Method of Characteristics Description of Brownian Motion Far from Equilibrium

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Method of Characteristics Description of Brownian Motion Far from Equilibrium

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Abstract

The far-from-equilibrium Brownian motion of small particles or heavy molecules inmersed in a carrier gas may be described by closed hydrodynamic equations in the limit where their speed of thermal agitation is much smaller than their convective velocity (a hypersonic closure). The corresponding hyperbolic governing equations are studied in this paper through the method of characteristics. In two-dimensional and axisymmetric problems, the original system of seven partial differential equations is reduced to a set of seven ordinary differential equations along five different characteristic directions that we determine algebraically. Three of the characteristic paths coincide with the particle trajectories, and the two other pairs originate from two distinct signal propagation modes. The method is implemented numerically in two problems (Prandtl-Meyer expansion and Gaussian wake), leading to an excellent agreement between the numerical results from the characteristic equations and analytical solutions derived by asymptotic integration of the kinetic Fokker-Planck equation. The Prandtl-Meyer problem illustrates the failure of the hypersonic closure, when used blindly in the vicinity of singular points, though the associated errors in the density are tolerably small.

I. Introduction

The motion of a far-from-equilibrium phase of small particles or heavy molecules inmersed in a light carrier gas cannot be described by the standard near-equilibrium Chapman-Enskog closure of the hydrodynamic equations for binary gas mixtures. Instead, more complex kinetic formulations such as those provided by the Fokker-Planck equation have to be used.[1] Fortunately, in many problems of interest, the smallness of the particles' thermal speed compared to typical values of the mean velocity, opens the door to a hypersonic closure of the hydrodynamic equations, even in situations where the carrier gas is subsonic.[2,3] The thesis of Fernández-Feria[2] (see also Ref. 3) reviews previous instances where the hypersonic condition of gases has been used to close the hydrodynamic equations. In particular, the moment equations can be closed by dropping the heat flux term in the equation for the pressure tensor while retaining (in contrast to previous deterministic formulations[4]) the pressure term in the momentum equation, thus accounting for the Brownian motion or diffusion of the particles[2,3]:

$$D\lambda_p + \nabla\cdot U_p = 0 \qquad (1)$$

$$DU_p + \frac{k}{m_p}[(T_p\cdot\nabla)\lambda_p + \nabla\cdot T_p] = (U - U_p)/\tau \qquad (2)$$

$$DT_p + (T_p\cdot\nabla)\, U_p + ((T_p\cdot\nabla)\, U_p)^T = 2(TI - T_p)/\tau \qquad (3)$$

where $\lambda_p = \log(\rho_p/\rho_{p0})$, ρ_{p0} is a reference density for the particles, U_p and U are the mean particle and fluid velocity, $D \equiv \partial/\partial t + U_p\cdot\nabla$ and τ is the relaxation time, related to the first approximation of the diffusion coef-ficient D given by the Chapman-Enskog theory for binary mixtures[5] by

$$\tau = m_p D(n + n_p)/(nkT)$$

The quantities n and n_p are the number densities of carrier gas and particles, respectively, k is Boltzmann's constant, m_p is the mass of the particles, and the superscript T denotes a transposed tensor. It can be shown[2] that, away from singular points, Eqs. (1-3) yield errors of the order of M_p^{-3} for the density and the mean velocity and $O(M_p^{-1})$ for the temperature, where

$$M_p = U_p/(kT_p/m_p)^{1/2} >> 1 \qquad (4)$$

is a sort of a Mach number or speed ratio of the particles and $T_p \equiv \mathrm{Trace}(T_p)/3$. Moreover, these errors are considerably reduced [to $O(M_p^{-4})$ and $O(M_p^{-2})$, respectively] when the heat flux term vanishes initially.

In this paper, the hyperbolic nature of Eqs. (1-3) when M_p is sufficiently large, is exploited to reduce them from a system of partial

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differential equations into a set of ordinary differential equations along the characteristics of the problem. In the case of two-dimensional (2D) and axisymmetric steady problems, the characteristic directions at a given point are obtained explicitly as a function of the local particle density, velocity and temperature tensor. We shall show in Sec. II, that three of the seven characteristic degenerate into the particle trajectories, and the remaining two pairs intersect the streamlines at angles whose interpretation is similar to that of the Mach angle in supersonic gas dynamics: the sine of these angles is the ratio between the transversal propagation of perturbations at a speed $c_i \approx (\gamma_i k T_{nn}/m_p)^{1/2}$ and the particles' mean velocity U_p. T_{nn} is the component of the temperature tensor perpendicular to the streamline and γ_i is 1 for one pair of characteristics and 3 for the other. The expression for c_i is an approximation based on the smallness of M_p^{-1}.

