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Higher Approximation in the Chapman-Enskog Expansion for Shock Structure*

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SUMMARY

The Chapman–Enskog expansion for the solution of the Boltzmann equation has been reexamined and certain inconsistencies in the procedure have been pointed out. For a steady state one-dimensional Boltzmann equation, the expansion is modified with the help of the PLK method. Macroscopic equations up to Burnett level of approximation are then obtained. Finally, these equations are used to examine the structure of a shock wave in a gas consisting of Maxwellian molecules. It is shown that new Burnett equations give solutions for all values of the Mach number.

1. Introduction

In order to obtain the steady state solution of the one-dimensional Boltzmann equation for the shock structure problem, various attempts using the Chapman–Enskog method, Grad's polynomial expansion and Mott–Smiths "Ansatz" method, have been made. Because of its simplicity and success with the strong shock structure problem, there have been efforts made to improve Mott–Smith's method; these have appeared in the form of the two fluid models of Glandsdroff, Yen, Ziering, etc. and the orthogonal polynomial expansion of Mintzer. Although Grad's Hermite polynomial expansion seems to have a mathematical basis as applied to the shock wave problem, its success has been limited to the case of weak shocks. Indeed, it is shown by Holway that Grad's expansion procedure is not convergent beyond Mach number 1.85.

The Chapman–Enskog expansion is usually presented as an expansion of the distribution function for the unsteady form of the Boltzmann equation. (Due to Hilbert's existence theorem). Due to the presence of the multiplicity of the time scales, one gets Euler's, Navier–Stokes and Burnett equations as the zero'th, 1st and 2nd approximations respectively. The higher approximations have not been carried out. As applied to the shock wave structure problem, the Navier–Stokes equations give continuous solutions for any Mach number but the Burnett equations do not give any solutions beyond Mach No. 2.1 (See Talbot and Sherman). Moreover, for the Burnett and higher levels of approximations the order of the governing equations increases, a feature which tends to complicate the meaning of the physical boundary conditions.

In the present paper an effort has been made to investigate the reason for the above result from the Burnett equations. It is found that for time-independent Boltzmann equation the expansion procedure does not satisfy certain compatibility relations. As a result the Boltzmann equations contain terms which are actually zero. Furthermore, it is found that the increase in the order of the differential equations is artificial and can be avoided by properly modifying the expansion procedure. The PLK method is used to find the Burnett level of conservation equations and it is shown that they give continuous solutions for any Mach number. This is carried out for only the one-dimensional case.

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2. Modified C–E Expansion

The steady state Boltzmann equation can be written as:

$$\xi_1 \frac{\partial f}{\partial x} = \int\int (f'f_1' - ff_1)\, gb\, db\, d\varepsilon\, d\zeta_i = J(f, f_1), \tag{1}$$

where f is the distribution function, ξ_i is the molecular velocity vector, g is the relative speed of the colliding molecules, b and ε are two geometric variables, f_1 is the value of f with ξ_i replaced by ζ_i, the velocity of the second particle. f' and f_1', are the values of f for velocities of two molecules after collisions. The Chapman–Enskog expansion amounts to expanding the distribution function as

$$f = f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \ldots . \tag{2}$$

In addition, we shall expand the independent variable as: (The reason for doing so will become clear later)

$$x = \frac{s}{\varepsilon} - x_1(s) + \varepsilon x_2(s) + \ldots , \tag{3}$$

where x_1, x_2 etc. are unknown functions to be determined later. Substituting (2) and (3) in (1) and equating like powers of ε, we get

$$\left.\begin{aligned} &J(f^{(0)}, f_1^{(0)}) = 0 , && \text{(i)} \\ &J(f^{(0)}, f_1^{(1)}) = \xi_1 \frac{\partial f^{(0)}}{\partial s} , && \text{(ii)} \\ &J(f^{(0)}, f_1^{(2)}) + J(f^{(1)}, f^{(1)}) = \xi_1 \left(\frac{\partial f^{(1)}}{\partial s} + x_1' \frac{\partial f^{(0)}}{\partial s} \right), && \text{(iii)} \end{aligned}\right\} \tag{4}$$

and etc., where prime over $x_1(s)$ stands for differentiation with respect to s. These are a set of linear singular integral equations. Comparing these with the usual C–E equation, we notice that the difference arises in equations for $f^{(2)}, f^{(3)}$ and etc. So the zero'th and first order solutions are similar in form to those obtainable by the ordinary expansion. As a consequence the conservation equations come out to be Euler's and Navier–Stokes respectively. It may be pointed out that this similarity of equations (4.i) and (4.ii) or the associated conservation equations with the corresponding C–E equations is only formal. In the present form either equations (4.i) and (4.ii) or the conservation equations are valid on a different length scale. The distribution functions for these cases may be written as:

$$f^{(0)} = \frac{n}{(2\pi RT)^{\frac{3}{2}}} \exp\{-[(\xi_1 - u)^2 + \xi_2^2 + \xi_3^2]/2RT\} , \tag{5}$$

$$f^{(1)} = f^{(0)} \left[\frac{p_{11}^{(1)}}{\frac{4}{3} pRT} (C_1^2 - \tfrac{1}{3} C^2) + \frac{q_1^{(1)}}{5pR^2T^2} C_1 (C^2 - 5RT) \right], \tag{6}$$

$$p = nkT, \quad R = k/m, \quad p_{11}^{(1)} = -\tfrac{4}{3}\mu \frac{du}{ds}, \quad q_1^{(1)} = -\tfrac{15}{4} R\mu \frac{dT}{ds},$$

where n, u and T are taken to be the local values of the number density, the x-component of mean velocity and the temperature respectively. μ is the coefficient of viscosity and for Maxwellian molecules it is proportional to the temperature T. Because of the definitions of n, u and T, all higher approximations contribute to the stress and heat flux only. The collision invariant moments of the Boltzmann equation with $f = f^{(0)} + f^{(1)}$ lead to Navier–Stokes equations with "s" as the independent variable.

