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A Synthetic View of the Mechanics of Rarefied Gases

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I. Introduction

1. Introductory Remarks

IT is a great privilege to join with you in commemorating the achievement of the Wright brothers who made the first mechanical flight of man on December 17, 1903. The underlying reason for their success was a strong desire to understand the science of flight before constructing a heavier-than-air vehicle to accomplish the feat. Through extensive studies of models in a wind tunnel and in the atmosphere and, through a careful reassessment of information published by others, they molded their concept of a successful airplane. This scientific procedure has become standard and it is regularly used to perfect the designs of modern aircraft with their ever-increasing performance requirements.

The Wright brothers recognized that they had to understand the mutual interaction of the atmosphere and their vehicles before a successful design could be devised. So today considerable energy is being expended to perfect our concept of flight in the upper atmosphere where the medium is highly rarefied and new physical effects occur, which must be understood. In current studies of this subject, not only models of aerospace vehicles are investigated, but also models of associated physical processes such as molecule-surface interactions and even models of the fundamental, but complex, equations which govern the flow.

We present here but one view of a rapidly developing subject which has many aspects. The objective is to outline a unified panorama of the mechanics of rarefied gases insofar as this is presently possible. In the headlong rush of modern science, it becomes more and more necessary to pause and try to put together the wider view. Even a limited state-of-the-art survey must reveal some of the gaps in our knowledge, a few of which are between overextensions of the subject; these areas require urgent attention.

For further aspects of the subject, the reader's attention is drawn to a number of excellent reviews.[1–4] An extensive bibliography up to 1961 is contained in Ref. 3. Many interesting papers on rarefied gasdynamics are found in Refs. 5–8.

2. Statistical Basis

A famous American mathematical physicist said: "In the present state of science, it seems hardly possible to frame a dynamic theory of molecular action which shall embrace the phenomena of thermodynamics, of radiation, and of the electrical manifestations which accompany the union of atoms." J. Willard Gibbs made that statement in the preface to his book on the *Elementary Principles in Statistical Mechanics*, published in 1902. Willard Gibbs understood the importance of unifying theories in physics. More than that, he did much to establish modern statistical mechanics that today gives some hope of reducing the fragmentation of fluid physics produced by the expedient extension of phenomenological methods into this field.

In considering the flow properties of a gas and its effect on a body or wall, we are concerned primarily with the macroscopic state. Although Newton's law is available to trace the motion of each particle of the gas, nevertheless the initial positions and velocities are not known, and the calculation of a subsequent state of the gas is not feasible by this method. Furthermore, such detailed information is not required. The method of statistical mechanics was invented to enable us to forecast the future conditions of an assemblage from an incomplete knowledge of the initial state.

As a basic concept from which to determine the "thermodynamic" (macroscopic) state of a gas, Willard Gibbs visualized an ensemble of replicas of the gas, having different states distributed over a wide range. The state of each replica (usually called a system) can be represented by a single point in a phase space having canonical coordinates $q_1, q_2, q_3 \ldots q_S$, $p_1, p_2, \ldots p_S$ where S is the number of degrees of freedom of a particle. The element of volume in this $2S$-dimensional "γ space" is

$$\mathbf{dq\ dp} = dq_1\, dq_2 \ldots dq_S\, dp_1\, dp_2 \ldots dp_S \qquad (1)$$

Then the probability that a particular state will have coordinates between q_α, p_α and $q_\alpha + dq_\alpha$, $p_\alpha + dp_\alpha$ is defined as $F(q_\alpha, p_\alpha, t)\mathbf{dq\ dp}$, where F is called the distribution function in the γ space. The Liouville theorem states that the density of a given group of adjacent phase points remains unaltered as we follow their motion. It is expressed mathematically in the form

$$\frac{\partial F}{\partial t} + \left[\frac{\partial H}{\partial p_\alpha}\frac{\partial F}{\partial q_\alpha} - \frac{\partial H}{\partial q_\alpha}\frac{\partial F}{\partial p_\alpha}\right] = 0 \qquad (2)$$

where H is the Hamiltonian function for a system.

When the density of representative points in each element of volume of the phase space is independent of time, then $\partial F/\partial t = 0$, and the probability function F has a stationary value. It will be noted that when F depends on p_α, q_α only, then $F(H)$ is a solution. More specifically, Gibbs deduced a macrocanonical distribution for the equilibrium state, based on the assumption that the energy (ϵ) of the entire ensemble remains constant, which he found led to all the well-known thermodynamic relations for a gas. Making use

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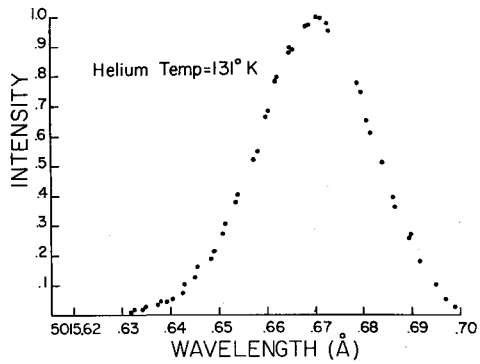

Fig. 1 Measurement of the equilibrium distribution function in helium using an electron gun technique.

of the H theorem (i.e., minimizing the integral $\int F \log F \, \mathbf{dq}\, \mathbf{dp}$), the constancy of ϵ and the condition

$$\int F \, \mathbf{dq}\, \mathbf{dp} = 1 \tag{3}$$

where the integrals are taken over the whole of the γ space, we deduce the following form for the probability distribution of the equilibrium state:

$$F(H) = \text{const}\ e^{-H/\theta} \tag{4}$$

where from thermodynamic considerations $\theta = kT$.

