Collisionless expansion of gases into vacuum

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The free-molecule limit of several free-flow problems is studied on the basis of the collisionless Boltzmann equation. It is shown that the density in the free expansion of a gas cloud obeys, under certain conditions, a diffusion equation with a coefficient directly proportional to the time, and the resulting flow field is described in terms of a thick 'diffusion front' travelling asymptotically at a definite velocity and growing linearly with time. It is also shown that in any free-molecule free expansion the stresses and heat flux can be expressed in terms of viscosity and conductivity coefficients, which however increase linearly with time but are such that the Stokesian relation is always valid and the Prandtl number has the value $\frac{5}{8}$.

The flow field due to sources and jets is also discussed, and it is found that the jet has a width inversely proportional to the Mach number if the Mach number is sufficiently high. Finally, a procedure is indicated for taking approximate account of collisions among the molecules.

1. Introduction

This paper is concerned with some problems in what may be called 'free gaskinetics', that is, with the kinetic theory of flows in which interactions with solid surfaces play no significant part. The free expansion of a gas cloud and the flow in a jet are two examples of this kind of problem. These problems are not only of practical interest in the space sciences and in astrophysics, but also have some fundamental interest in their own right, as they enable one to concentrate on the effect of intermolecular collisions to the exclusion of the uncertain effects of interaction with solid surfaces. However, as a necessary first step, even collisions among the molecules themselves will be neglected in most of the present report.

There has been some study, in the recent past, of the free expansion of gas clouds, though mostly on the basis of continuum gasdynamics of an inviscid fluid. Keller (1956) has investigated a class of solutions of the gasdynamic equations for certain types of initial and boundary conditions. Greifinger & Cole (1960) have found a very interesting exact solution for one-dimensional free expansion for some special (but realistic) values of γ (the ratio of specific heats), and have also studied the asymptotic flow field for arbitrary γ . Dyson (1958) has obtained some interesting results for the free expansion of non-spherical gas clouds with an initial Gaussian density distribution.

Attacks on the problem from the gaskinetic viewpoint seem far fewer. Molmud (1960) has calculated the density field in free-molecular free expansion of symmetric gas clouds by an intuitive method, using an 'analogy' with heat diffusion to evaluate his integrals. Keller (1948) has given the result for the free expansion of a 'half-space'.

Our purpose here is to study these problems very broadly, on the basis of the collisionless Boltzmann equation. The general free-flow problem we shall discuss can then be posed as follows: given an initial molecular velocity distribution function over all of space, and arbitrary time-dependent sources, what is the flow field at any later time?

When one thinks of actual physical problems, there is always a question about what a suitable initial distribution is. In principle the initial distribution is perfectly arbitrary (except possibly for some restrictions regarding its moments); in any specific problem it will have to be deduced, or guessed, from considerations other than those set forth here. However, it will be assumed in the following that there is some mechanism, apart from intermolecular collisions, which makes the initial distribution Maxwellian. For instance, when we consider the expansion of a gas cloud as an initial-value problem, the gas may be imagined as having been confined within a balloon whose size is much smaller than the mean free path; collisions with the surface of the balloon then ensure that the gas has a Maxwellian distribution. When the balloon is burst the gas expands freely into the vacuum, with no collisions among the molecules. In any case, the Maxwellian is the simplest and most obvious distribution to start with.

The flow field in the general problem is derived, using a method of characteristics, in §2; various particular cases are dealt with in later sections. The expansion of a gas cloud is treated as an initial-value problem in §3, and it is shown that, under certain conditions, the flow can be described as a kind of collisionless diffusion. In §4 steady and time-dependent sources are discussed, and the 'high Mach number' limit for a jet is briefly touched upon. Finally, in §5, a procedure is indicated for taking account of first collisions by extending the Willis method to general unsteady flows.

2. The general free-molecule free-flow problem

The basic unknown in a gaskinetic description of a flow is the molecular velocity distribution function $f = f(\mathbf{x}, t; \mathbf{v})$, giving the number density of molecules at position \mathbf{x} and time t, per unit volume in physical and velocity (\mathbf{v}) space. This function is governed by Boltzmann's equation, which, for a monatomic gas in the absence of external forces, can be written

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}\right) f(\mathbf{x}, t; \mathbf{v}) = \mathscr{G}(f) - f\mathscr{L}(f) + Q(\mathbf{x}, t; \mathbf{v}),$$
(2.1)

where $\mathscr{G}(f) - f\mathscr{L}(f)$ stands for the collision integrals (see e.g. Narasimha 1961), and where we have included a general source term Q, giving the number of molecules, per unit (\mathbf{x}, \mathbf{v}) -volume per unit time, introduced or created at \mathbf{x}, t . If we ignore collisions, (2.1) becomes

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q. \tag{2.2}$$

In this limit the function f is in general discontinuous in velocity space, which can often be divided into regions which are vacant (i.e. there are no molecules with

velocity vectors lying in them) and regions which are occupied by molecules of particular kinds, e.g. those coming from a solid surface if one is present. Though the distribution in the occupied regions may be like $e^{-\beta v^2}$, the β does not necessarily correspond to the local temperature, and moreover the distribution is usually not isotropic, so that it is not a local Maxwellian. The flow is in fact due to the development in time and physical space of these regions in velocity space.

This development is very generally described by equation (2.2) which is a linear, inhomogeneous first-order partial differential equation, with a vector parameter v which takes all possible values. To solve the equation completely one has in general to be given f on a three-dimensional hypersurface in \mathbf{x}, t space. In most practical problems this takes the form of an initial condition in physical space, say f(x, t, y) = f(x, y) + f(x, y)

$$f(\mathbf{x}, t = 0; \mathbf{v}) = f_0(\mathbf{x}; \mathbf{v}).$$
(2.3)

Here f_0 can, of course, be an arbitrary function of x and v.