In order to solve (4.iii) for $f^{(2)}$, the right hand side of it is required to satisfy certain solubility conditions. These are

$$\int \psi_i \xi_1 \left(\frac{\partial f^{(1)}}{\partial s} + x_1' \frac{\partial f^{(0)}}{\partial s} \right) d\xi_i = 0 , \tag{7}$$

where ψ_i are the collision invariants m, $m\xi_1$ and $\frac{1}{2}m\xi^2$. This gives us

$$\frac{d}{ds}(\rho u) = 0 ,$$

$$\frac{d}{ds}(p_{11}^{(1)}) + x_1'(s) \frac{d}{ds}(p + \rho u^2) = 0 ,$$

$$\frac{d}{ds}(q_1^{(1)} + u p_{11}^{(1)}) + x_1'(s) \frac{d}{ds}\left(\tfrac{5}{2} up + \rho \frac{u^3}{2} \right) = 0 . \tag{8}$$

In equation (8) ρ is the density, p the pressure, p_{11}^1 and $q_1^{(1)}$ are the Navier–Stokes stress and heat flux respectively and have been defined earlier. $x_1(s)$ is still unspecified. To the same degree of approximation, the ordinary Chapman–Enskog expansion leads to the Burnett equations and the corresponding solubility conditions for $f^{(2)}$ are then given as:

$$\frac{p_{11}^{(1)}}{dx} = 0 ,$$

$$\frac{d}{dx}(q_1^{(1)} + u p_{11}^{(1)}) = 0 . \tag{9}$$

In other words we can solve for $f^{(2)}$ provided equations (9) are somehow satisfied. Actually similar equations will have to by satisfied by $p_{11}^{(r)}$ and $q_1^{(r)}$ for the evaluation of $f^{(r)}$. Because of equation (9), the C–E expansion procedure becomes meaningless, as these are the expressions which appear in the form of stresses and heat flux in the conservation equations. Consequently, the Burnett equations not only contain certain terms which are actually zero but become meaningless. From a strict mathematical standpoint, it is the presence of these terms (which also increase the order of differential equations) which renders the Burnett, and thus higher approximation as well, more singular. In the present formulation the higher derivatives can be eliminated from the right hand side of (4.iii) by the use of equations (8). As a consequence $p_{11}^{(2)}$ and $q_1^{(2)}$ will not contain these higher order derivatives.

Now without actually solving equation (4.iii) for $f^{(2)}$, we can find out its contribution to the stress and heat flux. This we will do for Maxwellian molecules only.

Stress equation

Multiplying equation (4.iii) by ξ_1^2 and integrating over the velocity space we get

$$\frac{d}{ds}(\tfrac{6}{5} q_1^{(1)} + 3 u p_{11}^{(1)}) + x_1'(s) \frac{d}{ds}(3up + \rho u^3) = -\beta \rho p_{11}^{(2)} . \tag{10}$$

where $\beta = RT/\mu$.

Now using equations (8) to eliminate the derivatives of $p_{11}^{(1)}$ and $q_1^{(1)}$, we get

$$\tfrac{9}{5} p_{11}^{(1)} \frac{du}{ds} - x_1'(s) \left[\tfrac{9}{5} u \frac{dp}{ds} + \rho u^2 \frac{du}{ds} \right] = -\beta \rho p_{11}^{(2)} . \tag{11}$$

Heat flux

Again multiplying equation (4.iii) by $\xi^2 \xi_1$ and integrating over the velocity space, we get

$$\frac{d}{ds}(7RT p_{11}^{(1)} + 5u^2 p_{11}^{(1)} + \tfrac{32}{5} u q_1^{(1)}) + x_1'(s) \frac{d}{ds}(8u^2 p + 5pRT + \rho u^4) = -2\beta p (u p_{11}^{(2)} + \tfrac{2}{3} q_1^{(2)}) . \tag{12}$$

Using equations (8) and (11), we get

$$\left(\tfrac{32}{5}q_1^{(1)}\frac{du}{ds}+7p_{11}^{(1)}\frac{dRT}{ds}\right)+x_1'(s)\left[5p\frac{dRT}{ds}-2RT\frac{dp}{ds}-7up\frac{du}{ds}-3u^2\frac{dp}{ds}\right]=-\tfrac{4}{3}\beta\rho q_1^{(2)}. \tag{13}$$

Equations (11) and (13) are the requisite equations determining the Burnett stress and heat flux respectively. If we write

$$p_{11}=p_{11}^{(1)}+p_{11}^{(2)}, \qquad q_1=q_1^{(1)}+q_1^{(2)},$$

$$p_{11}^{(1)}=-\tfrac{4}{3}\mu\frac{du}{ds}, \qquad q_1^{(1)}=-\tfrac{15}{4}\mu\frac{dRT}{ds}, \qquad h=C_pT,$$

C_p being the specific heat at constant pressure, we get

$$-\beta\rho p_{11}=\tfrac{4}{3}p\frac{du}{ds}\left[\left(1-\frac{9}{5}\frac{\mu}{p}\frac{du}{ds}\right)-x_1'(s)\left(\frac{27}{20}\frac{u}{h}\frac{dh}{du}-\frac{27}{20}+\frac{15}{8}\frac{u^2}{h}\right)\right], \tag{15}$$

$$\beta\rho q_1=\tfrac{3}{2}p\frac{dh}{ds}\left[1-\frac{20}{3}\frac{\mu}{p}\frac{du}{ds}+x_1'\left\{\frac{3}{5}-\frac{3}{2}\frac{u^2}{h}+\left(\frac{2}{5}\frac{h}{u}-2u\right)\frac{du}{dh}\right\}\right]. \tag{16}$$

Equations (15) and (16) are the expression for stress and heat flux up to this order of approximation. $x_1(s)$ in these equations is still unspecified. Its choice is subject to two restrictions, viz. equation (8) does not reduce to (9) and the resulting conservation equations are no more singular then Navier–Stokes equations; consequently, its choice depends upon the particular problem we are dealing with. It may be pointed out that these restrictions do not help us to prescribe $x_1(s)$ uniquely. But this non-uniqueness in the choice of straining is inherent in the PLK method [see Van Dyke]. The best choice could be governed either by some physical criteria, e.g. resulting values of $p_{11}^{(2)}$ and $q_1^{(2)}$ should be maximum and positive or the rate of convergence of the asymptotic series be maximum. However, whatever value of $x_1(s)$ we choose which is compatible with the above requirements, the difference in the two asymptotic solutions should be of the order of the approximation.