Now we have seen that F is the distribution function for an ensemble of replicas of the subject system (or gas). Let us now introduce a six-dimensional space (called a μ space) having coordinates q_i, p_i ($i = 1, 2, 3$) in which the gas is represented by a cloud of points, each of which specifies the position and momenta of one of its particles. We define F_α as a single-particle distribution function referred to the αth particle. Thus F_α is the probability that the αth particle will have coordinates $q_{\alpha i}$, $p_{\alpha i}$ corresponding to the Hamiltonian (or total energy) H_α regardless of the states of all other particles. It is obtained by integrating F over the positions and momenta of all other particles except the αth. Thus we find for the equilibrium state

$$F_\alpha = \text{const}\ e^{-H\alpha/kT} \tag{5}$$

which is the well-known Maxwell law for the distribution of particle velocities. It should be noted that this distribution is a statistical fact and does not rely on specific forms of particle motions (i.e., collisions) to support it.

The form of Liouville's equation for a gas composed of neutral particles is readily obtained. The Hamiltonian has the form

$$H = \sum_{\alpha=1}^{N} \left[\frac{\mathbf{p}_\alpha^2}{2m_\alpha} + \varphi_\alpha(\mathbf{q}_\alpha) \right] \tag{6}$$

where $\varphi_\alpha(\mathbf{q}_\alpha)$ is a potential function from which the force on the αth particle can be derived, i.e.,

$$\mathbf{X}_\alpha = -(\partial \varphi_\alpha / \partial \mathbf{q}_\alpha) \tag{7}$$

The derivatives of H can now be determined and substituted in (2) to obtain Liouville's equation for a neutral gas

$$\frac{\partial F}{\partial t} + \sum_{\alpha=1}^{N} \left[\xi_\alpha \cdot \frac{\partial F}{\partial \mathbf{q}_\alpha} - \frac{\partial \varphi_\alpha}{\partial \mathbf{q}_\alpha} \cdot \frac{\partial F}{\partial \mathbf{p}_\alpha} \right] = 0 \tag{8}$$

In a rectangular coordinate system with $\mathbf{q}_\alpha$ replaced by $\mathbf{x}_\alpha$ and $\mathbf{p}_\alpha = m_\alpha \xi_\alpha$, Liouville's equation in this $6N$-dimensional $(\mathbf{x}_\alpha, \xi_\alpha)$ space becomes

$$\frac{\partial F}{\partial t} + \sum_{\alpha=1}^{N} \xi_\alpha \cdot \frac{\partial F}{\partial x_\alpha} + \sum_{\alpha=1}^{N} \frac{\mathbf{X}_\alpha}{m_\alpha} \cdot \frac{\partial F}{\partial \xi_\alpha} = 0 \tag{9}$$

The fundamental equation for the single-particle distribution function is obtained for the αth particle by integrating

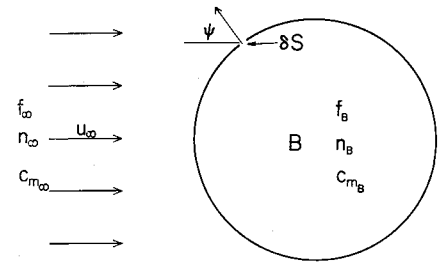

Fig. 2 Idealized orifice probe.

Liouville's equation with respect to all variables except $x_{\alpha i}$, $\xi_{\alpha i}$. Note that the definition of the singe-particle distribution function is

$$F_\alpha(\mathbf{x}_\alpha, \xi_\alpha, t) = \int F \, d\mathbf{x}_1 \ldots d\mathbf{x}_{\alpha-1}\, d\mathbf{x}_{\alpha+1} \ldots d\mathbf{x}_N d\xi_1 \ldots d\xi_{\alpha-1} d\xi_{\alpha+1} \ldots d\xi_N \tag{10}$$

where $d\mathbf{x}_1$ is the symbol for $dx_{11} dx_{12} dx_{13}$, etc. This is the probability that the αth particle will be at $\mathbf{x}_\alpha$, ξ_α irrespective of the coordinates of all remaining particles. We also need the definition of the binary distribution function which specifies the joint probability that the coordinates of the αth particle will be $\mathbf{x}_\alpha$, ξ_α at the time the βth particle has coordinates $\mathbf{x}_\beta$, ξ_β in the position-velocity phase space

$$F_{\alpha\beta}(\mathbf{x}_\alpha, \mathbf{x}_\beta, \xi_\alpha, \xi_\beta, t) = \int F \, d\mathbf{x}_1 \ldots d\mathbf{x}_{\alpha-1}\, d\mathbf{x}_{\alpha+1} \ldots d\mathbf{x}_{\beta-1}\, d\mathbf{x}_{\beta+1} \ldots d\mathbf{x}_N \, d\xi_1 \ldots d\xi_{\alpha-1}\, d\xi_{\alpha+1} \ldots d\xi_{\beta-1}\, d\xi_{\beta+1} \ldots d\xi_N \tag{11}$$

Then the integration of (9) with respect to all variables except $x_{\alpha i}$, $\xi_{\alpha i}$ over the whole $(\mathbf{x}_\alpha, \xi_\alpha)$ space yields the following equation for the single-particle distribution function:

$$\frac{\partial F_\alpha}{\partial t} + \xi_\alpha \cdot \frac{\partial F_\alpha}{\partial \mathbf{x}_\alpha} + \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N} \frac{1}{m_\alpha} \frac{\partial}{\partial \xi_\alpha} \cdot \int \mathbf{X}_{\alpha\beta} F_{\alpha\beta} \mathbf{dx}_\beta \mathbf{d}\xi_\beta = 0 \tag{12}$$

where the total force on the αth particle is the sum of the forces exerted by all other particles on the αth particle, i.e.,

$$\mathbf{X}_\alpha = \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N} \mathbf{X}_{\alpha\beta} \tag{13}$$

