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Shock Structure in a Simple Discrete Velocity Gas

JAMES E. BROADWELL
Thompson-Ramo-Wooldridge Space Technology Laboratories, Redondo Beach, California
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The structure of a shock wave in a simple discrete velocity gas—a gas in which the molecules move with a finite set of velocities—is discussed. The Boltzmann equation becomes, for this gas, a set of coupled differential equations which, in the present example, can be solved exactly. The solution describes an infinite Mach number shock in a gas consisting of hard elastic spheres. Although only six molecular velocities are considered, and the solution is easy to obtain, it compares remarkably well with those of other investigators.

I. INTRODUCTION

THE success of the simplest molecular model of a gas—molecules moving in the six directions along mutually perpendicular coordinates at constant speed—in predicting the equation of state and approximate expressions for the transport properties is well known. If the model is generalized by dropping the requirement that equal numbers of molecules move in all directions, then the gas can have fluid mechanical motion. Since the Boltzmann equation for such a gas is extremely simple, the resulting model may provide a useful approximate description of rarefied gas flows. This approach to the approximate solution of the Boltzmann equation, i.e., restricting the molecular velocities to a finite set, was suggested by Krook[1] in connection with his study of a similar approximation in radiative transfer problems. The idea was mentioned again by Gross[2] but apparently its only application has been to low-Mach-number Couette and Rayleigh flow.[3] The results of that study, in which the molecules were restricted to eight equal speed velocities, were both easy to obtain and in reasonable accord with what is known about these flows at low density. This outcome suggested that the method be applied to other gas dynamical problems for which Boltzmann equation solutions may be necessary. The structure of shock waves, especially at high Mach number, is, of course, such a problem.

This paper describes the structure of a shock wave in the "elementary kinetic theory" gas, a gas in which the molecules move in only six directions and at constant speed. To see that such a gas has the possibility of forming a shock wave, let the six allowed velocities, of magnitude c, be those shown in Fig. 1. Now consider a stream of molecules all moving with velocity (2) as indicated in Fig. 2. The stream has a fluid velocity equal to c and is at zero temperature and pressure. Now suppose that these molecules impinge on a wall, normal to the stream, from which they are emitted with velocity (1). If the impingement and emission rates are equal, the fluid velocity adjacent to the wall is zero. The upstream moving molecules, those in velocity cell 1, collide with those in cell 2, and these collisions populate cells 3, 4, 5, and 6. Thus a disturbance moves away from the wall within which the fluid velocity is brought to zero and the temperature and pressure rise from zero to finite values. It is shown in the following that this disturbance conforms remarkably well to our ideas about a shock wave in a monatomic, infinite Mach number, gas stream. The simple and exact solution to the Boltzmann equation for the model shows that the density ratio across the shock is four, the total enthalpy is constant across the wave (in steady flow) but rises slightly within, the maximum slope thickness is a few mean free paths, and so forth.

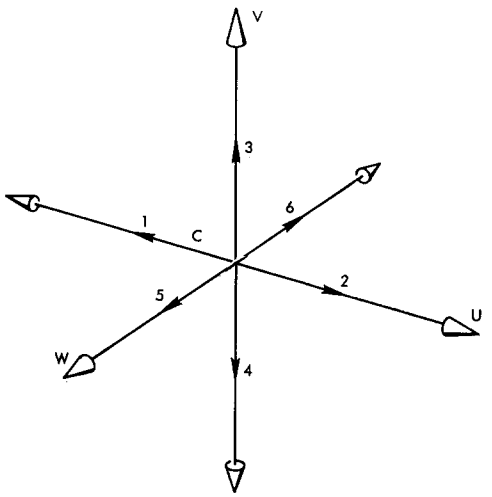

FIG. 1. The six molecular velocities.

[1] M. Krook, Astrophys. J. 122, 488 (1955).
[2] E. P. Gross, in *Proceedings of the First International Symposium on Rarefied Gas Dynamics*, edited by F. M. Devienne (Pergamon Press, Inc., New York, 1960).
[3] J. E. Broadwell, J. Fluid Mech. (to be published).

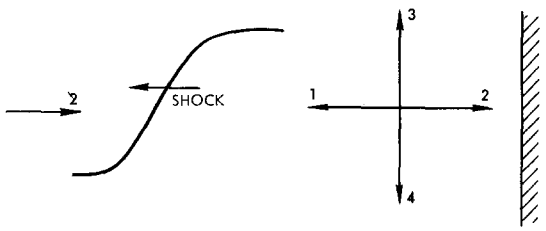

FIG. 2. Sketch of moving shock wave.