In the next section we shall use these equations to examine the structure of a shock wave.

3. Shock-Wave Structure

The conservation equations are

$$\text{Mass:} \qquad \frac{d}{dx}(\rho u)=0,$$

$$\text{Momentum:} \qquad \frac{d}{dx}[\rho u^2+p+p_{11}]=0,$$

$$\text{Energy:} \qquad \frac{d}{dx}\left[\rho u\left(h+\frac{u^2}{2}\right)+up_{11}+q_1\right]=0. \tag{17}$$

The equation of state for a perfect monatomic gas is

$$p=R\rho T.$$

p_{11} and q_1 are obtained in the last section. If the subscript "0" refers to free stream conditions, we get, after integration of equations (17):

$$\begin{aligned}&\rho u=\rho_0u_0,\\ &p_{11}+p+\rho u^2=p_0+\rho_0u_0^2,\\ &q_1+up_{11}+\rho_0u_0\left(h+\frac{u^2}{2}\right)=\rho_0u_0\left(h_0+\frac{u_0^2}{2}\right).\end{aligned} \tag{18}$$

Non-dimensionalizing the various quantities with respect to free stream conditions as

$$\frac{h}{h_0} = g\,, \quad \frac{u}{u_0} = v\,, \quad \frac{\mu}{\mu_0} = g\,,$$

$$\frac{sp_0}{\mu_0 u_0} = \eta\,, \quad \frac{x_1(s)p_0}{\mu_0 u_0} = y_1(\eta) \text{ and etc.},$$

utilizing equations (15) and (16), we get

$$g\frac{dv}{d\eta}\left[1-\tfrac{9}{5}v\frac{dv}{d\eta} - y_1'(\eta)\left(\tfrac{5}{4}M_\infty^2\frac{v^2}{g} + \frac{27}{20}\frac{v}{g}\frac{dg}{dv} - \frac{27}{20}\right)\right] = -\tfrac{5}{4}M_\infty^2 F(v,g)\,, \tag{19}$$

$$g\frac{dg}{d\eta}\left[1-\tfrac{20}{3}v\frac{dv}{d\eta} + y_1'(\eta)\left(\tfrac{3}{5}-M_\infty^2\frac{v^2}{g} + \frac{2}{5}\frac{g}{v}\frac{dv}{dg} - \tfrac{4}{3}M_\infty^2 v\frac{dv}{dg}\right)\right] = -\tfrac{10}{9}M_\infty^2 G(v,g)\,, \tag{20}$$

where $F(v,g) = 1-v + \dfrac{1}{\gamma M_\infty^2}(1-g/v)$,

$$G(v,g) = \left(\frac{1-g}{\gamma} - \frac{\gamma-1}{\gamma}v\right) + \frac{\gamma-1}{2}M_\infty^2(1-v)^2\,, \text{ with } \gamma = \tfrac{5}{3}\,,$$

and M_∞ is the free stream Mach number. In the present paper the following two choices of $y_1'(\eta)$ are considered:

$$\text{(i)} \quad \frac{dy_1}{d\eta} = -\frac{36}{25}\frac{g}{M_\infty^2 v}\frac{dv}{d\eta}\,,$$

$$\text{(ii)} \quad \frac{dy_1}{d\eta} = \frac{\tfrac{4}{3}v\dfrac{dv}{d\eta}}{1-\dfrac{v}{g}\dfrac{dg}{dv}} \tag{21}$$

Both of these expressions are obtained from equation (11). For these choices of y_1', $p_{11}^{(2)}$ and $q_1^{(2)}$ are positive throughout the shock wave structure although not necessarily maximum. Furthermore, $p_{11}^{(2)}$ and $q_1^{(2)}$ vanish when $p_{11}^{(1)}$ and $q_1^{(1)}$ tend to zero in the two boundary equilibrium states. Since, for the shock wave problem, $dv/d\eta < 0$, it can be seen very easily that equations (24) and (25) are no more singular than the corresponding Navier–Stokes equations. The only two singular points are the upstream and downstream states. The former or the supersonic state is a node while the subsonic state in the phase plane is a saddle point. Since the qualitative picture of the phase plane, in the present case, comes out to be the same as that for the Navier–Stokes case, the reasoning of Gilbarg and Paolucci can now be extended to the present case to show the existence of a unique integral curve joining the singular points. Utilizing their scheme of integration, equations (24) and (25) have been integrated numerically for various Mach numbers and the results of the calculations are presented in Figures 1. These plots are for density and the abscissa is $(\eta - y_1)$. The origin is taken to be the downstream end—the starting point of calculations and no effort is made to shift the origin or stretch the scale. The solid line corresponds to (21.ii) while the dashed curves are the corresponding Navier–Stokes profiles. The other set of the curves corresponds to the other choice of y_1'. Figures 2 are the plots of (y_1) *vs.* η. Again the solid curve is the solution of (21.ii) and the dashed curve corresponds to (21.i). Finally, in Figures 3, the present solution is compared with the Mott–Smith profiles. This has been achieved by shifting the origin appropriately.