The normalized value of the single-particle probability is one. Boltzmann has introduced another convenient single-particle distribution function that is the number density in the $(\mathbf{x}_\alpha, \xi_\alpha)$ space having the normalization for unit physical volume

$$\int f \mathbf{d}\xi = n \tag{14}$$

where n is the number density in physical space. The mean (macroscopic) velocity has the components

$$u_i(\mathbf{x}, t) = \frac{1}{n} \int \xi_i f \mathbf{d}\xi \qquad u_i = \xi_i - c_i \tag{15}$$

and the higher moments of f define the pressure tensor and components of the heat flow vector

$$p_{ij} = m \int c_i c_j f \mathbf{d}\xi \qquad \epsilon_i = m \int c_i c_j c_j f \mathbf{d}\xi \tag{16}$$

Thus a knowledge of the Boltzmann distribution function at a point in a gas is sufficient to determine the local macroscopic properties. Therefore, the determination of f is fundamental to our subject and we shall find that (12) provides a basis for relating the regimes of fluid mechanics.

II. Free Molecule Regime

1. Transfer Properties of Free Molecule Flow

We shall begin our discussion of the mechanics of rarefied gases with a consideration of the free-molecule regime. If

the motion is such that the forces between particles have a negligible effect, then the appropriate equation for the distribution function is obtained from (12) by dropping the force term, or in terms of Boltzmann's distribution function,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = 0 \tag{17}$$

In other words f remains constant following the motion of the particles in physical space. Thus f is a constant of the particle motion.

Calculations in free-molecule flow make frequent use of the equilibrium condition of a gas specified by (5), which has been verified by molecular beam methods. A technique for a direct determination of the velocity distribution function using electron beam excitation in low-density helium has been investigated recently by Muntz.[9] Observation of the electroluminescence produced a spectral line profile that was considered to be a close approximation to a true Doppler profile. Since a linear relation exists between Doppler shift and the relative velocity between an emitting atom and a detector, a direct determination of the velocity distribution function was possible. Preliminary tests gave the measured distribution shown in Fig. 1, which has the typical Maxwellian form.

We can illustrate the transfer properties of free-molecule flow by considering the theory of an orifice pressure probe[10-12] in a gas containing identical particles. We visualize in Fig. 2 a very low-density flow relative to an enclosure B having a small orifice of area δS (Fig. 2). The normal to δS is oriented at an angle ψ relative to the macroscopic motion of the external gas that is taken along the x_1 axis. We assume that the gas inside the enclosure is in equilibrium, the latter being unaffected by the small stream of particles entering through the orifice, i.e., in accordance with (5):

$$f_B = \frac{n_B}{(\pi^{1/2} c_{mB})^3} \exp\left(- \frac{c_i c_i}{{c_{mB}}^2} \right) \tag{18}$$

where $c_{mB} = (2RT_B)^{1/2}$ is the most probable particle speed and T_B is the temperature in the enclosure. Hence the number of particles emerging from the orifice in unit time is

$$[(n_B c_{mB})/2\pi^{1/2}]\delta S \tag{19}$$

We now specify that, in accordance with the properties of free-molecule motion, the distribution function for the particles entering the orifice is the same as the distribution function for the external gas "at infinity":

$$f_\infty = \frac{n_\infty}{(\pi^{1/2} c_{m\infty})^3} \exp\left(- \frac{c_i c_i}{{c_{m\infty}}^2} \right) \tag{20}$$

where $\xi_1 = u_\infty + c_1$, $\xi_2 = c_2$, $\xi_3 = c_3$, and the speed ratio is $S = u_\infty / c_{m\infty}$. Then the number of molecules entering the orifice in unit time is

$$\frac{n_\infty c_{m\infty}}{2\pi^{1/2}} [\exp(-S^2 \cos^2\psi) + \pi^{1/2} S \cos\psi (1 + \operatorname{erf} S \cos\psi)] \tag{21}$$

In the steady state there will be no accumulation of mass in the enclosure and (19) and (21) will be equal. Thus the orifice pressure probe is governed by the relation

$$\frac{p_B}{p_\infty}\left(\frac{T_\infty}{T_B}\right)^{1/2} = \exp(-S^2 \cos^2\psi) + \pi^{1/2} S \cos\psi (1 + \operatorname{erf} S \cos\psi) \tag{22}$$

A pressure probe of cylindrical shape having a small orifice was investigated experimentally for $S < 1$ in the University of Toronto, Institute for Aerospace Studies (UTIAS) low-density wind tunnel.[11] A typical test result is shown in Fig. 3. The agreement between theory (22) and experiment is satisfactory and our concepts of free-molecule flux appear to be verified in an over-all sense. Essentially this experiment indicates that at very low density there exists a flow such that the particles emerging from the orifice and the surrounding surface of the body neither collide among themselves nor interfere with those reaching the orifice from the external gas in the vicinity of the orifice.

We need to be more specific as to what is meant by "very low density." The particles at infinity in the external gas flowing relative to the probe will experience encounters among themselves, and a mean free path between collisions can be defined. We note that in the experiment the mean

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Gordon N. Patterson is the Director of the Institute for Aerospace Studies, University of Toronto. Born in Medicine Hat, Alberta, Canada, in 1908, he graduated from the University of Alberta with a B.Sc. in Engineering Physics (1931) and from the University of Toronto with the M.A. and Ph.D. in Physics (1935). He was Scientific Officer, Royal Aircraft Establishment, England, from 1935 to 1939, and participated extensively in improvements in the performance of the Spitfire fighter, which played such a significant role in the Battle of Britain. In 1939 he accepted an appointment as head of the Aerodynamics Section of the Aeronautical Research Laboratory, Melbourne, Australia, where he initiated the development of aerodynamic facilities in that country. He returned to the University of Toronto in 1947 and, in 1949, founded the Institute for Aerospace Studies.