The fact that the characteristic directions are known algebraically allows for a relatively simple numerical implementation of the method following the algorithm described in the Appendix. In Sec. III, the method is applied to two problems: The dispersion of an initially concentrated distribution of particles (we shall refer to it as the wake problem) and the two-dimensional version of this same problem when the initial distribution of particles is a step-function (which we shall denote as the a Prandtl-Meyer problem by analogy to the Prandtl-Meyer expansion of a pure gas into a vacuum). Explicit (asymptotic) kinetic solutions of the Fokker-Planck equation for these two problems are given here for the first time. The excellent agreement obtained when comparing the two pairs of kinetic and hydrodynamic solutions for both problems confirms the reliability (whenever no strong singularities are present) of the hypersonic approximation (1-3) as well as the usefulnessof the method of characteris-tics as a tool to analyze Brownian motion in more complex gas flow configurations. On the other hand, the limitations of Eqs. (1-3) used blindly in the vicinity of singular points are illustrated in the Prandtl-Meyer problem.

II. Method of Characteristics

A. Description of the method

The hypersonic truncation of the moment equations carried out in Eqs. (1-3) relies on the smallness of the particles' thermal speed compared to their mean velocity. Notice that, following the development in Ref. 2, the heat flux term, which is $O(M_p^{-1})$ compared to the convective term, has been dropped in Eq. (3), but the pressure term (proportional to k/m_p) in Eq. (2) has been retained so as to account for the Brownian motion of the particles, even though it is also small compared to the leading DU_p term. The close connection

between this pressure term and Brownian motion is physically evident from the fact that both are direct consequences of thermal agitation. Bringing Eqs. (1-3) to normalized form displays the small parameter underlying the truncation. The variables are replaced by their dimensionless counterparts

$$U_p \leftarrow U_p/U_R, \mathcal{T}_p \leftarrow \mathcal{T}_p/T_R, \ U \leftarrow U/U_R, \ T \leftarrow T/T_R, \ x \leftarrow x/L_R \qquad (5)$$

where U_R, L_R, T_R are characteristic values of the velocity, geometric scale, and temperature in the flow, respectively. Only steady problems are considered and the following parameters are introduced:

$$S = U_R\tau/L_R, \qquad \varepsilon^2 = kT_R/(m_p U_R^2) \qquad (6)$$

where S is the so-called Stokes number and ε, proportional to the inverse of M_p, is very small. Equations (1-3) then become

$$D\lambda_p = -\nabla\cdot U_p \qquad (7)$$

$$DU_p + \varepsilon^2 [(\mathcal{T}_p\cdot\nabla)\lambda_p + \nabla\cdot\mathcal{T}_p] = (U - U_p)/S \qquad (8)$$

$$D\mathcal{T}_p + (\mathcal{T}_p\cdot\nabla)U_p + [(\mathcal{T}_p\cdot\nabla)U_p]^T = 2(T\mathcal{I} - \mathcal{T}_p)/S \qquad (9)$$

Under the assumption that the geometry of the flow is 2D or axisymmetric, Eqs. (7-9) can be rewritten in a canonical matrix form. Let (x,y) be the axial and radial coordinates in axisymmetric problems (or any plane coordinates in 2D), and let z stand for the azymuthal coordinate or the direction perpendicular to the plane, respectively. From symmetry considerations, $T_{xz} = T_{yz} = 0$, and the velocity component along z is zero. If (u,v) are the components of the particle velocity at (x,y) and (u',v') their carrier gas counterparts, Eqs. (7-9) can be written as

$$\mathcal{A}\cdot\partial\omega/\partial x + \mathcal{B}\cdot\partial\omega/\partial y = b \qquad (10)$$

where

$$\omega = \{\lambda_p, u, v, T_{xx}, T_{xy}, T_{yy}, T_{zz}\}^T$$

$$b = \{-\beta v/y, (u'-u)/S - \varepsilon^2\beta T_{xy}/y, (v'-v)/S - \varepsilon^2\beta(T_{yy}-T_{zz})/y, 2(T-T_{xx})/S, -2T_{xy}/S, 2(T-T_{yy})/S, 2(T-T_{zz})/S - 2v\beta T_{zz}/y\}^T$$

β=0,1 for 2D and axisymmetric geometries, respectively, and

$$\mathcal{A} = \begin{bmatrix} u & 1 & 0 & 0 & 0 & 0 & 0 \\ \varepsilon^2 T_{xx} & u & 0 & \varepsilon^2 & 0 & 0 & 0 \\ \varepsilon^2 T_{xy} & 0 & u & 0 & \varepsilon^2 & 0 & 0 \\ 0 & 2T_{xx} & 0 & u & 0 & 0 & 0 \\ 0 & T_{xy} & T_{xx} & 0 & u & 0 & 0 \\ 0 & 0 & 2T_{xy} & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u \end{bmatrix}$$

$$B = \begin{bmatrix} v & 0 & 1 & 0 & 0 & 0 & 0 \\ \varepsilon^2 T_{xy} & v & 0 & 0 & \varepsilon^2 & 0 & 0 \\ \varepsilon^2 T_{yy} & 0 & v & 0 & 0 & \varepsilon^2 & 0 \\ 0 & 2T_{xy} & 0 & v & 0 & 0 & 0 \\ 0 & T_{yy} & T_{xy} & 0 & v & 0 & 0 \\ 0 & 0 & 2T_{yy} & 0 & 0 & v & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & v \end{bmatrix}$$