II. THE BOLTZMANN EQUATION FOR THE DISCRETE VELOCITY GAS

The Boltzmann equation may be written in the form

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} + w\frac{\partial f}{\partial z} = \left(\frac{\partial f}{\partial t}\right)_c = G - L, \quad (2.1)$$

in which f is the distribution function depending on the time and space variables t, x, y, z and on the molecular velocity $\mathbf{v}$ with components, u, v, w. The rate of change of f due to collisions, $(\partial f/\partial t)_c$, is written as the gain minus the loss, $G - L$. If the molecules occupy, between collisions, a finite set of cells located at $\mathbf{v}_i$ in velocity space, Eq. (2.1) can be written

$$\frac{\partial N_i}{\partial t} + u_i\frac{\partial N_i}{\partial x} + v_i\frac{\partial N_i}{\partial y} + w_i\frac{\partial N_i}{\partial z} = G_i - L_i, \quad (2.2)$$

in which N_i is the number of molecules per unit volume with velocity $\mathbf{v}_i$. Now consider the gas with the six molecular velocities in Fig. 1. Taking cell 1 as an example, let us compute $(G_1 - L_1)$, the rate of change of N_1 due to collisions. Loss of molecules from cell 1 occurs only when these molecules collide with those in cell 2, for when cell 1 occupants collide with occupants of any other cell, the collision partners must either return to their original cells or exchange places. The possible outcomes of a collision between molecules of cells 1 and 3, for instance, are indicated in Fig. 3. From a 1–2 collision, however, the partners may be deflected to cells 3 and 4, or 5 and 6, or may return to cells 1 and 2. For hard elastic spheres the scattering is spherically symmetric, and therefore these three pairs of cells are equally likely destinations for the colliding molecules. Hence, in two-thirds of the 1–2 collisions molecules are lost from cell 1, and

$$L_1 = \tfrac{2}{3}v_r S N_1 N_2 = \tfrac{4}{3}cSN_1N_2,$$

where v_r is the relative velocity between molecules 1 and 2 and S the mutual-collision cross section. These same considerations show that molecules are thrown into cell 1 from collisions 3–4 and 5–6; therefore

$$G_1 = \tfrac{2}{3}cSN_3N_4 + \tfrac{2}{3}cSN_5N_6.$$

With these expressions for G_1 and L_1, Eq. (2.2) for cell 1 is:

$$(\partial N_1/\partial t) - c(\partial N_1/\partial x) = \tfrac{2}{3}cS(N_3N_4 + N_5N_6 - 2N_1N_2). \quad (2.3)$$

Similar equations apply to the five other velocity cells.

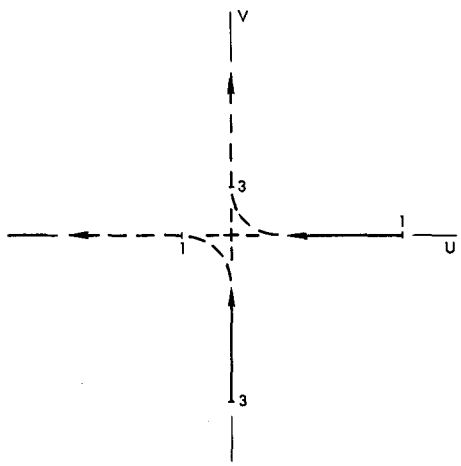

FIG. 3. The 1-3 collision.

III. THE INFINITE MACH NUMBER SHOCK WAVE

We wish to describe a shock wave in a flow from left to right along the x axis, i.e., in the u direction. While, as will be shown, it is possible to obtain such a wave in a gas with the molecular velocities in Fig. 1, the wave propagates at constant velocity. Since it is more convenient to work in shock-fixed coordinates, we add to the molecular velocities of Fig. 1, a velocity in the u direction, ξ, of magnitude to be determined later; the resulting velocities are shown in Fig. 4. For clarity only one of the velocity vectors is shown, $\mathbf{v}_3$; the others are indicated by the numbered points. As examples, $\mathbf{v}_3$ is the vector $[\xi, c, 0]$ and $\mathbf{v}_1$ is $[-(c - \xi), 0, 0]$.