Dr. Patterson is a Fellow Member of the American Institute of Aeronautics and Astronautics, and a Fellow of the Canadian Aeronautics and Space Institute, Royal Aeronautical Society, and the Royal Society of Canada. He has received the McCurdy Award, Canada's highest award in the aerospace sciences. He was selected as one of the three most outstanding graduates on the fiftieth anniversary of the University of Alberta and was presented with an honorary degree of Doctor of Laws. He has received the honorary degree of Doctor of Science from the University of Waterloo.

He has published a number of papers in the fields of the aerodynamics of ducted cooling, diffuser design, drag due to air leakage, heat regeneration, theory of ducted fans, and shock tubes, and has published a book on the *Molecular Flow of Gases*. Dr. Patterson has served as chairman of the Advisory Aeroballistics Panel, U. S. Naval Ordnance Laboratory; chairman of the Fourth International Symposium on Rarefied Gas Dynamics (Toronto, 1964); and is presently a member of the NASA Research Advisory Committee on Fluid Mechanics, the Advisory Committee on Plasma and Gas Dynamics, Defence Research Board of Canada, and the Technical Advisory Panel of the (Canadian) National Aeronautical Research Council.

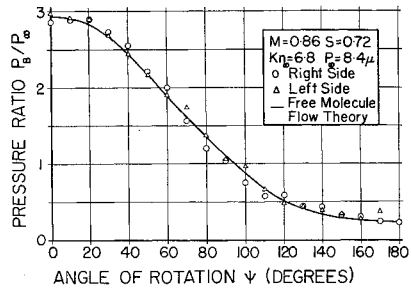


Fig. 3 Variation of orifice probe pressure with orientation.

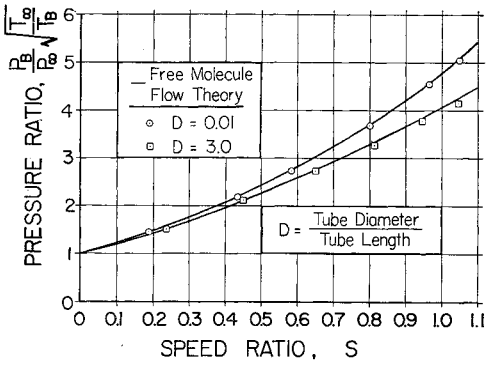


Fig. 5 Comparison of theoretically and experimentally determined impact pressure ratios for a cylindrical probe.

free path was 6.8 times the diameter of the probe (Kn_∞ = 6.8). This value was sufficiently large to ensure collisionless flow in the vicinity of the probe.

The significant feature of free-molecule flow is the emphasis that a study of this subject places on particle-surface interactions since this process dominates the motion. The orifice probe experiment was designed to avoid this complex subject initially. Nevertheless it suggests a simple model for particle reflection from a wall, which has been found to be useful in analyzing some low-density flows. We can imagine that the particles emerge from the surface as if they came from a gas in equilibrium having the temperature and macroscopic velocity of the surface analogous to the efflux of gas from the gage volume of the orifice probe. Thus the distribution function for the reflecting particles is given by (18), and is illustrated by Fig. 1; the process is called "perfectly diffuse reflection."

In order to investigate this kind of reflection, let us consider the free flux of particles through an axially symmetric tube which connects a gas in equilibrium with a vacuum (Fig. 4). Here a particle will collide many times with the walls of the tube and may eventually reach the vacuum or return to the gas.[13–15]

Let the total number of particles striking the annulus between x and $x + dx$ in unit time be $\zeta(x)dx$. If there is no adsorption or ablation, the number of particles reflecting from the wall between x and $x + dx$ in unit time is also equal to $\zeta(x)dx$. Now let $P(x, l)$ be the probability that a particle leaving the wall between x and $x + dx$ will pass through the exit opening at $x = l$ without further encounters with the wall. Then the number of particles reaching the vacuum space in unit time from the annulus between x and $x + dx$ is $P(x, l)\zeta(x)dx$, and the total number of particles that emerge in unit time from the tube in the vacuum space and that have collided with the wall of the tube is

$$\int_0^l P(x, l)\zeta(x)dx \tag{23}$$

Now some of the particles will proceed directly through the tube without striking the wall. Let this number be N_{cc} per unit time. Then the total number of particles that pass through the tube into the vacuum space in unit time is

$$N(l) = N_{cc}(l) + \int_0^l P(x, l)\zeta(x)dx \tag{24}$$

Proceeding along these lines we can calculate the formula for an impact pressure probe aligned antiparallel to the direction of the external macroscopic motion.[16] If the probe is cylindrical having a diameter d and length l, then

$$\frac{p_B}{p_\infty}\left(\frac{T_\infty}{T_B}\right)^{1/2} = \frac{W(S, d/l)}{W(o, d/l)} \tag{25}$$

The specific forms of $W(S, d/l)$ and $W(o, d/l)$ are rather extended and may be found in Ref. 12. A complete numerical solution over a wide range of Mach numbers is given in Ref. 15. This relation has been checked out experimentally[17] for speed ratios up to about 1 in the UTIAS low-density tunnel and found to be correct within experimental accuracy (Fig. 5). These experiments provided an over-all verification of theory. A more detailed study of the flux process, involving the use of an electron gun to determine the radial distribution of density at the exit of the tube,[18] is summarized in Fig. 6. We conclude that for the geometries and speed ratios tested, the assumption of perfectly diffuse reflection seems to work very well. Further calculations for other axially symmetric systems are reported in Ref. 19.