Equation (10) is a first-order system of nonlinear partial differential equations where all derivatives enter linearly. The slope y' of its characteristic direction results from solving the associated eigenvalue problem

$$\lambda \cdot B = y' \lambda \cdot A \qquad (11)$$

If Eq. (10) is multiplied on the left by one eigenvector λ, and y' is rewritten as

$$y' = \tan\theta \qquad (12)$$

the following results:

$$\lambda \cdot A \cdot (\cos\theta\, \omega_x + \sin\theta\, \omega_y) = \lambda \cdot b \cos\theta \qquad (13)$$

Then, along each characteristic direction θ (determined by each of theeigenvalues y'), an ordinary differential equation can be written as

$$\lambda \cdot A \cdot d\omega/ds = \lambda \cdot b \cos\theta \qquad (14)$$

where s is the length measured along the characteristic defined by y'.

Although the characteristic equation associated with the eigenvalue problem (11) is of order seven, the determinant of B - y'A may be factorized exactly to yield the following equation for y':

$$(v-y'u)^3\{(v-y'u)^2-\varepsilon^2(T_{yy}-2y'T_{xy}+y'^2T_{xx})\}$$
$$\{(v-y'u)^2-3\varepsilon^2(T_{yy}-2y'T_{xy}+y'^2T_{xx})\}=0 \qquad (15a)$$

Explicit expressions for each one of the seven eigenvalues and corresponding eigenvectors can be derived from Eqs. (11) and (15a):

$$y' = \frac{uv-\gamma\varepsilon^2T_{xy}\pm\varepsilon\sqrt{[\gamma^2\varepsilon^2(T_{xy}^2-T_{xx}T_{yy})+\gamma(v^2T_{xx}+u^2T_{yy}-2uvT_{xy})]}}{u^2-\gamma\varepsilon^2T_{xx}} \qquad (15b)$$

where γ takes the values 0, 1, or 3.

In particular, the eigenvalue $y'_0=\tan\theta_0 = v/u$ is triple, indicating that the particle trajectory is a triple characteristic. An alternative implicit expression for the remaining four eigenvalues y' is provided by the equation

$$\mu = \arcsin(1/M') \qquad (16a)$$

where, for a given characteristic, $y' = \tan(\theta_0 \pm \mu)$ and M' is a Mach number based on the temperature normal to the characteristic, defined as

$$M' = U_p/\sqrt{(\gamma k T_{pmm}/m_p)} \qquad (16b)$$

with $U_p=\sqrt{(u_p^2+v_p^2)}$, and the transversal speed of disturbances is, as one would expect, proportional to the square root of the component of the temperature tensor normal to the characteristic direction

$$T_{pmm} = \mathbf{m}\cdot \boldsymbol{T} \cdot \mathbf{m} = \sin^2\theta T_{xx} - 2\sin\theta\cos\theta T_{xy} + \cos^2\theta T_{yy}$$

where **m** is the unit vector normal to the characteristic direction given by y'. Equation (16a) is implicit because T_{pmm} is dependent on y'. It is informative to write the equation for y' in this form because it is strictly parallel to the definition of Mach angle in supersonic equilibrium flow of simple gases. An approximate form of Eq. (16a) can be helpful in the hypersonic limit where ε is very small. Then, with errors of order ε^2, the four characteristics cross the particle streamline at symmetric angles $\pm\mu_1$ and $\pm\mu_2$: $\theta_{1,2} = \arctan y'_{1,2} \approx \theta_0 \pm \mu_1$, $\theta_{3,4} = \arctan y'_{3,4} \approx \theta_0 \pm \mu_2$. The twin characteristics are deflected with relation to θ_0 by a small angle μ_i (of order ε) related to the Mach number of the particles by

$$\mu_i = \arcsin(1/M_i), \; i=1,2 \qquad (17a)$$

where two modes of propagation of signals give rise to corresponding Mach numbers. In physical magnitudes these Mach numbers may be expressed as

$$M_i = U_p/(\gamma_i k T_{pnn}/m_p)^{1/2}, \; \gamma_1=1, \gamma_2=3 \qquad (17b)$$

where the transversal speed of disturbances is now based on the normal component of the temperature tensor,

$$T_{pnn} = \mathbf{n}\cdot\boldsymbol{T}\cdot\mathbf{n} = \sin^2\theta_0 T_{xx} - 2\sin\theta_0\cos\theta_0 T_{xy} + \cos^2\theta_0 T_{yy}$$

where **n** is the unit vector normal to the particle streamline. It may be observed that Eqs. (16b-17b) are exactly coincident with the usual definition of the Mach angle if T_{pnn} is replaced by the scalar temperature and γ_i takes the value of the ratio of specific heat coefficients (γ = 5/3 for monatomic gases). It is clear that the two modes arise because of the breakdown of the isotropy in the temperature tensor, and that further modes would be present in a 3D problem lacking symmetry. Values of 1 and 3 for the coefficient γ correspond, respectively, to isothermal propagation and to a problem with only 1 degree of freedom (one-dimensional). This last situation arises when the mechanical work put by the pressure term in a particular direction is not redistributed by colisions, heating up only the corresponding component of the temperature tensor.