The flow is symmetrical about the u axis so that $N_3 = N_4 = N_5 = N_6$. Furthermore all the N's are independent of y and z. Thus with the molecular velocities in Fig. 4 and for steady flow, Eqs. (2.2) become

$$\begin{aligned} -(c - \xi)(dN_1/dx) &= \tfrac{4}{3}cS(N_3^2 - N_1N_2) \\ (c + \xi)(dN_2/dx) &= \tfrac{4}{3}cS(N_3^2 - N_1N_2) \\ \xi(dN_3/dx) &= -\tfrac{2}{3}cS(N_3^2 - N_1N_2), \end{aligned} \quad (3.1)$$

where N_3 has been taken as the representative velocity off the u axis. (The expressions for $G_i - L_i$ are unaffected by the coordinate shift.)

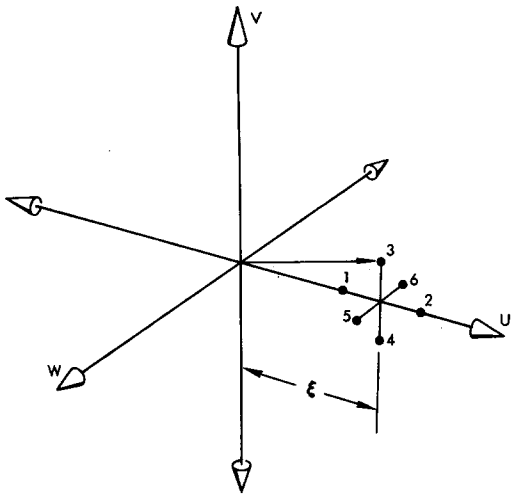

FIG. 4. The molecular velocities in shock-fixed coordinates.

It is convenient at this point to introduce the mean free path at some equilibrium reference state in which all the N_i's are equal. At such a state the collision rate of all the molecules in cell 1, for instance, is given by

$$\phi_1 = 2cSN_1N_2 + \sqrt{2}cSN_1(N_3 + N_4 + N_5 + N_6)$$
$$= 2(1 + 2\sqrt{2})cSN_1^2.$$

Then the collision frequency per molecule σ is determined by

$$\sigma = \phi_1/N_1 = 2(1 + 2\sqrt{2})cSN_1 = \tfrac{1}{3}(1 + 2\sqrt{2})cSn,$$

where n is the number density. By definition the mean free path, λ, is given by

$$\lambda = c/\sigma = 3/(1 + 2\sqrt{2})Sn.$$

Dividing Eqs. (3.1) by a reference number density, $n(r)$, and by c we get

$$-(1 - \xi/c)dn_1/d\eta = (n_3^2 - n_1n_2), \quad (3.2a)$$
$$(1 + \xi/c)dn_2/d\eta = (n_3^2 - n_1n_2), \quad (3.2b)$$
$$(-2\xi/c)dn_3/d\eta = (n_3^2 - n_1n_2), \quad (3.2c)$$

where

$$n_i = N_i/n(r), \qquad \eta = 4x/(1 + 2\sqrt{2})\lambda_r,$$

and λ_r represents the mean free path at the reference state.

Now let us look for a solution to Eqs. (3.2) representing an infinite-Mach-number shock wave, i.e., a wave with the upstream gas at zero temperature and pressure. Denote the upstream state, $x \to -\infty$, by (a) and the state for $x \to \infty$ by (b). If all the molecules at (a) are in cell 2 they constitute a stream with a fluid velocity $\bar{u}$ in the x direction, equal to $(\xi + c)$ and are at zero temperature. It is shown in the next paragraph that there is a state (b), connected to (a) by Eqs. (3.2), in which the molecules are equally distributed to the six cells and hence move with a fluid velocity equal to ξ, at a finite temperature and pressure. Then the solution connecting (a) and (b) will be found.

Division of Eqs. (3.2a) and (3.2c) by (3.2b) yields

$$\frac{(1 - \xi/c)}{(1 + \xi/c)}\frac{dn_1}{dn_2} = -1 \quad \text{and} \quad \frac{2\xi/c}{(1 + \xi/c)}\frac{dn_3}{dn_2} = -1.$$

Now let the reference state be (a); then $n_2(\text{a}) = 1$, $n_1(\text{a}) = n_3(\text{a}) = 0$, and thus

$$n_1 = \frac{(1 + \xi/c)}{(1 - \xi/c)}(1 - n_2) \quad \text{and} \quad n_3 = \frac{(1 + \xi/c)}{2\xi/c}(1 - n_2).$$

Next we look for a value of ξ/c such that there is a state (b) in which all the n_i's are equal. Equating n_1 to n_2 we find $\xi/c = \frac{1}{3}$. Then

$$n_1 = n_3 = 2(1 - n_2), \quad (3.3)$$

and the n_i's are equal when $n_2 = \frac{2}{3}$.