The most straightforward way of solving (2.2) is to write down the characteristics following Courant & Hilbert (1937). In terms of a parameter *s* along the characteristics, they are governed by the five ordinary differential equations

$$\frac{dt}{ds} = 1, \quad \frac{d\mathbf{x}}{ds} = \mathbf{v}, \quad \frac{df}{ds} = Q,$$
 (2.4)

which have the solution

$$t = s, \quad \mathbf{x} = \mathbf{v}s + \mathbf{\xi}, \quad f = \int_0^s Q \, ds + f_0,$$
 (2.5)

where Q is integrated with respect to s after being expressed as a function of s and the co-ordinates $\boldsymbol{\xi}$ of the initial surface. However, $\boldsymbol{\xi}$ can be eliminated from (2.5) and we can write f at any given time as

$$f(\mathbf{x},t;\mathbf{v}) = f_0(\mathbf{x} - \mathbf{v}t;\mathbf{v}) + \int_0^t Q\{\mathbf{x} - \mathbf{v}(t-s),s;\mathbf{v}\} ds.$$
(2.6)

This is the general solution of the initial-value problem that was posed earlier. The density, gas velocity and all other flow quantities can now be derived as appropriate moments of f.

3. Expansion of a gas cloud

Let us study briefly the case Q = 0. This includes the class of free expansion problems, in which one considers a cloud of gas confined within a certain region whose boundaries are suddenly removed at time t = 0. In such a problem $f_0 = 0$ outside the cloud. More generally an arbitrary initial distribution over all space may be given. In either case, the distribution at t > 0 is obtained simply from (2.6) by putting Q = 0 to give

$$f(\mathbf{x}, t; \mathbf{v}) = f_0(\mathbf{x} - \mathbf{v}t; \mathbf{v}).$$
(3.1)

The corresponding flow quantities are most conveniently worked out by making the transformation $\mathbf{x} - \mathbf{v}t = \mathbf{x}',$

$$D\mathbf{x}' = dx_1' dx_2' dx_3' = -t^3 dv_1 dv_2 dv_3 = -t^3 D\mathbf{v}.$$
(3.2)

(The notation $D\mathbf{x}$ stands for an element of volume in \mathbf{x} -space.) Thus the density is given by

$$\rho(\mathbf{x},t) = \int f_0(\mathbf{x} - \mathbf{v}t; \mathbf{v}) D\mathbf{v} = \frac{1}{t^3} \int f_0\left(\mathbf{x}'; \frac{\mathbf{x} - \mathbf{x}'}{t}\right) D\mathbf{x}', \qquad (3.3)$$

where the integration is performed over all \mathbf{x}' . (Note that $D\mathbf{x}'/D\mathbf{v}$ is just the Jacobian of the transformation, and only its absolute value appears in (3.3).) The gas velocity \mathbf{u} , defined as

$$\mathbf{u}(\mathbf{x},t) = \frac{1}{\rho(\mathbf{x},t)} \int \mathbf{v} f(\mathbf{x},t;\mathbf{v}) D\mathbf{v},$$

is given by

$$\mathbf{u} = \frac{1}{\rho} \int \frac{\mathbf{x} - \mathbf{x}'}{t} f_0\left(\mathbf{x}'; \frac{\mathbf{x} - \mathbf{x}'}{t}\right) D\mathbf{x}' = \frac{\mathbf{x}}{t} - \frac{1}{\rho t^4} \int \mathbf{x}' f_0\left(\mathbf{x}'; \frac{\mathbf{x} - \mathbf{x}'}{t}\right) D\mathbf{x}'.$$
(3.4)

Any other flow quantity can be similarly calculated as some transformed moment of the initial distribution function.

Equation (3.4) shows what is apparently a general feature of free gaskinetic flows, namely, that the gas velocity can be split into two parts, one of which (like \mathbf{x}/t) is purely kinematic, in the sense that it does not depend on any dynamic variable (like temperature, e.g.), and another part which is thermal and tends to have a characteristic value like $1/\sqrt{\beta} \sim (\Re T)^{\frac{1}{2}}$ (where \Re is the gas constant and T is the temperature). Physically the kinematic part arises from the presence at \mathbf{x} of molecules which took exactly the time t to get there. It of course vanishes in steady free flow. In unsteady flows it seems to be the counterpart of the asymptotic similarity component of the velocity that one encounters in gasdynamics. Some interesting examples of free expansion are worked out below.

The 'point' cloud

At sufficiently large distances any cloud must look like a point. Thus suppose there are N molecules all concentrated at the origin at t = 0 and having a Maxwellian velocity distribution, so that

$$f_0(\mathbf{x}; \mathbf{v}) = \delta(\mathbf{x}) N(\beta/\pi)^{\frac{3}{2}} e^{-\beta v^2}.$$
(3.5)

 $\delta(\mathbf{x})$ is the Dirac delta function such that $\int \delta(\mathbf{x}) D\mathbf{x} = 1$ if the integral includes the origin. Then from (3.1), (3.3) and (3.10),

$$f(\mathbf{x},t;\mathbf{v}) = \delta(\mathbf{x} - \mathbf{v}t) N(\beta/\pi)^{\frac{3}{2}} e^{-\beta v^{2}},$$

$$\rho(\mathbf{x},t) = \frac{1}{t^{3}} \int \delta(\mathbf{x}') N\left(\frac{\beta}{\pi}\right)^{\frac{3}{2}} \exp\left\{-\beta\left(\frac{\mathbf{x} - \mathbf{x}'}{t}\right)^{2}\right\} D\mathbf{x}'$$

$$= \frac{N}{t^{3}} \left(\frac{\beta}{\pi}\right)^{\frac{3}{2}} \exp\left(-\frac{\beta x^{2}}{t^{2}}\right),$$