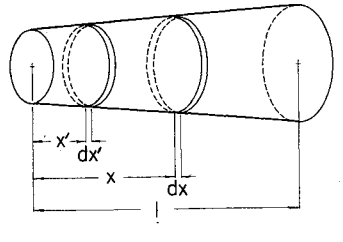


Fig. 4 Particle flux through axially symmetric tubes.

However, considerable evidence has now been accumulated to show that although the assumption of perfectly diffuse reflection may be adequate in some applications (in particular, internal flux systems), in general the subject of particle-surface interactions is highly complex and still not understood. Until research produces an improved technique, low-density aerodynamicists will continue to use empirical accommodation coefficients in their calculations. To introduce these coefficients let us recall first that in perfectly diffuse reflection the particles emerge as if they had come from a gas having the same macroscopic state (temperature and velocity) as the surface, i.e., the reflected gas was fully accommodated to the wall. Thus each incident particle appears to be temporarily "trapped" by the surface and many encounters with wall constituents occur before the particle joins the emerging gas. We can also imagine a mirror-like or specular reflection in which each particle reflects as if it came from a gas having a state identical with that of the incident gas so that the emerging gas shows no accommodation toward the condition of the wall. In diffuse reflection, the ultimate angle of departure of a given particle from a surface bears no relation to the incident direction, and the probability that a particle will leave the surface with a particular orientation is proportional to the cosine of the angle made with the normal to the surface. On the other hand, in specular reflection the normal component of velocity of the incident particle is reversed in direction but unchanged in magnitude, and the tangential components remain unchanged.

Maxwell[20] suggested that some particles might reflect specularly and others diffusely. In other words, the emergent gas was only partially accommodated to the state of the surface. Proceeding along these lines, it is useful to consider the reflected momentum and energy from an element of surface as a linear combination of the corresponding quan-

tities for specular and perfectly diffuse reflection. Thus the normal momentum, tangential momentum, and energy of the emergent gas are represented empirically as

$$\begin{aligned} p_r &= (1 - \sigma')p_\infty + \sigma' p_B \\ \tau_r &= (1 - \sigma)\tau_\infty \qquad (\tau_B = 0) \\ \epsilon_r &= (1 - \alpha)\epsilon_\infty + \alpha\epsilon_B \end{aligned} \tag{26}$$

where σ', σ, and α are the normal momentum, tangential momentum, and energy accommodation coefficients, respectively, and are regarded as constant. Note that, in particular, σ', σ, and α are all zero for completely specular reflection and all have the value 1 for perfectly diffuse reflection.

The value of the accommodation coefficients to the aerodynamicist is readily seen when we write down the expressions for normal pressure and shearing stress on the surface element:

$$\begin{aligned} p &= p_\infty + p_r = (2 - \sigma')p_\infty + \sigma' p_B \\ \tau &= \tau_\infty - \tau_r = \sigma\tau_\infty \end{aligned} \tag{27}$$

where p_∞, p_B, τ_∞ can be found using the appropriate distribution function [see (18) and (20)]. Introducing measured values of σ', σ, and α, and integrating these expressions over the whole surface of a body, we can determine the resultant force. These calculations are based on the assumption that there is no outgassing, adsorption, or ablation involved in the reflection process so that the number of reflected particles equals the number of incident molecules. This condition permits the calculation of n_B for prescribed values of n_∞, the component of S perpendicular to the surface element and T_∞. An abbreviated form of the drag coefficient for an "infinite" cylinder transverse to the flow is given by[3]

$$C_D = \frac{\sigma'\pi^{3/2}}{4S}\left(\frac{T_B}{T_\infty}\right)^{1/2} + \frac{4 + \sigma - 2\sigma'}{S}\,\pi^{1/2} e^{-1/2S^2} F(S) \tag{28}$$

Thus the free-molecule force on a body depends on surface temperature T_B and α, as well as on the undisturbed conditions of the gas flow, body geometry, σ' and σ.

In a given low-density flow various forms of energy are received and given up by the element of surface. There will be impinging and actual reflected fluxes of molecular energy ϵ_∞, ϵ_r, incident and emergent radiant energies R_∞, R_B, and heat conducted to or from the element of surface due to sources inside the body, Q. Thus the balance of energy at the element of surface requires that

$$\epsilon_\infty + R_\infty = \epsilon_r + R_r + Q \tag{29}$$

This equation specifies T_B for given conditions at infinity and known values of α and Q. In most aerodynamic calculations T_B is taken to be constant over the whole surface. This is acceptable if internal heat conduction is very rapid. Of special interest is the equilibrium value of T_B, which is attained when $Q = 0$. This value of T_B applies to wind tunnel tests in which no heat is supplied to the model. On the other hand, the ambient value of T_B, for which $T_B = T_\infty$, is characteristic of high-speed flight conditions in which radiant cooling is dominant.

Not many experiments on the aerodynamics of bodies strictly in the free-molecule regime have been made. However, the pioneering work of Stalder, Goodwin, and Creager reported in Refs. 21 and 22 provides a comparison of theory and experiment (Fig. 7) which must be regarded as satisfactory when we consider the practical difficulties in measuring very small drag forces. The theory indicated in Fig. 7 is based on an assumption of diffuse reflection such that $\sigma' = \sigma = 1$ but $\alpha = 0.9$, i.e., the particles emerge diffusely from a gas which has a temperature different from the wall value.