Note from the right-hand sides of Eqs. (3.2) that (a) and (b) are equilibrium states. Furthermore an observer moving with the gas (at velocity ξ) at (b) sees a symmetrical molecular distribution. It was to meet this latter condition that a state with equal n_i's was sought in the preceding determination of ξ. (There are no other pairs of symmetrical states in the present model.)

Recall that (a) has been chosen as the reference state. Then the number density at (b) is given by

$$n(\text{b}) = \sum N_i(\text{b}) = n(r) \sum n_i(\text{b}) = 4n(\text{a}),$$

and the density ratio across the shock is four as it is for a real monatomic gas.

With $\xi/c = \frac{1}{3}$ and with the help of Eq. (3.3), Eq. (3.2b) can be written in the form:

$$dn_2/d\eta = \tfrac{3}{2}(3n_2 - 2)(n_2 - 1). \quad (3.4)$$

The solution is

$$n_2 = (1 + 2e^{3\eta/2})/(1 + 3e^{3\eta/2}),$$

when the arbitrary constant has been chosen to make $n_2 = \frac{3}{4}$ at $\eta = 0$. Since n_1 and n_3 are given by Eq. (3.3), the solution is complete.

Remembering that $n_i = N_i/n(\text{a})$, we see that N_2, the number density of cell 2, falls from its initial value, $n(\text{a})$, to $\frac{2}{3}n(\text{a})$ as $x \to \infty$. The number density of each of the other five cells rises simultaneously from zero to $\frac{2}{3}n(\text{a})$. Hence as stated above, the total number density n increases by the factor four

through the wave. Within the wave, n is related to n_2 by the equation

$$n = \sum N_i = n(\mathrm{a})(n_1 + n_2 + 4n_3) = n(\mathrm{a})(10 - 9n_2).$$

The fluid velocity is determined by

$$\bar{u} = \frac{1}{n}\sum N_i u_i = \tfrac{2}{3}c(-n_1 + 2n_2 + 2n_3)\frac{n(\mathrm{a})}{n} = 4c/3(10 - 9n_2).$$

If we let $u^* = \bar{u}/c$ and observe that $u^*_{\mathrm{a}} = \frac{4}{3}$ and $u^*_{\mathrm{b}} = \frac{1}{3}$, we can put Eq. (3.4) in the form

$$du^*/dx = -[6/(1 + 2\sqrt{2})\lambda_{\mathrm{a}}](u^*_{\mathrm{a}} - u^*)(u^* - u^*_{\mathrm{b}}), \tag{3.5}$$

where λ_{a} is the mean free path in the hypersonic stream.[4] This equation is of the same form as that found by Mott-Smith[5] and by others,[6-9] using the two-fluid model.

The maximum slope shock thickness, Δ, defined by

$$\Delta = \frac{(u^*_{\mathrm{a}} - u^*_{\mathrm{b}})}{(du^*/dx)_{\max}},$$

is, from Eq. (3.5), equal to 2.55 λ_{a}. The Mott-Smith shock thickness is not unique; the arbitrariness arises in the choice of a function to be used with the collisional invariants in deriving a determinate equation system from the transport equation. Solutions are obtained for two functions and lead, for hard elastic spheres and infinite Mach number, to $\Delta = 2.14\ \lambda_{\mathrm{a}}$ and $\Delta = 1.58\ \lambda_{\mathrm{a}}$. The detailed quantitative results of the present model are probably not to be taken seriously, and therefore an extensive comparison with the other analyses will not be made.

Next it is of interest to examine the variation of the pressure, the normal viscous stress, and the total enthalpy through the wave.

Defining the pressure as the average normal momentum flux through planes perpendicular to axes moving with the fluid velocity $\bar{u}$, we have

$$p = \tfrac{1}{3}m\sum(V^2_{xi} + V^2_{yi} + V^2_{zi})N_i = \tfrac{1}{3}mn(\mathrm{a})\sum V_i^2 n_i,$$

where $\mathbf{V}_i = \mathbf{v} - \bar{u}$, $V_i = |\mathbf{V}|$, and m is the molecular weight.