$$\mathbf{u} = \mathbf{x}/t.$$
(3.6)

and

The result for the velocity is quite obvious, as only molecules with velocity $\mathbf{v} = \mathbf{x}/t$ can reach \mathbf{x} at time t, so $\mathbf{v} = \mathbf{x}/t = \mathbf{u}$. Also the thermal or peculiar velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$ is then zero, so the temperature T = 0. At any point \mathbf{x}

the velocity shoots up suddenly to infinity at t = 0+, then drops off as t^{-1} . The density, on the other hand, builds up gradually from zero to a maximum (of $27N/8x^3e^{\frac{3}{2}} = 0.07361N/x^3$) at $t = x(\frac{2}{3}\beta)^{\frac{1}{2}}$, and drops off like t^{-3} at large times. Thus the decay in density is exponential in space and algebraic in time.

As may be expected and will be shown later the same solution is obtained if $f_0 = 0$ but $Q = \delta(\mathbf{x}) \, \delta(t) \, N(\beta/\pi)^{\frac{3}{2}} e^{-\beta v^{\frac{3}{2}}}$, which represents a pulse source. Incidentally, it may be worth noting that as all molecules at \mathbf{x} have the single velocity \mathbf{x}/t , the relative velocity g between any two of them is zero, and hence they will never collide. Thus, in so far as one can speak of a point cloud with an initial Maxwellian distribution expanding into perfect vacuum, equations (3.6) given an exact fundamental solution of the full Boltzmann equation, because the collision integrals vanish identically for (3.6). However, as the full Boltzmann equation is non-linear, it is not possible to superpose these fundamental solutions to derive solutions for more complicated problems.

Symmetric clouds

We discuss the one-dimensional case in some detail, especially because an exact solution of the problem in the gasdynamic limit has been obtained by Greifinger & Cole (1960). Suppose the gas is confined between two planes $x_1 = \pm l$ and is allowed to expand into vacuum at t = 0. We can then write, assuming the initial distribution to be Maxwellian,

$$f_0(\mathbf{x}; \mathbf{v}) = \left[\mathscr{H}(x_1+l) - \mathscr{H}(x_1-l)\right] n_0(\beta_0/\pi)^{\frac{3}{2}} e^{-\beta_0 v^2},$$

where \mathscr{H} is the Heaviside step function. Due to the symmetry, the co-ordinates x_2, x_3 at the point of observation **x** can be taken to be zero; then, from (3.3), it is easily seen that

$$\rho(\mathbf{x},t) = \frac{n_0}{t^2} \left(\frac{\beta_0}{\pi}\right)^{\frac{3}{2}} \int_{-l}^{+l} \exp\left\{-\beta_0 \frac{(x_1 - x_1')^2}{t^2}\right\} dx_1' \\ \times \int_{-\infty}^{+\infty} \exp\left(-\beta_0 x_2'^2\right) dx_2' \int_{-\infty}^{+\infty} \exp\left(-\beta_0 x_3'^2\right) dx_3',$$

or, introducing $\xi = x_1/l$ and $\tau = t/l\sqrt{\beta_0}$,

$$\rho = \frac{1}{2}\rho_0 \left\{ \operatorname{erf} \frac{\xi + 1}{\tau} - \operatorname{erf} \frac{\xi - 1}{\tau} \right\},\tag{3.7}$$

where $\rho_0 = mn_0$ is the initial density. This result is the same as that given by Molmud (1960), but we want to give it a different interpretation here. A typical density profile is shown in figure 1.

Now for large times, i.e. for $t \gg \beta_0^{\frac{1}{2}}(x_1 \pm l)$, (3.7) reduces to

$$\frac{\rho}{\rho_0} = \left(\frac{10}{3\pi}\right)^{\frac{1}{2}} \frac{l}{a_0 t} \simeq 1.03 \frac{l}{a_0 t}, \qquad (3.7a)$$

where $a_0 = (5\Re T_0/3)^{\frac{1}{2}}$ is the initial speed of sound in a cloud of monatomic particles. The density is roughly constant in x, provided x is not too large, and drops off as 1/t.

As might be expected from general similarity considerations, Greifinger & Cole find an asymptotic relation identical in form with (3.7a), but with a different numerical constant. Their calculation gives, when $\gamma = \frac{5}{3}$,

$$\rho/\rho_0 \simeq \frac{1}{2}(l/a_0 t), \tag{3.7b}$$

i.e. about half of what one expects in free molecule flow.



FIGURE 1. Typical density profile in one-dimensional free expansion.

Differentiating (3.7) with respect to ξ , one obtains

$$\frac{1}{\rho_0}\frac{\partial\rho}{\partial\xi} = -\frac{2}{\tau\sqrt{\pi}}\sinh\frac{2\xi}{\tau^2}\exp-\frac{\xi^2+1}{\tau^2},$$
(3.8)

which is always negative, so ρ decreases monotonically; but differentiating once more it is easily verified that $\partial \rho / \partial \xi$ is a maximum at a point $\overline{\xi} = \overline{\xi}(\tau)$ such that

$$\xi = \coth\left(2\xi/\tau^2\right). \tag{3.9}$$

 $\bar{\xi}$ is plotted versus τ in figure 2. For large times (which means, as it will turn out, $t \gg l_{\lambda}/\beta_{0}$), equation (3.9) can be approximated by

$$\bar{\xi} = \frac{1}{2}\tau$$
 or $\bar{x}_1/t = (2\beta_0)^{-\frac{1}{2}}$. (3.10)