2. Estimates of Satellite Drag

To the aerodynamicist, the hypersonic condition in low-density flows is most important. According to the theory discussed previously, the drag coefficient for a spherical satellite moving in an orbit, where the motion involves essentially the interaction of neutral particles with the surface of the satellite, should have the form

$$C_D = 2 - \sigma' + \sigma \tag{30}$$

This relation is obtained from the expression for the free-molecule drag coefficient of a sphere by allowing the speed ratio S to approach infinity while T_B/T_∞ remains finite. We see at once that $C_D = 2$ for both purely specular and completely diffuse reflection. Schaaf[3] considers this result to be misleading, but concludes that it does point up the importance of particle-surface interactions.

Let us examine the estimates of the satellite drag coefficient based on physical models of the surface interactions proposed by Schaaf[23] and Schamberg.[24] Schaaf suggested a tentative, high-energy interaction in which dissociation plays a role. He assumed the satellite to be in an orbit where the at-

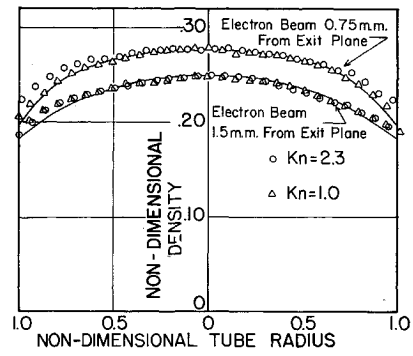
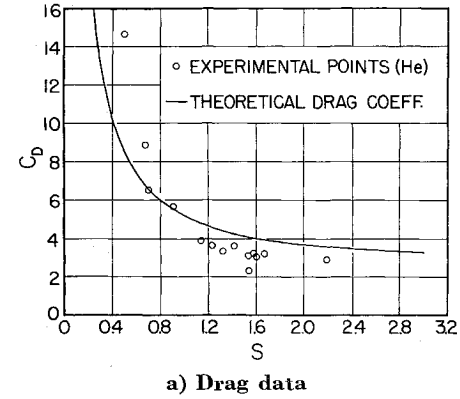
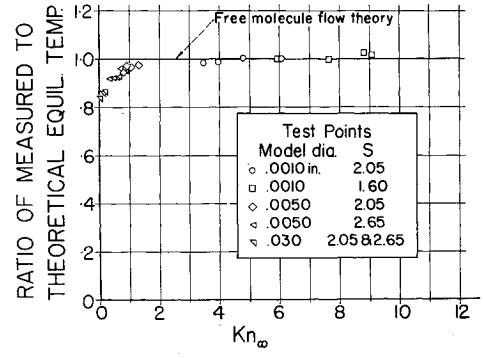


Fig. 6 Radial distribution of density at the exit of a tube measured with an electron gun and compared with free-molecule theory.



a) Drag data



b) Equilibrium temperature data

Fig. 7 Low-density aerodynamic data for transverse cylinders and a comparison with free-molecule theory.

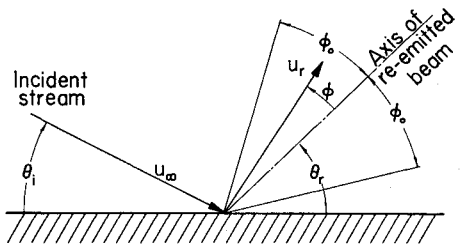


Fig. 8 Schamberg's model of the particle-surface interaction.

mospheric oxygen is completely dissociated into atoms but the nitrogen remains essentially in the molecular state. The oxygen atoms reflect diffusely with respect to direction but the energy accommodation is incomplete. The interaction of oxygen atoms with the wall is characterized, therefore, by a single accommodation coefficient α_o. A similar interaction is assumed for the nitrogen molecules except that some of them (a fraction β) dissociate on contact with the surface. The energy of the reflected nitrogen atoms is regarded as negligible compared with the dissociation energy. Thus the interaction of nitrogen with the surface is specified by the two parameters α_{N_2} and β. Schaaf then deduced the following expression for the drag coefficient of a sphere in orbit:

$$C_D = 2 + \frac{2^{1/2}\pi}{3}\left[\frac{\rho_0}{\rho}(1-\alpha_o)^{1/2} + (1-\beta)\frac{\rho_{N_2}}{\rho}(1-\alpha_{N_2})^{1/2}\right] \quad (31)$$

where ρ, ρ_0, and ρ_{N_2} are the densities of the atmosphere, oxygen atoms, and nitrogen molecules, respectively.

In using (31) to obtain an estimated drag coefficient under the conditions assumed, it is necessary to forecast values for α_0 and α_{N_2} on typical engineering materials. We have noted a value of 0.9 in the experiments of Stalder, Goodwin, and Creager. But it is now realized that this value pertained to the experimental conditions that were influenced by an adsorbed layer of gas on the test surface. Considerable experimental work has been done to determine α. A compilation made by Hurlbut is reviewed in Ref. 3 where it will be seen that the surface condition is all-important. A review of the subject given by Hartnett[25] led to the conclusion that most investigations suffered from one or more deficiencies such as failure to specify the true surface condition, ensure free-molecule flow, or eliminate the necessity for large radiation corrections. Add to this the fact that no tests have been reported as yet at the particle energies appropriate to space flight and we understand the aerodynamicists' problem in choosing a value for α. However, it is felt that the very low pressure surrounding orbiting vehicles, compared with that reported so far in laboratory tests, and the scouring effect of the high energy particles impinging on a surface in space will produce a "clean" surface such that incident particles will interact primarily with the bare surface constituents. It seems likely, therefore, that α will be somewhat less than 0.9. Schaaf found that for $\alpha_O \cong 0.45$, $\alpha_{N_2} \cong 0.5$, C_D was about 2.6 for no dissociation and 2.1 with complete dissociation. The significance of these results lies in the stress they place on a better knowledge of particle-surface interactions since the latter has an overriding influence on the aerodynamics of hypersonic vehicles in the upper atmosphere.