Likewise the internal energy per unit mass e is the molecular kinetic energy in the moving coordinates. Thus

$$e = \frac{1}{2n}\sum V_i^2 N_i = \frac{n(\mathrm{a})}{2n}\sum V_i^2 n_i,$$

and the enthalpy, $h = e + p/\rho$, where $\rho = mn$, is given by

$$h = \frac{5}{6}\frac{n(\mathrm{a})}{n}\sum V_i^2 n_i.$$

With the above derived values for $\bar{u}$ and n_i, it is straightforward to show that

$$\sum n_i V_i^2 = \tfrac{8}{9}c^2[1 + n/n(\mathrm{a}) - 2n(\mathrm{a})/n].$$

Then

$$p = \tfrac{8}{27}mn(\mathrm{a})\,c^2[1 + n/n(\mathrm{a}) - 2n(\mathrm{a})/n].$$

The direct procedure for finding the normal viscous stress τ on a plane normal to the flow would be to derive an expression for the normal momentum flux through such a plane moving with velocity $\bar{u}$, and then to subtract the pressure. It is much simpler, however, to find τ from the hydrodynamical momentum equation. If Eqs. (3.1) are multiplied successively by the collisional invariants, m, mu_i, $\frac{1}{2}m|\mathbf{v}_i|^2$, and summed, the right-hand sides vanish, a consequence of the conservation of number, momentum, and energy in the collisions. The remaining terms can be written in the standard form:

$$(d/dx)(\rho\bar{u}) = 0, \tag{3.6a}$$

$$(d/dx)(\rho\bar{u}^2 + p - \tau) = 0, \tag{3.6b}$$

$$(d/dx)[\rho\bar{u}^2(h + \tfrac{1}{2}\bar{u}^2) + q - \tau\bar{u}] = 0, \tag{3.6c}$$

in which q is the heat flux in the x direction.

Now with the expressions for $\bar{u}$, ρ, and p derived above, τ can be found from Eq. (3.6b) to be

$$\tau = \tfrac{8}{27}mn(\mathrm{a})\,c^2[-5 + n/n(\mathrm{a}) + 4n(\mathrm{a})/n].$$

As expected τ vanishes at $n/n(\mathrm{a}) = 1$ and 4; it is a maximum at $n/n(\mathrm{a}) = 2$. It is also of interest to compare the behavior of $|\tau/p|$ with that derived by Liepmann, Narasimha, and Chahine[10] from the conservation equations and the condition $q - \tau u =$ constant. They show that for an infinitely strong shock in a monatomic gas $|\tau/p|$ has a maximum value of $\frac{3}{2}$ at the shock front and falls smoothly to zero at the downstream side. In the present case, $|\tau/p|$ has a maximum value of unity at the front and also falls to zero monotonically.

[4] Since the mean free path was defined for a state in which the N_i's were equal, it would perhaps be more rigorous to use state (b) as the reference state instead of (a). It is usual, however, to refer the shock thickness to λ_a, and in the present case it seems justified to apply formally the equation $\lambda = 3/(1 + 2\sqrt{2})Sn$ in state (a).

[5] H. M. Mott-Smith, Phys. Rev. **82**, 885 (1951).

[6] P. Glansdorff, in *Proceedings of the Second International Symposium on Rarefied Gas Dynamics*, edited by L. Talbot (Academic Press, Inc., New York, 1961).

[7] N. Rott and C. G. Whittenbury, Douglas Aircraft Company Report SM-38524 (1961).

[8] S. Ziering, F. Ek, and P. Koch, Phys. Fluids **4**, 975 (1961).

[9] P. Glansdorff, Phys. Fluids **5**, 371 (1962).

[10] H. W. Liepmann, R. Narasimha, and M. T. Chahine, Phys. Fluids **5**, 1313 (1962).

The total enthalpy $h_0 = h + \frac{1}{2}\bar{u}^2$ can be shown to be described by

$$h_0 = \tfrac{4}{27}c^2\{5 + 5n(\mathrm{a})/n - 4[n(\mathrm{a})/n]^2\}.$$

Thus h_0 has the value $8c^2/9$, equal to $\frac{1}{2}(u_a)^2$, at (a) and (b) and rises to a maximum of $8.75c^2/9$ within the shock. This is an increase of about 8% compared with a maximum of about 2% in the Navier–Stokes approximation (see Ref. 10).