As sketched in the Appendix, the seven differential equations (along different paths) obtained from Eq. (14) can be solved numerically by means of a characteristic mesh. The only additional difficulty with respect to traditional characteristic solutions is the increassed complexity of the grid. In the next section the characteristic method is applied to two problems for which asymptotic analytical solutions are available.

III. Examples: Gaussian Wake and Prandtl-Meyer Expansion

In this section, two problems are considered for which asymptotic analytical solutions are available. The building unit is an expression describing the spread of particles emanating from a steady point source in a uniform background gas at temperature T_b which travels at velocity U_b in the x direction.[3] This exact solution results from a numerical convolution integral of a known solution of the Fokker-Planck equation for the evolution in time of a pulse of particles.[6,7] In the limit $\varepsilon<<1$, the convolution integrals reduce asymptotically to simple algebraic expressions for n_p and U_p. These results may also be obtained by a near-axis boundary layer analysis of the hypersonic Eqs. (1-3), which provides also explicit expressions for T_{xx} and T_{yy}.[3] The asymptotic results for the steady source problem are summarized here: If particles at the source are produced at a rate n' and with a Maxwellian distribution with mean velocity U_0 (also in the x direction) and temperature T_0, the particle phase magnitudes at a point (x, y) [where $y \le O(\varepsilon x)$] can be written in terms of parametric variables as[3]

$$x=x_0(s); \qquad u=u_0(s); \qquad T_{xx}=\xi(s); \qquad T_{yy}=d(s)/a(s)$$

$$n=\frac{N'}{u_0(s)}[2\pi\varepsilon^2 a(s)]^{(1-n_d)/2}\exp(-\frac{y^2}{2a(s)\varepsilon^2}); \qquad v=\frac{c(s)}{a(s)}y \qquad (18)$$

where n_d = 2 or 3 in 2D and axisymmetrical problems, respectively. In the preceding equations, the same normalization defined in Eq. (5) is used, with $U_R = U_b$, $L_R = U_b\tau$, $T_R = T_b$, so that S = 1, and the

following functions are introduced:

$$x_0(s) = s + \delta(1 - e^{-s}); \qquad u_0(s) = x_0'(s) = 1+\delta e^{-s} \qquad (19a,b)$$

$$a(s) = \alpha\,(1 - e^{-s})^2 + 2s - 3 - e^{-2s} + 4e^{-s} \qquad (19c)$$

$$c(s) = a'(s)/2 = (1 - e^{-s})\,(1 - e^{-s} + \alpha e^{-s}) \qquad (19d)$$

$$d(s) = \alpha[1-4e^{-s}+(2s+3)e^{-2s}]+2s-4+8e^{-s}-(2s+4)e^{-2s} \qquad (19e)$$

$$\xi(s) = e^{-2s}[e^{2s}-1+\alpha(1+\delta)^2+4\delta(e^{s}-1)+2\delta^2 s]/u_0(s) \qquad (19f)$$

with $\alpha = T_0/T_b$, $\delta = (U_0 - U_b)/U_b$, $N' = n'\tau$. No closed-form expression for T_{xy} has been yet obtained, but in the vicinity of the source (s<<1), $T_{xy} = \alpha y/[(1 + \delta)s]$ for $\alpha \neq 0$ and $T_{xy} = 5y/[3(1 + \delta)]$ otherwise. Equations (18) can be considered a fundamental solution, from which more complicated problems can be solved by convolution. The fundamental solution for N' = 1 is denoted with a subscript F: $n_F = n$, $U_F = ue_x + ve_y$, $\mathcal{T}_F = T_{xx}e_xe_x + T_{yy}e_ye_y + T_{xy}(e_xe_y + e_ye_x)$.

A. Dispersion of an Initially Gaussian distribution of particles (Gaussian Wake)

Particles are seeded in the plane x = 0 at a dimensionless rate N' with a Gaussian concentration profile, so that at s = 0,

$$n = \frac{N'}{u_0(s)}(2\pi\varepsilon^2 a_0)^{(1-n_d)/2}\exp(-\frac{y^2}{2a_0\varepsilon^2}), \quad u_0 = 1+\delta, \quad v=0$$

$$T_{xx} = T_{yy} = T_{zz} = \alpha, \quad T_{xy} = 0 \qquad (20)$$

where a_0 is a constant. As particles evolve in the uniform (T_b,U_b) back-ground, their Brownian motion broadens the concentration profile. From a convolution argument, the field quantities are