Another approach to the subject of hypersonic drag in free-molecule flow has been outlined by Schamberg. He proposed a new model of the particle-surface interaction for the case in which the flight speed is much greater than the most probable speed of the random motion of the particles in the atmosphere ($S \to \infty$). In fact, the random motion of the incident particles is neglected, and they are assumed to approach the surface in the form of a parallel, uniform beam with velocity u_∞ and angle of incidence θ_i. Schamberg then assumed that the most probable angle of reflection of a particle (θ_r) lies between the most probable direction of diffuse reflection ($\theta_r = 90°$ for all θ_i) and the angle of specular reflection ($\theta_r = \theta_i$) (Fig. 8). Suggested by surface interaction experiments made by Hurlbut[26] on the clean surface of a lithium fluoride crystal in which the re-emission differed appreciably from the diffuse reflection (cosine) law, Schamberg further assumed that the distribution of reflected particles is symmetric about the axis of the beam. Finally the lack of adequate experimental information necessitated the interim assumption that the speeds of all emerging particles is the same, independent of φ (Fig. 8). Schamberg then deduced a "hyperthermal" drag coefficient having the general form

$$C_D = 2 + f(\alpha, \nu, \varphi_0, \text{body shape})$$
$$\cos\theta_i = (\cos\theta_r)^\nu \qquad u_r/u_\infty \cong (1-\alpha)^{1/2} \quad (32)$$

The first term is the contribution to the drag coefficient due to the incident beam of particles. It would be the value of C_D if all particles stuck to the surface and it is independent of body shape and the surface interaction. The second term is the contribution made by the reflected particles and, here, the surface interaction parameters and body shape play a significant role. In the case of the sphere Schamberg estimates that for $\alpha = 1$, $C_D = 2$, but for $\alpha < 1$, $C_D > 2$. It is interesting that in this hypersonic model of the surface interaction α is the accommodation coefficient retained in the theory. A calculation of C_D for a flat plate and a finite cylinder in addition to the sphere led to the conclusion that the drag coefficient is influenced much more by the changes in surface interaction than by variations in body geometry. Schamberg further concludes that questions of atmospheric composition are secondary to the accurate prediction of α.

3. Thermal Accommodation Coefficient

The preceding speculation on the drag of a sphere in hypersonic, free-molecule motion has been useful in emphasizing the importance of the energy accommodation coefficient to the aerodynamicist. We will now give some attention to recent experimental investigations and theoretical studies of this coefficient. Our previous considerations lead us to suspect that in the free-molecule, hypersonic regime two essential requirements must be met in laboratory tests: 1) the surface must be clean, its condition fully specified and reproducible; and 2) incident particles must have energies appropriate to hypersonic motion. Some excellent reviews of the literature are available[27, 28] and we must conclude from these that, because of practical difficulties, conditions 1 and 2 have not yet been met. It is clear that the laboratory simulation of aerodynamic conditions in space is now an urgent requirement of considerable importance.

The subject of the effect of surface conditions on the accommodation coefficient of the inert gases has received at-

Table 1 Accommodation coefficients for helium on various prepared metal surfaces at room temperature obtained by a number of authors[27]

Metal	Accommodation coefficient α
Tungsten	0.017
Platinum	0.038
Aluminum	0.073
Beryllium	0.145
Potassium	0.083
Sodium	0.090

tention by a number of experimenters and the most reliable results from various references have been summarized by Wachman.[27] Table 1 shows the results for helium on various clean metals. The surfaces in the first and second items in Table 1 were prepared by flashing, and the remainder by evaporation on platinum or tungsten. It is noted that α is very much below the value 0.9 inferred previously for air from wind tunnel tests.

The importance of surface condition is further emphasized by the more recent work of Datz, Moore, and Taylor.[29] As a beam source they used a tungsten furnace which could be heated to about 3000°K corresponding to a particle energy approaching 0.5 ev. Angular distributions measured for helium and deuterium reflecting from a polished polycrystalline platinum surface showed interesting properties. The effect of both surface and beam temperatures is illustrated in Fig. 9 for the case of helium. It will be seen that at room temperature the reflection was diffuse but an increase in surface temperature to over 1000°C produced a strong tendency toward fully specular reflection. This tendency was further increased by raising the beam temperature. The authors concluded that the test surface was smooth down to atomic dimensions, that the essential effect of higher surface temperature was to drive off adsorbed contaminant gases, and that the effect of higher beam temperatures was to reduce the "residence time" of the impinging particles on the surface. The authors also investigated the effect of angle of incidence on the reflection of the relatively energetic particles on a clean surface and found that the tendency toward specular reflection increased with the angle of incidence. It is interesting that the pattern of angular distributions obtained in this experiment gave support to Schamberg's reflection model discussed previously.

A number of theoretical studies of particle-surface interactions have been made. Both quantum and classical formulations of the problem have been attempted. The quantum method was initiated by Jackson[30] and developed by Devonshire.[31] Mathematical complexity led to the introduction of many simplifying assumptions with a resultant loss in physical insight. Furthermore, Devonshire's results do not appear to give results consistent with clean surface measurements. Both objections are alleviated by a classical approach[28, 32, 33] using appropriate potential fields around participating particles and a lattice representation of the solid.