IV. THE SPEED OF SOUND

To find the Mach number behind the shock and also to illustrate another interesting property of the six-cell gas, let us find the speed of sound in the gas, i.e., the speed of propagation of a weak disturbance. To do this, let the gas be at rest with a uniform number distribution. Again consider the wave to propagate along the x axis so that $N_3 = N_4 = N_5 = N_6$. Then Eqs. (2.2) become

$$(\partial N_1/\partial t) - c(\partial N_1/\partial x) = \tfrac{4}{3}cS(N_3^2 - N_1N_2),$$
$$(\partial N_2/\partial t) + c(\partial N_2/\partial x) = \tfrac{4}{3}cS(N_3^2 - N_1N_2),$$
$$(\partial N_3/\partial t) = -\tfrac{2}{3}cS(N_3^2 - N_1N_2).$$

Now if these equations are linearized by setting

$$n_i = N_i/n_0 = n^0 + n_i',$$

where n_0 is the initial total number density, n^0 the initial number fraction in each cell, and n_i' is a small perturbation, the resulting system of equations leads to a single equation for n_1', say,

$$\beta\frac{\partial}{\partial t}\left[\frac{\partial^2 n_1'}{\partial t^2} - c^2\frac{\partial^2 n_1'}{\partial x^2}\right] + \left[\frac{\partial^2 n_1'}{\partial t^2} - \frac{c^2}{3}\frac{\partial^2 n_1'}{\partial x^2}\right] = 0, \quad (4.1)$$

where

$$\beta = (1 + 2\sqrt{2})\lambda_0/2c.$$

This equation is of the general type treated by Whitham[11] and in particular has been shown to govern wave propagation in a chemically reacting gas.[12,13] In this latter application, β would be an effective reaction relaxation time, while c and $c/\sqrt{3}$ would be called the frozen and equilibrium sound speeds, respectively. Here the relaxation is associated with the flow of energy from the molecular motion directly induced in the x direction by the wave into the other two modes. Whitham shows that in general the lower-order terms in Eq. (4.1) cause an exponential decay of the wave propagating at speed c and that for times large compared with λ_0/c, the main disturbance moves at $c/\sqrt{3}$. In the latter situation the higher order terms cause the lower speed wave to diffuse.

To compare the equilibrium sound speed in Eq. (4.1) with the propagation of weak disturbances in a real gas, we must assign a meaning to c. Up to this point, c has been an arbitrarily chosen molecular speed and the results are independent of its magnitude. Here it seems reasonable to equate c to the mean thermal speed in the gas with which the model is being compared. (This is the usual assumption in elementary kinetic theory). Then, since the temperature of the six-cell gas cannot change in a weak disturbance, it is perhaps not surprising that the equilibrium speed, $c/\sqrt{3}$, is closer to the real isothermal speed, $(\pi/8)^{\frac{1}{2}}c$, than to the isentropic speed, $(\pi\gamma/8)^{\frac{1}{2}}c$. It is interesting that the disturbance moving with the molecular speed c succeeds, through the first term in Eq. (4.1), in producing at least one of the molecular effects on weak waves, i.e., the diffusion of the equilibrium wave.

Returning to the calculation of the Mach number, we call $c/\sqrt{3}$ the speed of sound in the six-cell gas, and hence find that the Mach number at (b) is given by

$$M(\mathrm{b}) = \sqrt{3}\bar{u}(\mathrm{b})/c = 1/\sqrt{3} = 0.58$$

compared with the correct value

$$[(\gamma - 1)/2\gamma]^{\frac{1}{2}} = 0.45.$$

V. CONCLUSION

The number of velocity cells in this example is so limited that the study should be considered mainly as an illustration of the method. The general reasonableness of the results and the ease with which they were obtained, however, strongly suggest the possibility of useful extensions. Increasing the number of molecular velocities is an improvement which is certainly possible, especially for linear problems or if numerical computation, for which the model is naturally suited, is considered. The effects of other intermolecular forces laws should be easily determined—varying the law simply varies the cell assignments of the molecules leaving the collisions—and it may even be possible to consider collisions in which internal degrees of freedom are excited. Finally, a method which leaves the physics of the collisions in such plain view should be helpful in developing intuitive ideas about flows for which the Navier–Stokes approximation may be inadequate.

[11] G. B. Whitham, Comm. Pure and Appl. Math. **XII**, 113 (1959).
[12] W. G. Vincenti, J. Fluid Mech. **6**, 481 (1959).
[13] F. K. Moore and W. E. Gibson, J. Aerospace Sci. **27**, 117 (1960).