$$n(x) = \int ds^i(x')\, n^i(x')u_0^i(x')\, n_F(x-x') \qquad (21a)$$

$$n(x)\, U(x) = \int ds^i(x')\, n^i(x')u_0^i(x')\, n_F(x-x')\, U_F(x-x') \qquad (21b)$$

$$n(x)\mathcal{T}(x) = \varepsilon^{-2}[\int ds^i(x')n^i(x')u_0^i(x')n_F(x-x')U_F(x-x')U_F(x-x') - U(x)U(x)] + \int ds^i(x')\, n^i(x')u_0^i(x')\, \mathcal{T}_F(x-x') \qquad (21c)$$

where the superscript i refer to the initial condition given in Eqs. (20), and the integration is carried over the seeding plane [$ds^i(x')$ is the differential element of surface centered around x']. Performing the integrals (21), the following is obtained for the particle magnitudes

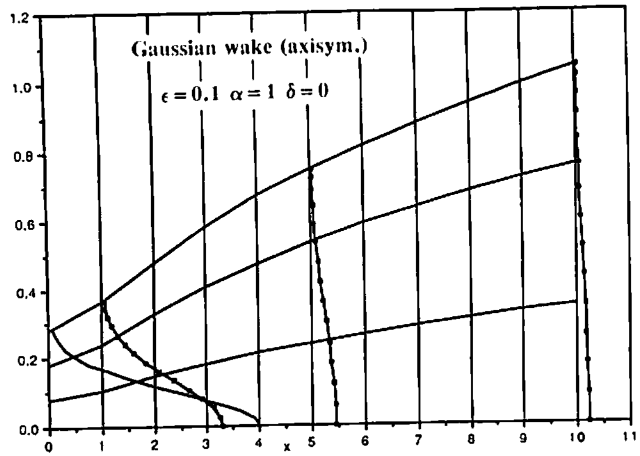

Fig. 1. Trajectories and density profiles for axisymmetric Gaussian wakes. Marked curves correspond to Eq. (22). —— numerical integration of the hypersonic equations by the method of characteristics. ε=0.1; α=1; δ=0.

downstream from the seeding plane:

$$n=\frac{1}{u_0}[2\pi\varepsilon^2(a+a_0)]^{(1-n_d)/2}\exp\left[-\frac{y^2}{2(a+a_0)\varepsilon^2}\right] \qquad (22a)$$

$$U = u_0 e_x + e_y\frac{yc}{(a+a_0)},\quad T_{yy}=\frac{d}{a}+\frac{a_0c^2}{a(a+a_0)},\quad T_{xx}=\xi \qquad (22b)$$

No expression for T_{xy} is given because it is not available in the fundamental solution. As before, a, c, d, ξ, and u_0 are functions of x, implicitly defined as $x_0(s)=x$ [Eqs. (19)].

Figures 1 and 2 show density profiles and trajectories as calculated from Eqs. (22) compared with the results from the numerical integration of the hypersonic equations using the method of characteristics (see the Appendix). Two different initial conditions (both with ε=0.1) are displayed for axisymmetric flows. A very close agreement is observed in the density profiles for both cases, as well as for the corresponding 2D situations (not shown). The agreement in the velocity and the temperature, not shown, is even better than for the densities. The mesh size used in the numerical method was $\Delta x=0.01$ for $x\leq 5$ and $\Delta x=0.1$ for $x>5$. The convergence of the numerical method (see the Appendix) was very fast: typically, after two iterations the error was smaller than $0.1(\Delta x)^2$.

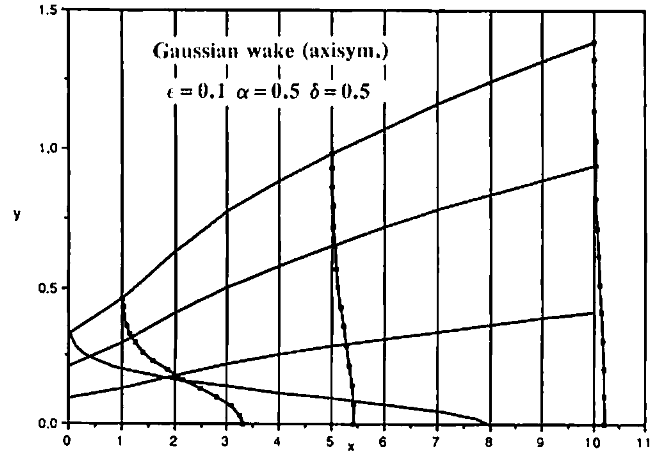

Fig. 2 Like Fig. 1, but with ε=0.1; α=0.5; δ=-0.5.