4. Discussion

In this report the method of Chapman and Enskog for the solution of the Boltzmann equation is reexamined. As applied to a steady state one-dimensional problem, certain inconsistencies

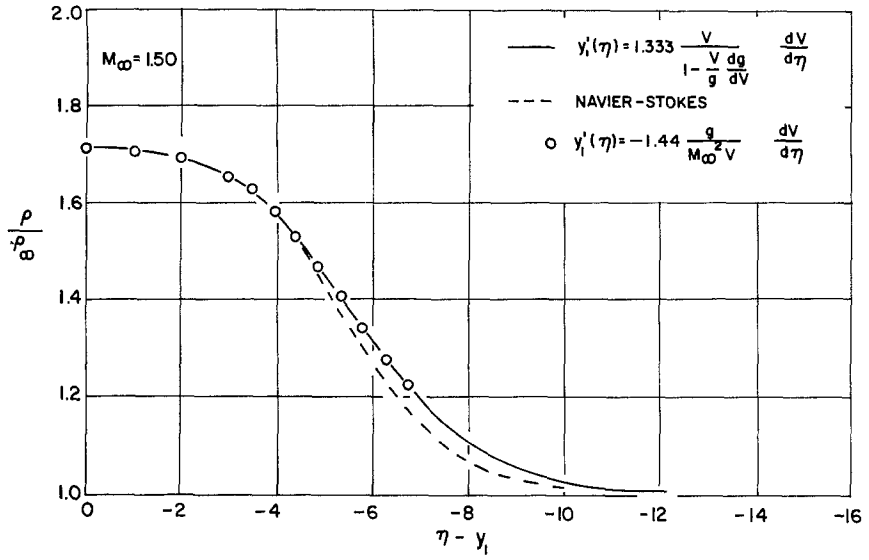

Fig. 1a

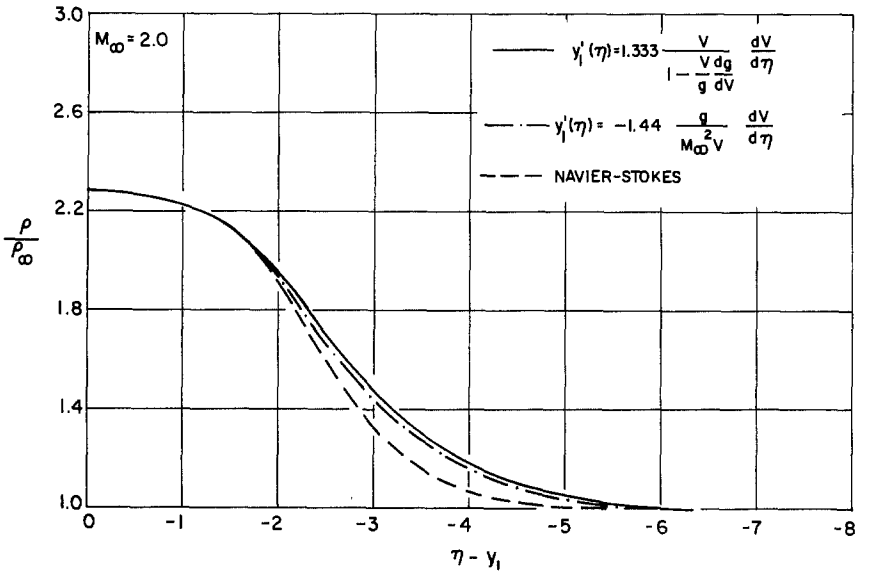

Fig. 1b

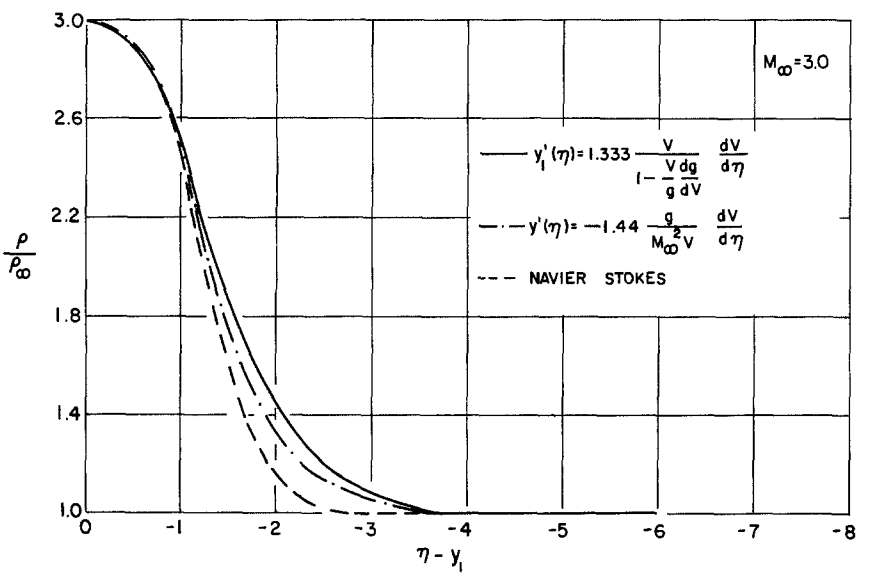

Fig. 1c

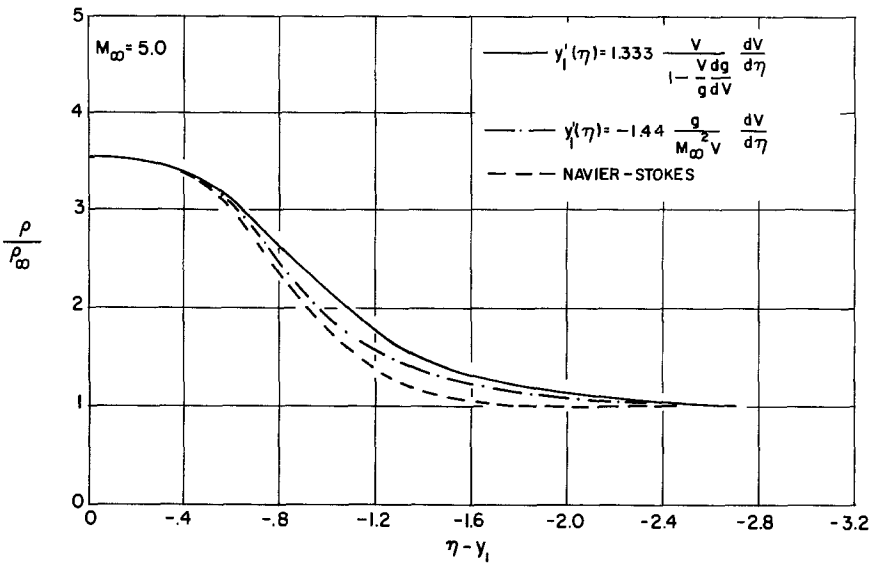

Figure 1d. Density distribution.