That is, the region of most rapid change in density travels asymptotically at a definite velocity $(2\beta_0)^{-\frac{1}{2}} = (\mathscr{R}T_0)^{\frac{1}{2}}$, which is equal to the isothermal speed of sound in the initial cloud. To find out how this region is spreading, one can define a thickness of the region by $\delta = \Delta o/(2\sigma/2\pi)$ (2.11)

$$\delta = \Delta \rho / (\partial \rho / \partial x_1)_{\bar{x}_1} \tag{3.11}$$

where $\Delta \rho$ is the difference in densities across the region, or (what amounts to the same thing) the density at $x_1 = 0$; this is given by (3.7*a*). Putting (3.10) into (3.8), one obtains

$$\delta = t(e/2\beta_0)^{\frac{1}{2}} \simeq 1 \cdot 17t\beta_0^{-\frac{1}{2}}.$$
(3.12)

Finally one can work out the gas velocity from (3.4). It is

$$u_{1} = \frac{2}{(\pi\beta_{0})^{\frac{1}{2}}} \frac{\sinh\left(2\xi/\tau^{2}\right)\exp\left\{-(\xi^{2}+1)/\tau^{2}\right\}}{\operatorname{erf}\left\{(\xi+1)/\tau\right\} - \operatorname{erf}\left\{(\xi-1)/\tau\right\}}.$$
(3.13)

At large times $(t \ge (x_1 \pm l)\sqrt{\beta_0})$, this reduces to $u_1 \simeq x_1/t$ and at small times $(t \le (x_1 \pm l)\sqrt{\beta_0})$, to $u_1 \simeq (x_1 \mp l)/t$. It may also be verified easily that at

$$x_1 = \overline{x}_1, \quad u_1 = \overline{u}_1 \to (2\beta_0)^{-\frac{1}{2}}$$

for $t \gg l \sqrt{\beta_0}$; and that the mass flow ρu_1 is a maximum at \bar{x}_1 .

To summarize, the flow field can be roughly described as follows. At large times there is a growing region of practically uniform density near the centre, but this density is falling in time as 1/t. Most of the density change occurs in a layer which is travelling with a definite velocity given by $(\mathcal{R}T_0)^{\frac{1}{2}}$ and whose thickness is increasing linearly with time. The gas velocity in this layer is also of order $(\mathcal{R}T_0)^{\frac{1}{2}}$, and the largest mass flow is taking place there.



FIGURE 2. Propagation of the 'diffusion front' in one-dimensional free expansion.

One can carry out an exactly similar analysis of a spherically symmetric cloud, to obtain

$$\frac{\rho}{\rho_{0}} = \frac{1}{2} \left\{ \operatorname{erf} \frac{\xi + 1}{\tau} - \operatorname{erf} \frac{\xi - 1}{\tau} \right\} - \frac{\tau}{\xi \sqrt{\pi}} \sinh \frac{2\xi}{\tau^{2}} \exp \left(-\frac{\xi^{2} + 1}{\tau^{2}}\right), \\
u_{1} = \frac{1}{\rho(\pi\beta_{0})^{\frac{1}{2}}} \sinh \frac{2\xi}{\tau^{2}} \exp \left(-\frac{\xi^{2} + 1}{\tau^{2}}\right) \left\{ \frac{1}{\xi} \coth \frac{2\xi}{\tau^{2}} - \frac{\tau^{2}}{\xi^{2}} \right\},$$
(3.14)

where x is now the distance from the origin, and l is the radius of the original cloud. The maximum density gradient is located at the solution of

$$\tau^{2}(\overline{\xi}^{2} + \tau^{2}) + 2\overline{\xi}^{2} = 2\overline{\xi}(\overline{\xi}^{2} + \tau^{2}) \coth(2\overline{\xi}/\tau^{2}); \qquad (3.15)$$

for large τ we obtain again, by expanding the coth to two orders, exactly the same result as before: a velocity of $(2\beta_0)^{-\frac{1}{2}}$ and a thickness of $t(e/2\beta_0)^{\frac{1}{2}}$. We shall return to a more basic discussion of these flows later.

Asymmetric clouds

It is obvious, from equations (3.3) and (3.4), that the expansion of any arbitrary cloud can, at worst, be numerically computed. All the same it is desirable to have at least some simple model for asymmetric clouds so that one can get a rough idea of any tendencies toward symmetry, if in fact such tendencies exist. For this purpose we consider a distribution function of the form

$$f_0(\mathbf{x}; \mathbf{v}) = n_0 \{ \exp - (a_1 x_1^2 + a_2 x_2^2 + a_3 x_3^2) \} (\beta_0 / \pi)^{\frac{3}{2}} \exp (-\beta_0 v^2), \qquad (3.16)$$

as a model for an asymmetric isothermal cloud. The cloud is actually supposed infinite in extent, but the density falls off exponentially with distance. The density contours are the ellipsoids

$$a_1x_1^2 + a_2x_2^2 + a_3x_3^2 = \text{const.},$$

assuming the a are all positive. The advantage of the form assumed in (3.16) is that the variables are separable.

From equation (3.3) we can work out the density at later times as

$$\rho = \frac{n_0 \beta_0^3}{\left[\left(\beta_0 + a_1 t^2\right) \left(\beta_0 + a_2 t^2\right) \left(\beta_0 + a_3 t^2\right) \right]^{\frac{1}{2}}} \exp - \left\{ \frac{\beta_0 a_1 x_1^2}{\beta_0 + a_1 t^2} + \frac{\beta_0 a_2 x_2^2}{\beta_0 + a_2 t^2} + \frac{\beta_0 a_3 x_3^2}{\beta_0 + a_3 t^2} \right\}.$$
(3.17)

It thus appears that the contours of ρ are always ellipsoids, but the eccentricity of the contours is a function of time. Equation (3.17) shows that as $t \to \infty$ the contours become spheres.