B. Dispersion of a Step-like Particle Distribution (Prandtl-Meyer Problem)

In this section we consider the analog of a 2D Prandtl-Meyer expansion. Particles are uniformly seeded only in the upper half of the plane x=0, so that there is a discontinuous step in their concentration at x=0. The properties of the carrier fluid are uniform everywhere. Although it is not included here, the axisymmetric counterpart of this problem corresponds to the expansion of particles uniformly seeded in a circle at plane x=0. With the help of Eqs. (24) and (25), and carrying out similar integrations as before, the following asymptotic results are obtained:

$$n = \mathrm{erfc}(-\eta)/2,\quad T_{xx}=\xi \qquad (23a)$$

$$U=u_0e_x+e_y\frac{c}{a}\left(\frac{2\varepsilon^2 a}{\pi}\right)^{1/2}\exp(-\eta^2)/\mathrm{erfc}(-\eta) \qquad (23b)$$

$$T_{yy}=\frac{d}{a}+\frac{c^2}{a}\left[1-\frac{2\eta}{\sqrt{\pi}}\frac{\exp(-\eta^2)}{\mathrm{erfc}(-\eta)}-\frac{2}{\pi}\left(\frac{\exp(-\eta^2)}{\mathrm{erfc}(-\eta)}\right)^2\right] \qquad (23c)$$

where we have defined the variable

$$\eta=y/\sqrt{(2a\varepsilon^2)} \qquad (23d)$$

and erfc is the complementary error function.[8] To avoid the singularity at the origin, the numerical integration is started slightly downstream from x=0 (at x=0.25 in Fig. 3) using Eqs. (23) as initial conditions (from the starting behavior of the fundamental solution $T_{xy}F$, it

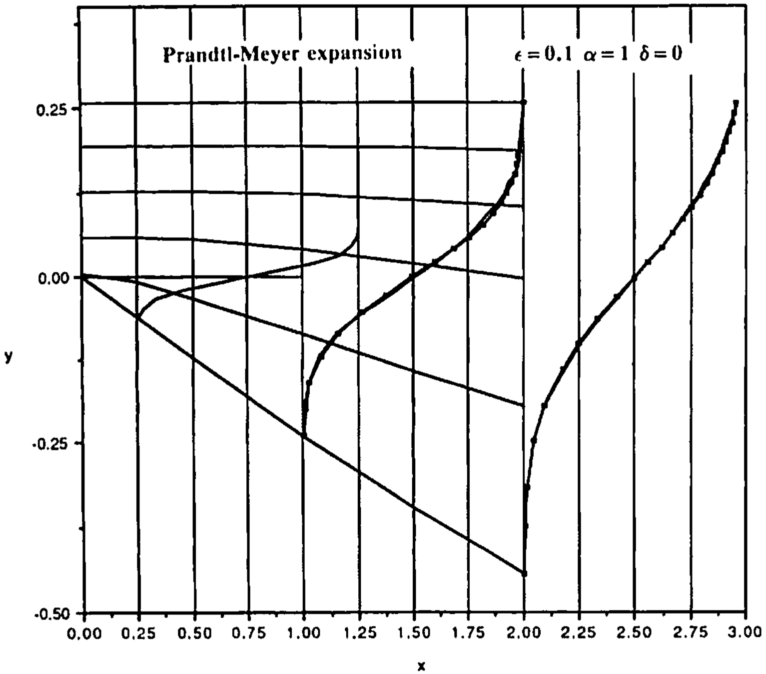

Fig. 3. Trajectories and density profiles for a Prandtl-Meyer expansion with $\varepsilon=0.1$, $\alpha=1$ and $\delta=0$. Marked curves correspond to the analytical solution (Eqs. 23) of the Fokker-Planck equation; —— numerical integration by the method of characteristics, started at x=0.25 using the analytical solution (23).

follows that $T_{xy} \approx 2\alpha v/(1+\delta)$ for small x) and the results for $\varepsilon=0.1$ are presented in Fig. 3, together with the solution (23). The mesh size used in the numerical integration was $\Delta x=0.01$. The agreement between both solutions for the velocities and temperatures (not shown) is also excellent.

While Eqs. (23) are only restricted to small values of ε, a note of caution is required when using the hypersonic truncated set of Eqs. (1-3) in problems such as the Prandtl-Meyer expansion where very large gradients occur near the origin[2,3] (this is why our numerical integration has to be started downstream from x=0). Indeed, from Eqs. (1-3) and through a boundary layer analysis near y=0, a solution can be obtained for x<<1 for $v=U_p.e_y$, λ, and T_{yy} in terms of the similarity variable κ