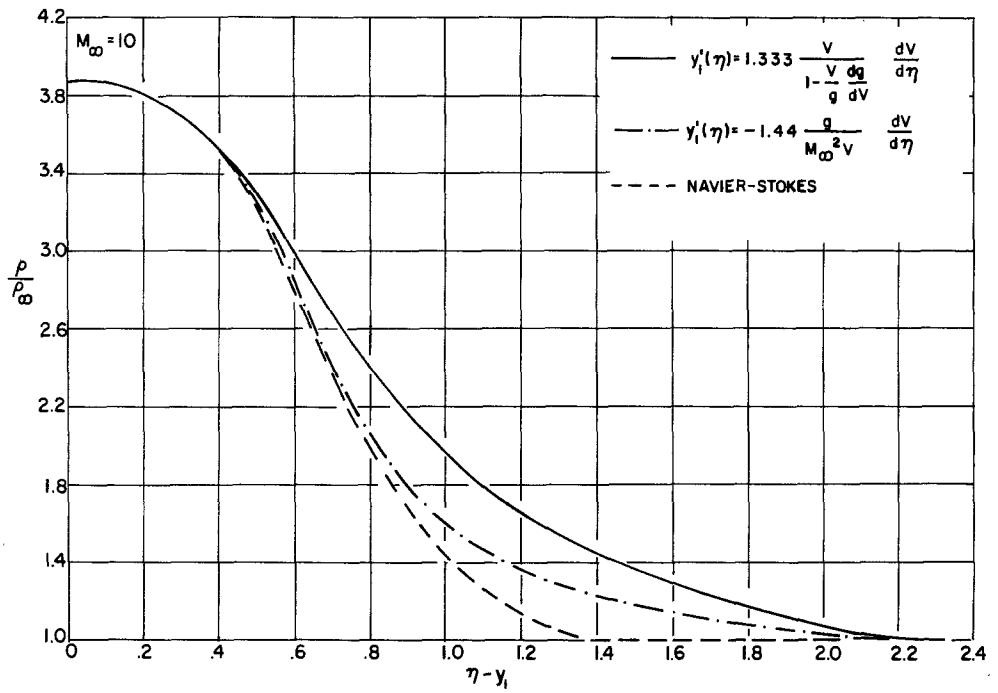

Figure 1e. Density distribution.

Figure 1a. Density distribution.

◀ Figure 1b. Density distribution.

Figure 1c. Density distribution.