Consider an ellipsoid of revolution, given initially by

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$$a_1 x_1^2 + a_2 R^2 = \text{const.} = x_1^2 / l_1^2 + R^2 / l_2^2,$$

where l_1 and l_2 are now proportional to the axes of the ellipsoid, and R is the cylindrical radius. From (3.17) the axes of the contours at later times are related by

$$l_{1}^{\prime 2} \propto (\beta_{0} + a_{1}t^{2})/\beta_{0}a_{1}, \quad l_{2}^{\prime 2} \propto (\beta_{0} + a_{2}t^{2})/\beta_{0}a_{2},$$
$$\frac{l_{1}^{\prime}}{l_{2}^{\prime}} = \left\{ \frac{l_{1}^{2}/l_{2}^{2} + t^{2}/\beta_{0}l_{2}^{2}}{1 + t^{2}/\beta_{0}l_{2}^{2}} \right\}^{\frac{1}{2}}.$$
(3.18)

so their ratio is

This equation is plotted in figure 3, as l'_1/l'_2 vs. $t/l_2\sqrt{\beta_0}$ for some values of l_1/l_2 . The limit $l_1/l_2 = 0$ corresponds to a flat cloud. For oblate spheroids (i.e. $l_1/l_2 < 1$) the shape of the expanded cloud is almost spherical at $t \sim 2l_2/\sqrt{\beta_0}$, and this time depends only slightly on the initial eccentricity. The narrow portions of the cloud expand out much faster than the other parts. It is interesting to note that the flatter the initial cloud, the *higher* is the rate at which it tends to symmetry, though the actual time taken is longer.

For prolate spheroids $(l_1/l_2 > 1)$, (3.18) can be written

$$\frac{l_2'}{l_1'} = \begin{cases} l_2^2/l_1^2 + t^2/\beta_0 l_1^2 \\ 1 + t^2/\beta_0 l_1^2 \end{cases}^{\frac{1}{2}}, \tag{3.18a}$$

which has the same form as (3.18) except that l_1/l_2 is replaced by the reciprocal, and t is non-dimensionalized with l_{γ}/β_0 . With this interpretation, therefore, figure 3 also describes the expansion of prolate spheroids.

We may then generalize the above results as follows: an asymmetric cloud in free-molecule expansion always tends to symmetry, which is roughly achieved at times of order $2l\sqrt{\beta}$, where *l* is the *longest* initial dimension of the cloud.

This result is somewhat different from the conclusion reached by Dyson (1958) after a gasdynamic analysis of the same problem. He found that an initially oblate spheroid actually becomes prolate after expansion, and vice versa.



FIGURE 3. Eccentricity of expanding ellipsoidal clouds.

Free-molecule diffusion

It will be noticed that some of the integrals written down in previous sections show a superficial resemblance to those encountered in heat-diffusion problems; and this fact has actually been used by Molmud to evaluate them. We want to show here that, under certain conditions, there is in fact a peculiar diffusive mechanism in the flow.

We have already expressed the density in free expansion as the integral (3.3); differentiating this integral with respect to \mathbf{x} ,

$$\frac{\partial \rho(\mathbf{x},t)}{\partial \mathbf{x}} = \frac{1}{t^3} \int \frac{1}{t} \frac{\partial f_0(\mathbf{x}';\mathbf{y})}{\partial \mathbf{y}} D\mathbf{x}', \qquad (3.19)$$

where $\mathbf{y} = \mathbf{y}(\mathbf{x}') = (\mathbf{x} - \mathbf{x}')/t$. Comparing (3.19) with the expression (3.4) for \mathbf{u} , it is seen that $\partial \rho / \partial \mathbf{x}$ is proportional to $\rho \mathbf{u}$, if, and only if,

$$\frac{\partial f_0(\mathbf{x}'; \mathbf{y})}{\partial \mathbf{y}} = k \mathbf{y} f_0, \qquad (3.20)$$

where k is a constant, independent of x. Thus only if f_0 can be written as $g(\mathbf{x}) e^{-\beta_0 v^2}$, and so is an isothermal Maxwellian with constant β_0 , is (3.20) satisfied; and in this case the mass flux is indeed proportional to the density gradient,

$$\rho \mathbf{u} = -\frac{t}{2\beta_0} \frac{\partial \rho}{\partial \mathbf{x}},\tag{3.21}$$

and the flow is irrotational. Putting this relation in the equation of conservation of mass $\partial \rho / \partial t + \operatorname{div} (\rho \mathbf{u}) = 0$,

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one obtains

$$\frac{\partial \rho}{\partial t} - \frac{t}{2\beta_0} \nabla^2 \rho = 0. \tag{3.22}$$

This is a diffusion equation for the density with a time-dependent diffusion coefficient. It can be transformed to a diffusion equation with a constant coefficient of unity if we put $t^2/4\beta_0 = \tilde{t}$. Then (3.22) becomes

$$\partial \rho / \partial t - \nabla^2 \rho = 0. \tag{3.23}$$

It is thus no surprise to see integrals looking like those in heat diffusion.

The mechanism of the 'diffusion' exhibited in (3.22) and (3.23) has nothing in common with the other familiar phenomena, namely, ordinary diffusion which depends on intermolecular collisions, or Knudsen diffusion which depends on collisions with surfaces. The mechanism of free expansion can in fact be best described as a kind of collisionless or kinematic diffusion. All the peculiar features noted earlier, like the diffusive front travelling at a definite velocity and growing linearly with time, can be explained now as simple consequences of the diffusion coefficient in (3.22) being proportional to time.

The limitations of this interpretation should be clearly understood. In particular, it should be noted that if β is not constant, one does not get a diffusion equation with a correspondingly variable diffusion coefficient; there simply is no diffusion equation in that case, as ρu and $\partial \rho / \partial x$ cannot be related. Also, if the Maxwellian is centred about a non-zero mean velocity, additional terms are introduced into the equations. Finally, as we shall see later, the solutions when there are time-dependent sources have no simple analogy.