$$\kappa=y/(\sqrt{3}\,\varepsilon x) \tag{24a}$$

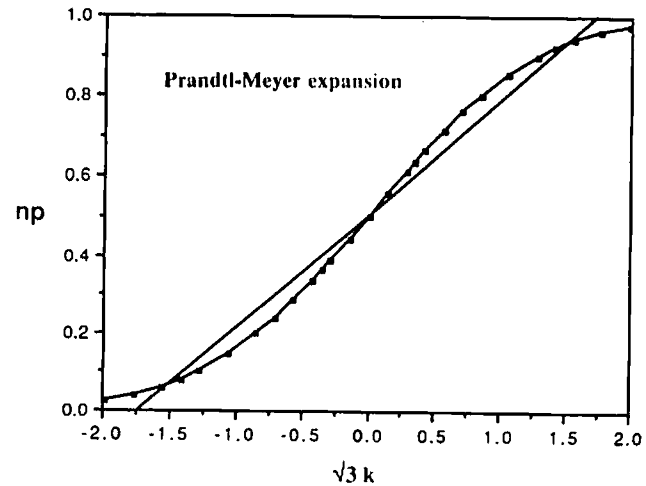

Fig. 4. Comparison of the solution via the Fokker-Planck equation [Eq. (23)] with the direct solution [Eq.(24)] to the hypersonic equations in the vicinity of the Prandtl-Meyer corner.

which for $\kappa\leq\sqrt{3}$ can be written as

$$w_0=\frac{v}{\varepsilon}=\frac{\sqrt{3}}{2}(\kappa-1);\quad \exp(\lambda_0)=\frac{1}{2}(1+\kappa);\quad T_{yy0}=\frac{1}{4}(\kappa+1)^2 \tag{24b}$$

This solution, though rigorously derived from Eqs. (1-3), is incorrect because the temperature and density jumps at the start of the expansion give rise to a singular transversal heat flux that cannot be neglected in the energy equation. Nonetheless, as shown in Fig. 4, even in this irregular case the hypersonic solution (24) is not intolerably different from the asymptotic solution (23).

Appendix: Sketch of the Numerical Method

After solving the eigenvalue problem (11) with y' given by Eq. (15), Eq. (13) yields the following three equations on the trajectories (defined by $y'=\tan\theta_0=v/u$):

$$U\, dT_{zz}/ds_0 = 2\,(T - T_{zz})/S \tag{A.1}$$

$$C_1\frac{d\omega}{ds_0}=\frac{-\beta v}{y}+\frac{\sin\theta_0\,(T-T_{xx})}{ST_a}-\frac{\cos\theta_0\,(T-T_{yy})}{ST_b} \tag{A.2}$$

$$C_2\frac{d\omega}{ds_0}=\frac{-\cos\theta_0}{S}\left[\frac{T_b}{T_a}(T-T_{xx})+2T_{xy}+\frac{T_a}{T_b}(T-T_{yy})\right] \tag{A.3}$$

where

$$C_1=(U,\frac{1}{\cos\theta_0}+\frac{T_{xx}\tan\theta_0}{T_a},\frac{-T_{xy}}{T_b},\frac{u\tan\theta_0}{2T_a},0,-\frac{u}{2T_b},0) \quad (A.4)$$

$$C_2=(0,T_{xy}-\frac{T_{xx}T_b}{T_a},T_{xx}-\frac{T_{xy}T_a-uT_b}{T_b},\frac{}{2T_a},u,-\frac{uT_a}{T_b},0) \quad (A.5)$$

$$U=\sqrt{(u^2+v^2)}=u/\cos\theta_0;\quad T_a=\cos\theta_0 T_{xy}-\sin\theta_0 T_{xx} \quad (A.6,7)$$

$T_b=\cos\theta_0 T_{yy}-\sin\theta_0 T_{xy}$, (A.8)
and s_0 is the coordinate along the trajectory. The other four equations along the characteristics defined by $y'_i=\tan\theta_i$, $i=1,2,3,4$, may be written as

$$D_i\frac{d\omega}{ds_i}=\{-\frac{\beta v}{y}\lambda_{1i}+\frac{u'-u}{S}-\frac{\varepsilon^2\beta}{y}T_{xy}+\lambda_{3i}[\frac{v'-v}{S}-\frac{\varepsilon^2\beta}{y}(T_{yy}-T_{zz})]+$$
$$+2\lambda_{4i}\frac{T-T_{xx}}{S}-2\lambda_{5i}\frac{T_{xy}}{S}+2\lambda_{6i}\frac{T-T_{yy}}{S}+\lambda_{7i}[2\frac{T-T_{zz}}{S}-2v\beta\frac{T_{zz}}{y}]\cos\theta_i \quad (A.9)$$

with

$$D_i=\{u\lambda_{1i}+\varepsilon^2(T_{xx}+T_{xy}\lambda_{3i}),\ \lambda_{1i}+u+2T_{xx}\lambda_{4i}+T_{xy}\lambda_{5i},\ u\lambda_{3i}+v\lambda_{5i}$$
$$+2T_{xy}\lambda_{6i},\ \varepsilon^2+u\lambda_{4i},\ \varepsilon^2\lambda_{3i}+u\lambda_{5i},\ u\lambda_{6i},\ u\lambda_{7i}\}$$

$$\lambda_{1i}=[a_i^2+\varepsilon^2(b_iy_i'-c_i)]/(2a_iy'_i)$$

$$\lambda_{3i}=-[a_i^2+\varepsilon^2(3b_iy_i'-c_i)]/(2\varepsilon^2c_iy'_i);\quad \lambda_{4i}=\varepsilon^2y_i'/a_i$$