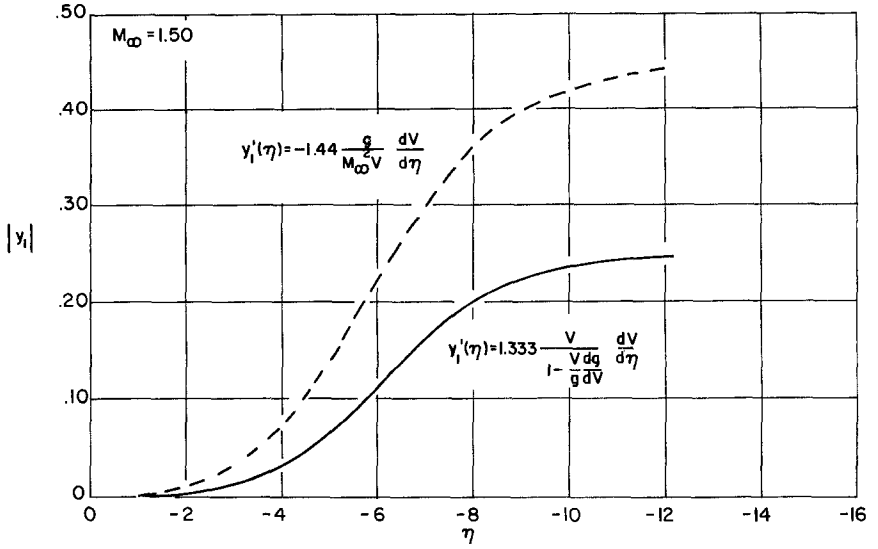

Fig. 2a

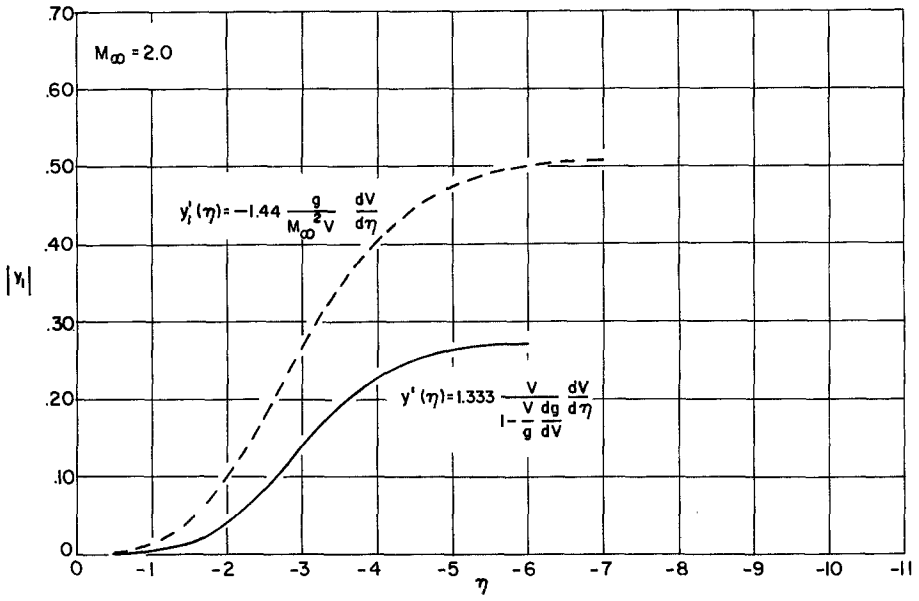

Fig. 2b

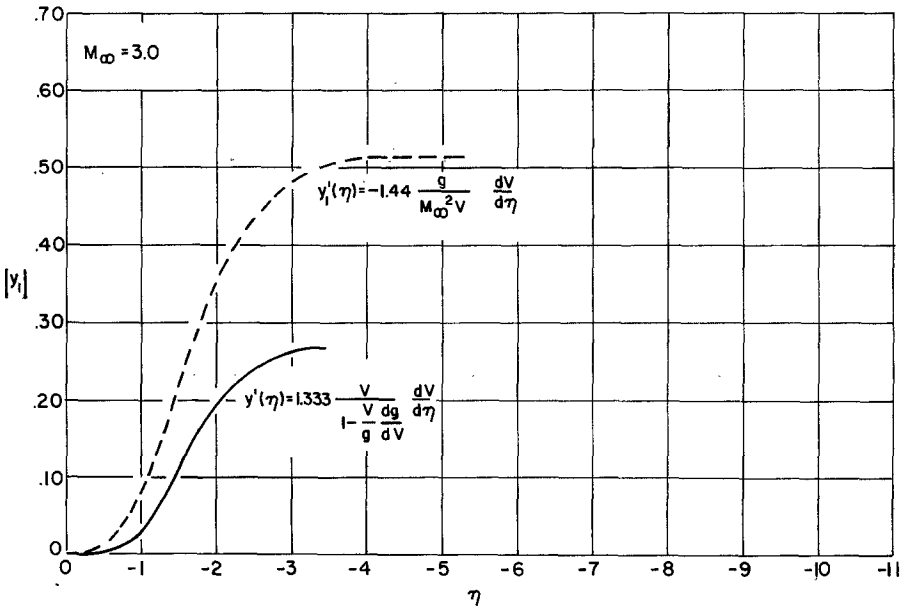

Fig. 2c

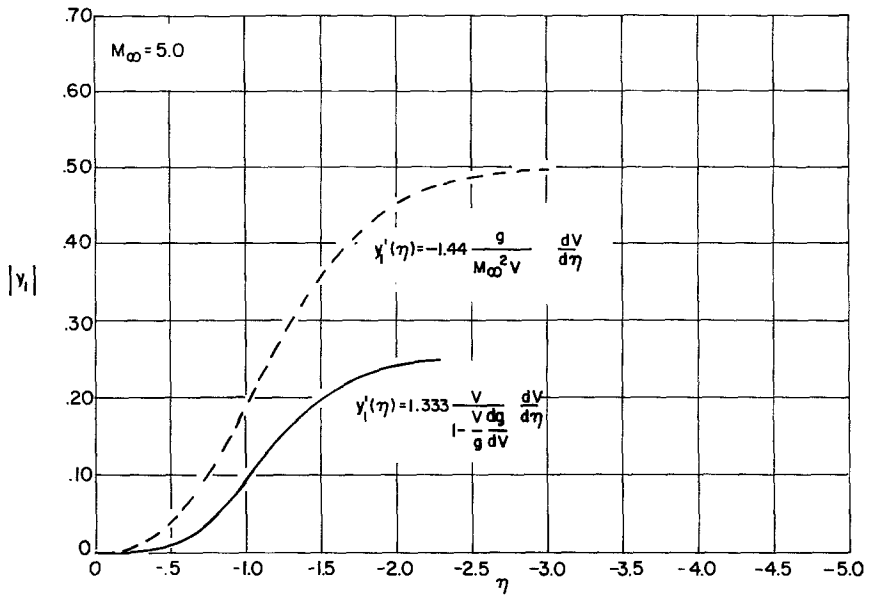

Figure 2d. Normalized straining.

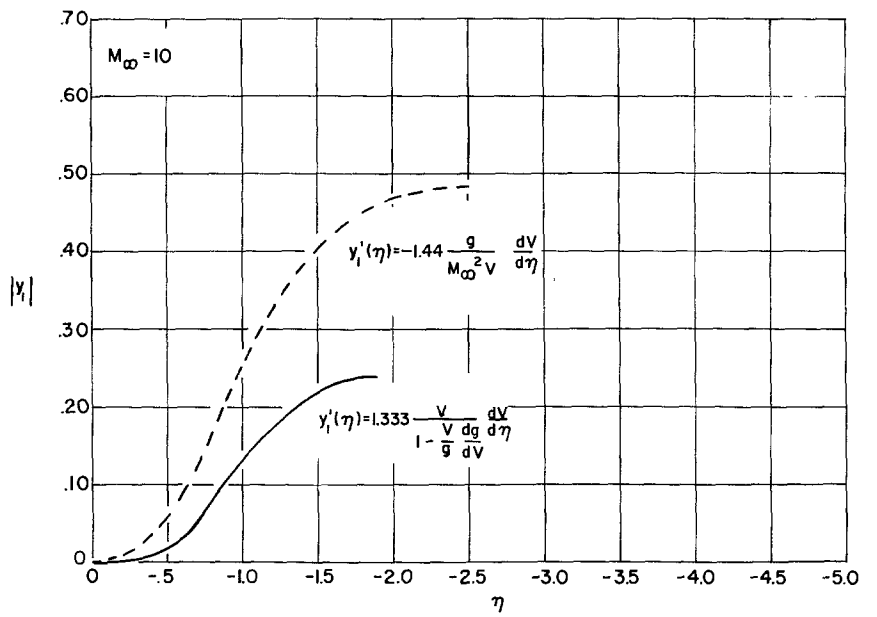

Figure 2e. Normalized straining.

