet and reaching steady state at ξ_0 where the discrete number density n_0 is well defined locally there. Let $\hat{R} = S(N_2N_4 - N_1N_3)$, or $\bar{R} = (n_2n_4 - n_1n_3)$, where $n_i = N_i/n_0$; and then use non-dimensional $U = u/c_0$, $Y = \eta/d$, d is the channel width. c_0 could be related to a non-boundary-driven unit force [4, 13, 14, 17].

The system of equations (2)–(5) above can thus be simplified to

$$\frac{\partial n_1}{\partial Y} = \frac{\bar{R}}{\beta K_n} \qquad \frac{\partial n_2}{\partial Y} = -\frac{\bar{R}}{\alpha K_n} \qquad \frac{\partial n_3}{\partial Y} = -\frac{\bar{R}}{\beta K_n} \qquad \frac{\partial n_4}{\partial Y} = \frac{\bar{R}}{\alpha K_n}$$

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

$$\frac{\partial n/n_0}{\partial Y} = 0 \qquad \text{and} \qquad \frac{\partial(nu/c)}{\partial \eta} = \frac{2}{\alpha\beta}\hat{R}.$$

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

$$\frac{nc_0}{cn_0}\frac{\partial U}{\partial Y} = \frac{2}{K_n\alpha\beta}\bar{R} = \frac{2}{\alpha}\frac{\partial n_1}{\partial Y} = \frac{2}{\beta}\frac{\partial n_4}{\partial Y} = -\frac{2}{\beta}\frac{\partial n_2}{\partial Y} = -\frac{2}{\alpha}\frac{\partial n_3}{\partial Y}. \tag{9}$$

Integrating the above equation we then obtain

$$2n_1 = AU + K_1 \qquad 2n_4 = BU + K_4 \qquad 2n_2 = -BU + K_2 \qquad 2n_3 = -AU + K_3$$

where

$$A = \alpha \frac{nc_0}{cn_0} \qquad B = \beta \frac{nc_0}{cn_0}. \tag{10}$$

When the state of interest is selected as the fully developed state (a stationary state with balancing between externally non-boundary-driven unit-force and dissipations from confined boundaries [2–5]), or $n = n_0$, $c = c_0$, then we obtain $A = \alpha$, $B = \beta$.

To include the effect of grazing collisions, especially near the region of gas–solid reflections or interactions, we define the ratio $= n/n_0$. If the ratio is unity, there is no effect from grazing collisions. Meanwhile, we fix $c = c_0$ for simplicity.

As for the general boundary conditions [5], we use the idea that the number density $N_i = N_{\rm wall}|_i$ (the Maxwellian density) at the wall for $i = 1, 2, 3, 4$, which means molecules are in a Maxwellian equilibrium with the boundary just before they re-emit from the confined boundary, e.g. the wall. Derivations of this kind of Maxwellian density have been mentioned above.

From these boundary conditions, with $V = 0$, i.e. $B(n_1 - n_3) = A(n_4 - n_2)$, and $n = n_1 + n_2 + n_3 + n_4 =$ ratio, we thus obtain $K_1 = K_3$, $K_2 = K_4$, $K_1 + K_2 =$ ratio and

$$\frac{\mathrm{d}U}{\mathrm{d}Y} = \frac{A^2 - B^2}{2K_n AB}\left(U^2 - \frac{K_1 - K_2}{A^2 - B^2}\right) \qquad A \neq B \qquad AB \neq 0. \tag{11}$$

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

$$\frac{\mathrm{d}U(0)}{\mathrm{d}Y} = 0 \qquad U\left(Y = \frac{1}{2}\right) = U_{\rm s} = \frac{2K_2 - \text{ratio}}{A + B}$$

where $U_{\rm s}$ is the velocity slip at the wall. $U_{\rm wall} = 0$ here.