$$\lambda_{5i}=-[a_i^2+\varepsilon^2(3b_iy_i'+c_i)]/(2c_ia_i);\lambda_{6i}=[a_i^2+\varepsilon^2(3b_iy_i'-c_i)]/(2c_iy_i'a_i)$$

$$a_i=v-y_i'u;\quad b_i=T_{xy}-y_i'T_{xx};\quad c_i=T_{yy}-y_i'T_{xy}$$

To solve these equations numerically, a grid is adapted to the particle flow as follows: in the first place a set of curves $x=\xi_k(y)$ ($k = 0,1,2...$) is defined in such a way that they are not tangent to the trajectories at any point. For instance, in the case of the examples in Sec. III, these curves are vertical straight lines $x = x_k =$ const. The first of these lines $x=\xi_0(y)$ has to be coincident with the boundary at which initial conditions are given, so that ω is known at $k = 0$. Along the first line, grid points (0, m) are defined (see Fig.5): the next row of grid points (1, m) is located by intersecting the particle trajectories through the corresponding points in the previous row (0, m) with the curve $\xi_1(x)$. The properties ω at the new points are still unknown, but an iterative technique allows to determine them: the iteration is started by assuming $\omega(1, m) = \omega(0, m)$, from which the slope of the characteristics through (1,m) can be obtained. The intersection of

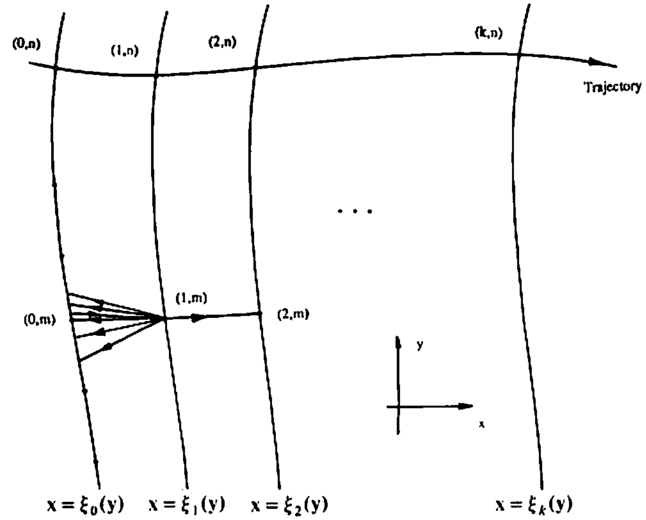

Fig. 5. Sketch of the grid and the procedure used in the numerical implementation of the method of characteristics.

the curve $\xi_0(x)$ with straight lines shot from (1,m) with the characteristic slopes identifies five *predecessor* points whose properties can be evaluated by means of a spline interpolation along the $\xi_0(x)$ curve. Now, a finite-difference formulation of Eq. (A9) can be written linking the properties at (1,m) with those at the predecessor points along $\xi_0(x)$. A first nontrivial approximation for $\omega(1,m)$ is thus obtained, and the process of backward shooting, interpolation, and finite-difference reevaluation of $\omega(1,m)$ can be repeated until a convergence criterion is met. In our case, the iterations have been stopped when the euclidean norm of the difference between two consecutive values of $\omega(1,m)$ is less than $(\Delta s_0)^2$, where Δs_0 is the increment in the streamline coordinate s_0 between the two points (0,m) and (1,m). This process is repeated each time when jumping from a curve ξ_{k-1} into a new ξ_k.

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References

[1]Fernández de la Mora, J. and Fernández-Feria, R., "Kinetic Theory of Binary Gas Mixtures with Large Mass Disparity," Physics of Fluids, Vol. 30, pp.740-751, March 1987.

[2]Fernández-Feria, R., "On the Gas Dynamics of Binary Gas Mixtures with Large Mass Disparity," Ph.D. Dissertation, Yale University, New Haven, CT, 1987.

[3]Riesco-Chueca, P. and Fernández de la Mora, J., "Brownian Motion Far from Equilibrium: a Hypersonic Approach," (to be published in Journal of Fluid Mechanics, 1989).

[4]Friedlander, S. K., Smoke, Dust and Haze, Wiley, New York, 1977.

[5]Chapman, S. and Cowling, T. G., The Mathematical Theory of Non-Uniform Gases, Cambridge Univ. Press, Cambridge, UK, 1970.

[6]Rice, S. A. and Gray, P., The Statistical Mechanics of Simple Liquids, Interscience, New York, 1965.

[7]Nguyen, T. K.and Andres, R. P., "Fokker-Planck Description of the Freejet Deceleration Flow," Progress in Astronautics and Aeronautics: Rarefied Gas Dynamics, Vol.74, AIAA, New York, 1981.

[8]Abramowitz, M. and Stegun, I. A., Handbook of Mathematical Functions, Dover, New York, 1972.