Figure 2a. Normalized straining.

◀ Figure 2b. Normalized straining.

Figure 2c. Normalized straining.

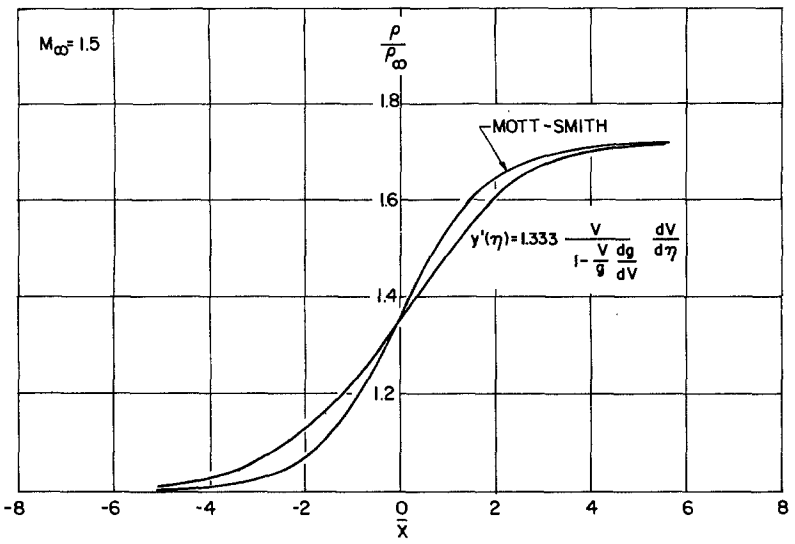

Fig. 3a

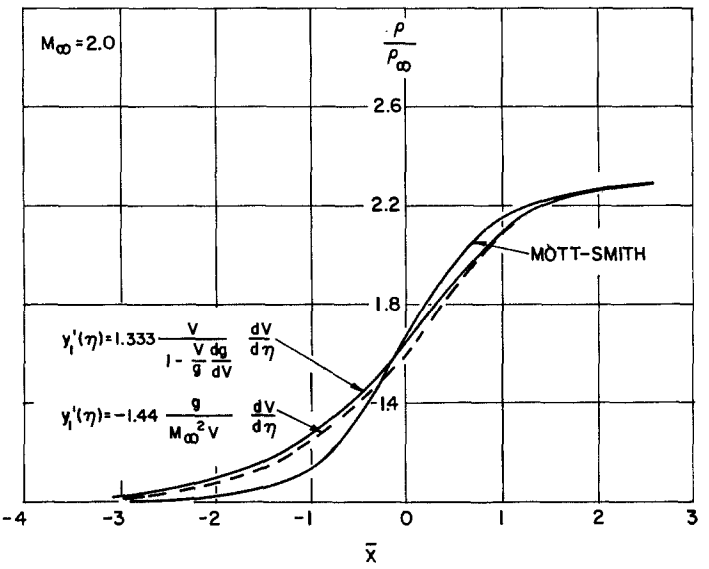

Fig. 3b

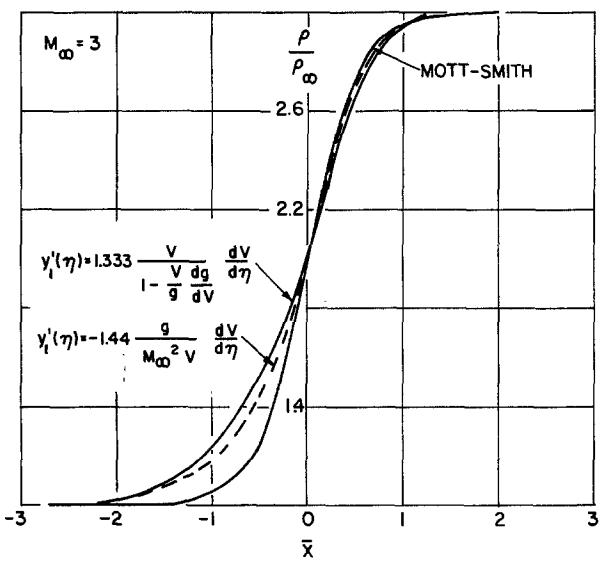

Fig. 3c

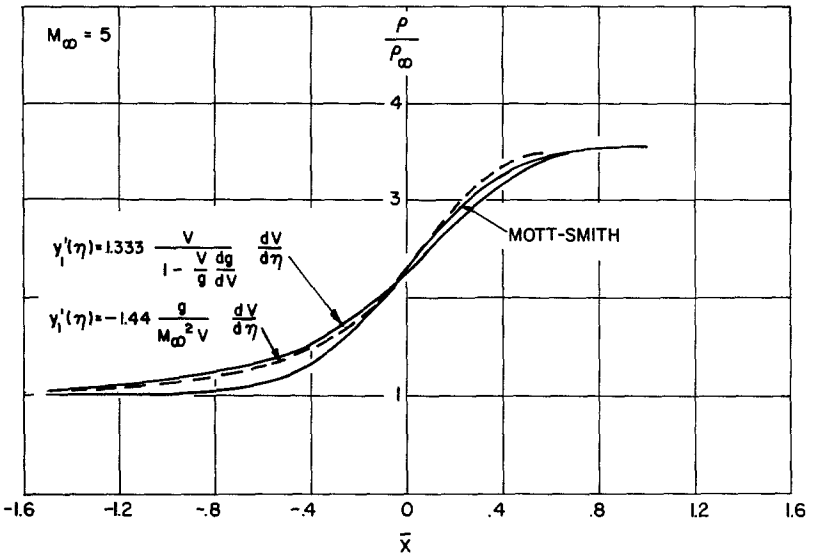

Figure 3d. Density distribution.