It thus seems that while the resemblance to diffusion is useful in some problems, it is not very general; as the approach through the basic differential equations is at least as simple and vastly more general and fundamental, it will be adopted in the rest of the following work.

However, relations similar to (3.21) can also be derived for all flow quantities. These are interesting as they enable us to find any moment of f if one of them (e.g. the density) is known. Assuming again that the initial distribution is an isothermal Maxwellian, it can be shown, from the corresponding expressions for the moments and from the equations of motion, that the temperature, pressure tensor and heat flow are given by

$$\frac{T}{T_0} = 1 - \frac{1}{3} \left(\beta_0 u^2 - \frac{t}{\rho} \frac{\partial \rho}{\partial t} \right) = 1 - \frac{1}{3} t \operatorname{div} \mathbf{u}, \qquad (3.24a)$$

$$p_{ij} = \rho \overline{c_i c_j} = p \delta_{ij} + \frac{\rho t}{6\beta_0} \frac{\partial u_k}{\partial x_k} \delta_{ij} - \frac{\rho t}{4\beta_0} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \qquad (3.24b)$$

$$q_i = -\frac{3\rho \mathscr{R}t}{4\beta_0} \frac{\partial T}{\partial x_i}.$$
(3.24c)

These expressions can be put in many other equivalent forms. The pressure tensor has the Navier–Stokes form; and though the viscosity coefficients are now timedependent, the Stokesian relation between them is still valid. (An expression like (3.24b) was given by Keller 1948 for the special case of an expanding half-space,

in which flow the off-diagonal terms of p_{ij} are zero.) Finally, the conductivity also increases with time, but the Prandtl number of the flows has the constant value $\frac{5}{6}$.

4. Flow due to sources

In this section we are concerned with the flow due to free-molecule sources, and so with the non-homogeneous equation (2.2), $Q \neq 0$, and its solution given by (2.6). If $f_0 = 0$ and we have a pulse source

$$Q = Q(\mathbf{x},t;\mathbf{v}) = \delta(\mathbf{x})\,\delta(t)\,N(eta/\pi)^{rac{3}{2}}e^{-eta v^2}$$

we obtain again the point-cloud solution

$$f(\mathbf{x},t;\mathbf{v}) = \delta(\mathbf{x} - \mathbf{v}t) \,\mathscr{H}(t) \, N(\beta/\pi)^{\frac{3}{2}} e^{-\beta v^2}.$$

One problem of particular interest is the continuous point source which emits molecules with a given mean velocity \mathbf{u}_0 at a certain rate $\dot{N}(t)$ molecules per unit time. This would, for example, give the flow field due to a free-molecule jet at large distances from the exit. The source in this case has the form

$$Q = \delta(\mathbf{x}) \dot{N}(t) \left(\beta/\pi\right)^{\frac{3}{2}} \exp\left\{-\beta(\mathbf{v}-\mathbf{u}_0)^2\right\}.$$
(4.1)

Putting this in (2.6), one gets

$$f(\mathbf{x},t;\mathbf{v}) = \left(\frac{\beta}{\pi}\right)^{\frac{3}{2}} \exp\left\{-\beta(\mathbf{v}-\mathbf{u}_0)^2\right\} \int^t \delta\{\mathbf{x}-\mathbf{v}(t-s)\}\,\dot{N}(s)\,ds.$$
(4.2)

If we introduce the transformation

$$\sigma = 1/(t-s), \quad \delta\{\mathbf{x} - \mathbf{v}(t-s)\} = -\sigma^3 \delta(\mathbf{v} - \mathbf{x}\sigma) \tag{4.3}$$

in (4.2) and integrate over v, we get

$$\rho(\mathbf{x},t) = \int^{\infty} \left(\frac{\beta}{\pi}\right)^{\frac{3}{2}} \exp\left\{-\beta(\mathbf{x}\sigma - \mathbf{u}_{0})^{2}\right\} \dot{N}(t-1/\sigma) \sigma d\sigma,$$

$$\mathbf{u}(\mathbf{x},t) = \frac{\mathbf{x}}{\rho} \int^{\infty} \left(\frac{\beta}{\pi}\right)^{\frac{3}{2}} \exp\left\{-\beta(\mathbf{x}\sigma - \mathbf{u}_{0})^{2}\right\} \dot{N}(t-1/\sigma) \sigma^{2} d\sigma.$$
(4.4)

The lower limit in these integrals is $\sigma = 1/t$ if the source starts emitting at t = 0, and $\sigma = 0$ if the source has been emitting since $t = -\infty$.

The simplest case is when $\dot{N}(t) = \dot{N}\mathscr{H}(t)$ is a step function in time, \dot{N} being a constant. The integrals in (4.4) can then be evaluated explicitly, and give

$$\rho(\mathbf{x},t) = (N/2\beta x^{2}) (\beta/\pi)^{\frac{1}{2}} \exp(-\beta v^{2} \sin^{2}\theta) \{\exp[-\beta(x/t - u_{0} \cos\theta)^{2}] + (\pi\beta)^{\frac{1}{2}} u_{0} \cos\theta \operatorname{erfc} [\beta^{\frac{1}{2}}(x/t - u_{0} \cos\theta)]\},$$

$$\mathbf{u}(\mathbf{x},t) = (2\mathbf{x}/x\sqrt{\beta}) \{\beta^{\frac{1}{2}}(x/t + u_{0} \cos\theta) \exp[-\beta(x/t - u_{0} \cos\theta)^{2}] + \frac{1}{4}\pi^{\frac{1}{2}}(1 + 2\beta u_{0}^{2} \cos^{2}\theta) \operatorname{erfc} [\beta^{\frac{1}{2}}(x/t - u_{0} \cos\theta)]\}$$

$$+ \{\exp[-\beta(x/t - u_{0} \cos\theta)^{2}] + (\pi\beta)^{\frac{1}{2}} u_{0} \cos\theta + \operatorname{erfc} [\beta^{\frac{1}{2}}(x/t - u_{0} \cos\theta)]\}.$$

$$(4.5)$$

Here θ is the angle between x and \mathbf{u}_{0} and $x = |\mathbf{x}|$ is the distance from the source.