After direct integration of ordinary differential equation (8), we obtain one family of solutions for certain A (α), B (β), K_n; A (α), B (β) being strongly linked to maximum admissible orientations (θ) (whereas the minimum θ corresponds to $U_{\rm s} = 0$)

$$U = G \tanh(C - GKY) \qquad \text{where} \quad G = \left(\frac{2K_2 - \text{ratio}}{A^2 - B^2}\right)^{1/2} \qquad K = \frac{A^2 - B^2}{2A\,BK_n} \tag{12}$$

where C will depend on the specific gas–surface interface. The principle of fixing θ is similar to that adopted in [18]. We also take the data of Gaede [19] into consideration to fix C since his data are for a kind of non-boundary-driven stationary flow which is similar to ours and could be a guideline for our macroscopic velocity field. Thus, C could be fixed once the gas and the solid boundary are known [14].

With these velocity fields, we also can calculate the kinetic temperature and/or pressure fields following the procedures in [4] from the modified discrete kinetic theory [20]. The direct integration of U then gives us the dimensionless volume (or mass) flow rate

$$Q_m = -2\frac{2A\,BK_n}{A^2 - B^2}\left\{\log\left[\cosh\left(C - \frac{GK}{2}\right)\right] - \log[\cosh(C)]\right\} \tag{13}$$

which could be compared with previous data (as in [3, 4]; please see especially the references cited in [3] for the application to the plane Poiseuille flow of rarefied gases).

3. Results and discussion

To check the effect of grazing collisions for the stationary flow in consideration, i.e. a non-boundary-driven case, we plot Q_m versus K_n for different ratios in figure 1, with data of previous attempts included [3]. We can observe the significant contributions or shifts of Q_m

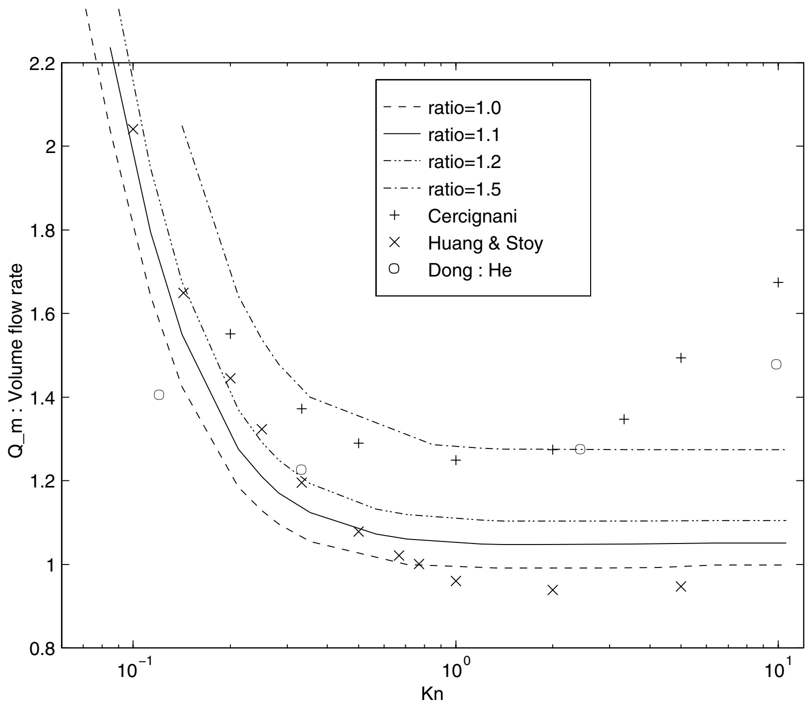

Figure 1. Comparison with other approaches and experiments for different ratios due to grazing-collision enhanced flow.

due to different ratios or effects of grazing collisions. Experimental data, such as Dong's and/or other numerical approaches, such as that of Cercignani (using continuous Boltzmann model) or Huang and Stoy could be quantitatively approximated by our approaches (using θ and the ratio based on the arguments in [13, 14]). The minor differences may be due to the discrete equilibrium Maxwellian (distribution) we used as the boundary condition [10, 11] or other open problems of the four-velocity model [4, 13, 14, 16], for example, one-speed limitation of the four-velocity model. Note that the measurements for comparison as shown in figure 1 or obtained in [3] or [4] were conducted around the mid-1950s for monatomic gases flowing along glass-walled channels.

As we know, for the boundary conditions, the most suitable state along the boundary (wall) should be a non-equilibrium one which is more direct for the solution of a stationary state [2] (already balanced between the viscous shear and non-boundary-driven external force) for many particles subjected to binary collisions only.

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