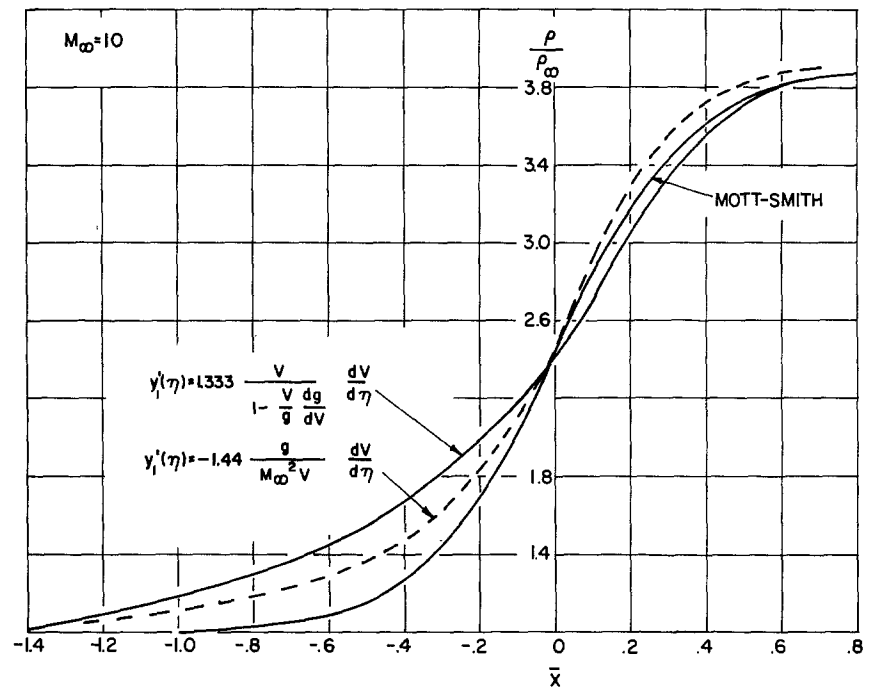

Figure 3e. Density distribution.

Figure 3a. Density distribution.

Figure 3b. Density distribution.

Figure 3c. Density distribution.

in the use of the method are pointed out. The Burnett equations, rather the whole expansion procedure becomes meaningless when it is applied to a steady state problem. In order to remove these inconsistencies, the expansion procedure is modified by the use of the PLK method. To the Burnett level of approximation it is found that the governing equations are no more singular than the Navier–Stokes equations and so the continuous solutions exist for all Mach numbers.

From the figures one can easily notice that higher order stresses and heat fluxes tend to thicken the shock.

For a weak shock the various choices of $y_1'(\eta)$ (including one which blows up for higher Mach numbers) did not improve very much upon the corresponding Navier–Stokes solution other than for few points on the upstream side of the shock. For $M_\infty = 1.2$, these solution curves could not be distinguished from the Navier–Stokes profile. This supports the earlier conclusions of other investigators about the validity of the Navier–Stokes equations for the shock wave problem. For higher Mach numbers the choice of y_1' does influence the density profiles. If the maximum value of $|x_1(s)|/s$ achieved within the shock is taken to be some criteria for the rate of convergence of the asymptotic series, then the solution with minimum $|x_1|/s$ should give a better approximation to the actual solution to the problem. Although the relative importance of various choices of $x_1(s)$ could be examined beforehand from equations (21), we have made a plot of $y_1(\eta)$ *vs.* η (Figures 2) for both the choices of y_1'. According to the above-mentioned criteria, the choice (21.ii) for y_1' should give a better approximation than the other choice. Figures 3 shows a fairly good agreement with Mott–Smith's solutions. The relative position of the solid curve with respect to Mott–Smith's profiles is in agreement with other approximate solutions. This gives some support to our criteria for the choice of the straining.

The application of this method to any other intermolecular potential is straightforward and does not lead to any conceptual difficulties. Omitting the small terms due to $J(f^{(1)}f^{(1)})$, a sample calculation for hard sphere molecules was made and results do show considerable improvement over the Navier–Stokes solution. Two basic questions about the present method are left open—some physical criteria for the choice of $x_1(s)$ and how the method takes into account the behavior of fast particles.

REFERENCES

[1] H. Grad, The Profile of a Steady Shock Wave, *Comm. Pure and Appl. Maths.*, 5, 3, 257 (1952).
[2] H. M. Mott–Smith, Solution of the Boltzmann Equation for a Shock Wave, *Phys. Rev.* series 2, 82, 6, 885 (1951).
[3] P. Glandsdorff, Solution of the Boltzmann Equation for Strong Shock Waves by the Two Fluid Model. *Phys. Fluids*, 5, 6, 1371 (1962).
[4] S. M. Yen, Approximate Solution of the Boltzmann Equation for a Shock Wave. AVCO Corporation, Technical Memo. RAD-TM-66-9, March 1966.
[5] S. Ziering and others, Extension of the Mott-Smith Method for a One-Dimensional Shock Wave. *Phys. Fluids*, 7, 2, 180 (1964).
[6] D. Mintzer and S. H. Radin, Orthogonal Polynomial Solutions of the Boltzmann Equation for a Strong Shock Wave. *Phys. Fluids*, 9, 9, 1621 (1966).
[7] L. H. Holway, Jr., Existence of Kinetic Theory Solutions to the Shock Structure Problem, *Phys. Fluids*, 7, 911 (1966).
[8] S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases, Cambridge University Press, London (1960).
[9] D. Gilbarg and D. Paolucci, The Structure of Shock Waves in the Continuum Theory of Fluids. *J. Rational Mech. Anal.*, 2, 4, 617 (1954).
[10] F. S. Sherman and L. Talbot, Experiment versus Kinetic Theory for Rarefied Gases, *Proc. of 1st International Symposium on Rarefied Gas Dynamics* (1960), Pergamon Press.
[11] M. Van Dvke, Perturbation Methods in Fluid Mechanics, Academic Press, Inc., 1964.