Consider first the symmetric source, $u_0 = 0$. Equations (4.5) then simplify considerably to $\dot{N} (R)^{\frac{3}{2}} (R)^{\frac{3}{2}}$

$$\rho(\mathbf{x},t) = \frac{N}{2\beta x^2} \left(\frac{\beta}{\pi}\right)^{\frac{1}{2}} \exp\left(-\frac{\beta x^2}{t^2}\right),\tag{4.6a}$$

$$\mathbf{u}(\mathbf{x},t) = \frac{\mathbf{x}}{t} + \frac{\mathbf{x}}{2x} \left(\frac{\pi}{\beta}\right)^{\frac{1}{2}} \exp\left(\frac{\beta x^2}{t^2}\right) \operatorname{erfc} \frac{x\sqrt{\beta}}{t}.$$
(4.6b)

First of all it is seen that the gas velocity splits into two parts again, one part containing $\sqrt{\beta}$ and the other not. At small times or large distances $(x\sqrt{\beta}|t \ge 1)$, using the asymptotic expansion for erfc,

$$\mathbf{u} \simeq (\mathbf{x}/t) + (\mathbf{x}t/2\beta x^2) \simeq \mathbf{x}/t,$$

the same as for the pulse source, of course. Secondly, the time t enters into (4.6a) only in the combination $x\sqrt{\beta/t}$, and disappears when $x\sqrt{\beta/t} \ge 1$. Thus at any time a steady state prevails at sufficiently small x, and an unsteady state at sufficiently large x.



FIGURE 4. Comparison of source flows.

Naturally, at any given point x the flow becomes steady at very large times and the kinematic part of the velocity then vanishes. The field of the steady symmetric source is given by

$$\rho = \dot{N} \sqrt{\beta/2\pi^{\frac{3}{2}} x^2}, \quad \mathbf{u} = \frac{1}{2} (\pi/\beta)^{\frac{1}{2}} \mathbf{x}/x, \quad u = |\mathbf{u}| = \frac{1}{2} (\pi/\beta)^{\frac{1}{2}} = \frac{1}{4} \pi \bar{c}.$$
(4.7)

The total mass flux at any radius is $4\pi x^2 \rho u$, = \dot{N} . It is very interesting to note that the gas velocity is constant throughout, and it is the density that drops off as the inverse square of the distance—in contrast to the ordinary incompressible hydrodynamic source. The proper thing to compare it with is actually the supersonic source, for which the velocity tends to a constant at infinity. A general comparison of the velocity field of gasdynamic and free-molecule sources is made in figure 4.†

 $\dagger x_0$ in the figure is defined by $\tilde{Q} = 4\pi a_0 \rho_0 x_0^2$, where \tilde{Q} is the total mass flux from the source. For the gasdynamic sources ρ_0 , a_0 are the stagnation point values of density and sonic speed, and for the free-molecule source a_0 is the sonic speed at the origin.

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Let us return now to the case $u_0 \neq 0$. From (4.5) it is obvious that the streamlines still radiate in straight lines from the centre, but now they tend to crowd around an axis in the direction \mathbf{u}_0 . The remarks made above concerning the unsteady character of the field still apply. They are quite general, in fact. The steady field is given by

$$\rho = \frac{1}{2} \frac{N \beta^{\frac{1}{2}}}{\pi^{\frac{3}{2}} x^{2}} [\exp(-U_{0}^{2}) + \pi^{\frac{1}{2}} U_{0} \cos\theta \exp(-U_{0}^{2} \sin^{2}\theta) \{1 + \operatorname{erf}(U_{0} \cos\theta_{0})\}], \\ \mathbf{U} = \mathbf{u} \sqrt{\beta} = \frac{\mathbf{x}}{x} \frac{U_{0} \cos\theta \exp(-U_{0}^{2} \cos^{2}\theta) + (\frac{1}{2}\pi^{\frac{1}{2}})(1 + 2U_{0}^{2} \cos^{2}\theta) \{1 + \operatorname{erf}(U_{0} \cos\theta)\}}{\exp(-U_{0}^{2}) + \pi^{\frac{1}{2}} U_{0} \cos\theta \{1 + \operatorname{erf}(U_{0} \cos\theta)\}}.$$

$$(4.8)$$

Here $\mathbf{U}_0 = \mathbf{u}_0 \sqrt{\beta}$, and is proportional to the initial Mach number. At right angles to the axis the density is reduced by the factor exp $(-U_0^2)$ in comparison with the symmetric source, but the velocity remains the same.



FIGURE 5. Approximate density distribution in a free-molecule jet, with a comparison with exact expression.

The 'high Mach number' limit

The case of $U_0 \ge 1$ is of some practical interest, and an asymptotic expression for the integrals in (4.4) can be obtained using the method of steepest descents (see e.g. Jeffreys 1950) in the limit $U_0 \rightarrow \infty$. One then gets

$$\rho(\mathbf{x},t) \approx \frac{\sqrt{\beta}}{\pi x^2} U_0 \cos\theta \dot{N} \left(t - \frac{x\sqrt{\beta}}{U_0 \cos\theta} \right) \exp\left(- U_0^2 \sin^2\theta \right), \quad \mathbf{u}(\mathbf{x},t) \approx \frac{\mathbf{x}}{x} u_0 \cos\theta. \quad (4.9)$$

It will be noticed that ρ at (x, t) depends only on the strength of the source at the time $(t - x\beta^{\frac{1}{2}}/U_0 \cos \theta)$; obviously the expressions are valid only when $t > x/u_0 \cos \theta$ and are thus not correct at $\theta \sim \frac{1}{2}\pi$. As we shall see below, however, the density is so small at $\theta \sim \frac{1}{2}\pi$ that (4.9) is practically good everywhere.

In the case when N is constant the density given by (4.9) has been plotted in figure 5, for a few values of U_0 . The exact solution is also included for $U_0 = 1$ and the closeness of the approximation for $\theta \sim \frac{1}{2}\pi$ is quite impressive. The agreement is of course very much better at the higher U_0 for which the density falls off so rapidly with increasing θ that the error committed in using (2.22) for all angles is hardly noticeable. It is obvious from (4.9) that the angle of the spread of the jet is of order U_0^{-1} .

5. Effect of collisions

We sketch here an extension of the Willis method for taking approximate account of collisions, so that it can be applied to the unsteady problems discussed in previous sections. Even the first departure from free-molecular flow becomes very complicated in the general unsteady case, however, and can only be solved with the aid of a computer.

The basic idea involves iteration in which one approximates to f by successive iterates f^0 , f^1 , etc., where each f^n is obtained from the previous one from the equation (see (2.1))

$$(\partial f^n / \partial t) + \mathbf{v} \cdot (\partial f^n / \partial \mathbf{x}) = \mathscr{G}(f^{n-1}) - f^n \mathscr{L}(f^{n-1}) + Q,$$
(5.1)

with f^{0} being the free-molecule solution:

$$(\partial f^0/\partial t) + \mathbf{v} \cdot (\partial f^0/\partial \mathbf{x}) = Q.$$

It is of course hoped that the first iterate f^1 will already be a good approximation to the departure from free-molecule flow. As we will mostly be concerned only with the first iterate, we will study the equation

$$(\partial f^{1}/\partial t) + \mathbf{v} \cdot (\partial f^{1}/\partial \mathbf{x}) = \mathscr{G}(f^{0}) - f^{1}\mathscr{L}(f^{0}) + Q.$$
(5.2)

It will be noticed that $\mathscr{G}(f^0)$ acts as a source distribution so that it can be lumped with Q. In the following Q will be omitted for the sake of brevity, as all one has to do to take account of it is to replace \mathscr{G} by $\mathscr{G} + Q$.

Writing $\mathscr{G}(f^0) = \mathscr{G}^0$ and $\mathscr{L}(f^0) = \mathscr{L}^0$, equation (5.2) becomes

$$(\partial f^{1}/\partial t) + \mathbf{v} \cdot (\partial f^{1}/\partial \mathbf{x}) + f^{1} \mathscr{L}^{\mathbf{0}} = \mathscr{G}^{\mathbf{0}}, \qquad (5.2a)$$

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a quasi-linear, first-order differential equation. The characteristics of (5.2a) are given by

$$dt/ds = 1$$
, $d\mathbf{x}/ds = \mathbf{v}$, $df^{1}/ds + \mathscr{L}^{\mathbf{0}}f^{1} = \mathscr{G}^{\mathbf{0}}$;

using the initial condition

$$f(\mathbf{x}, t = 0; \mathbf{v}) = f_0(\mathbf{x}; \mathbf{v})$$

their solution can be written

$$t = s, \quad \mathbf{x} = \mathbf{v}s + \mathbf{\xi},$$
$$f^{1} = \exp\left\{-\int_{0}^{s} \mathscr{L}^{\mathbf{0}} ds'\right\} \cdot \left[\int_{0}^{s} \mathscr{G}^{\mathbf{0}}\left\{\exp\int_{0}^{s'} \mathscr{L}^{\mathbf{0}} ds''\right\} ds' + f^{\mathbf{0}}\right].$$

Eliminating x and ξ as was done with equation (2.5) and putting x' = x - vt, we get

$$f^{1}(\mathbf{x}, t; \mathbf{v}) = f_{0}(\mathbf{x}'; \mathbf{v}) \exp\left[-\int_{0}^{t} \mathscr{L}^{0}(\mathbf{x}' + \mathbf{v}t', t'; \mathbf{v}) dt'\right] \\ + \int_{0}^{t} \mathscr{G}^{0}(\mathbf{x}' + \mathbf{v}t', t'; \mathbf{v}) \left\{\exp\left[-\int_{t'}^{t} \mathscr{L}^{0}(\mathbf{x}' + \mathbf{v}t'', t''; \mathbf{v}) dt''\right]\right\} dt' \quad (5.3)$$
Here
$$\mathscr{L}^{0}(\mathbf{x}, t; \mathbf{v}) \equiv \mathscr{L}\{f^{0}(\mathbf{x}, t, \mathbf{v})\}$$

wh

etc. Note that $f_0(\mathbf{x}'; \mathbf{v})$ is just the free-molecule solution $f^0(\mathbf{x}, t; \mathbf{v})$.

To proceed further from (5.3) one has to postulate some molecular model. If we use the model for scattering proposed by Bhatnagar, Gross & Krook (1954), we take $\mathscr{G}(f)$ and $\mathscr{L}(f)$ to have the form

$$\begin{aligned} \mathscr{L}(f) &= An, \\ \mathscr{G}(f) &= AnF = An^2(\beta/\pi)^{\frac{3}{2}} \exp\left\{-\beta(\mathbf{v}-\mathbf{u})^2\right\}, \end{aligned}$$

$$(5.4)$$

where n, **u** and β are the corresponding moments of f.

Even with this simplified form for the collision terms the calculation turns out to be extremely complicated in most cases. Computer calculations are now in progress and it is hoped to be able to report on them in the near future.

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