Goodman's perturbation theory for the thermal accommodation of light gases has led to quantitative agreement between classical theory and experiment. He adopted a reflection model such that the impinging flux of molecules is represented as a stream of particles, each having the same velocity consistent with the gas temperature. Thus no account is taken of an initial distribution of particle velocities. The surface is represented as a three-dimensional semi-infinite lattice initially at rest (0°K). An incident particle is assumed to impinge on a surface particle in a direction normal to the surface such that no other surface particles "feel" the influence of the force field around the incident particle. In the first approximation the lattice is considered to remain

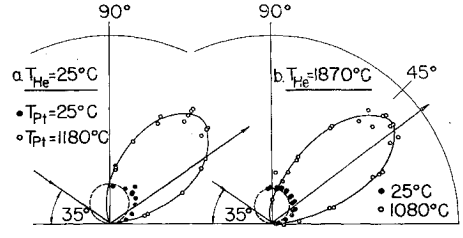


Fig. 9 Angular scattering of helium particles from a polished polycrystalline platinum surface.

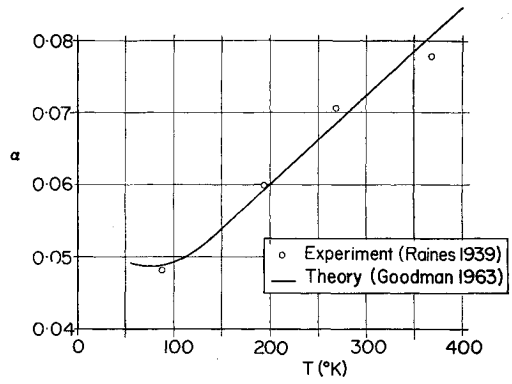


Fig. 10 Thermal accommodation of helium particles on nickel vs gas temperature.

at rest throughout the interaction and the force on the lattice due to an approaching and receding gas particle is a known function of time. In the second operation this force is permitted to act on the free lattice. The resulting increment in lattice energy is determined and assumed to be equal to the energy lost by the particle. Inherent errors in this perturbation method restricted the theory to light gases and small thermal accommodation coefficients. A comparison of the theory with experiment involved a choice of a characteristic quantity of the Morse potential function to obtain the best fit. The variation of the thermal accommodation coefficient with gas temperature (T) calculated by Goodman agrees well with experiment for He/N_i, He/W, and Ne/W.[34] The case He/N_i is illustrated in Fig. 10. Further comparisons appear to be necessary, however, in view of the uncertainty of the cleanness of the surface in the experiments.

Of special interest to the hypersonic aerodynamicist is the theoretical work of Oman, Bogan, Weiser, and Li,[33, 35] which applies to hypervelocity flight where incident molecular energies are much larger than the thermal energies in the atoms of the solid and the collision is of short duration. Starting with a wide range of initial input conditions they have calculated a large number of molecular trajectories for particles interacting with an ideal crystal surface using a digital computer. The solid is represented by an Einstein lattice, i.e., each surface atom is regarded as a three-dimensional harmonic oscillator with a linear restoring force. A Lennard-Jones 6–12 potential is adopted for the interaction between an impinging particle and each lattice atom. The total force on the incident particle arises from all the forces exerted by the surface atoms, each of which interacts only with the gas particle. At large distances between the gas particle and the lattice, the solid medium was represented as a semi-infinite continuum exerting a van der Waals force of attraction. At intermediate distances, a composite of the continuum potential and the Lennard-Jones potential was used. No account is taken at this stage of the calculations of effects due to surface roughness and contaminants, internal degrees of freedom of the particles, electron interactions, sputtering or chemical effects. The general conclusion of the authors was that full-scale numerical computations of gas-surface interactions were practicable and useful. The method opens the way to a systematic study of the various parameters controlling the interaction. A study of flux and energy distributions after interaction showed that the representation of the process as a linear combination of specular and diffuse reflection was oversimplified. Their calculations also indicated that any comparison of theory and experiment was possible only if the experimental conditions could be accurately assessed. In particular, a measurement of an accommodation coefficient at ordinary thermal energies could hardly be applied to the case of a satellite.

In some later work, Oman, Bogan, and Li[35] have made a series of calculations for the inert gases argon, neon, and helium impinging on nickel over a range of incident energies. Table 2 presents a comparison of some of the results for helium in rounded-off figures for one incident angle. Such a calculation is useful in showing the importance of the ratio of incident particle mass to the lattice atom mass. It is interesting that the results showed several "bounces" under some conditions, each involving a decrease in particle energy, and the possible failure of the gas particle to separate from the wall. Thus the possibility of a "trapped state" was suggested by these calculations. The momentum accommodation coefficients σ', σ are noticeably different from each other and from the frequently assumed value of 1.0.

Despite the usefulness of the accommodation coefficients and the promise of more recent research, a rigorous formulation of the boundary conditions for a kinetic theory of free-molecule flow requires an expression for the distribution of velocities for particles leaving the surface of a body or wall. Thus the macroscopic properties of the motion around a body can be calculated at any prescribed point if f_∞ and f_B are given and used within their respective cone angles. At present, experiments on particle-surface interactions yield only a measurement of the number density of particles within a specified angle of reflection and at most the associated average particle velocity.

III. Transition Regime

1. Boltzmann Equation

We have seen that the solution of problems in the free-molecule regime involved a reduced form of the equation for the single-particle distribution function (17) and the appropriate boundary conditions. If now interparticle collisions are to be considered, we must return to (12) and obtain an expression for the force term. We note first that although $F(t)$ can be determined for an initial $F(0)$ from the Liouville equation (9), the equation for the single-particle distribution function F_α involves the unknown $F_{\alpha\beta}$, which must be found before $F_\alpha(t)$ can be calculated for an initial $F_\alpha(0)$. An attempt to find an equation for $F_{\alpha\beta}$ by the method used to obtain (12) would yield a relation containing $F_{\alpha\beta\gamma}$, and so on. In fact we would deduce a sequence of equations for F_α, $F_{\alpha\beta}$, $F_{\alpha\beta\gamma}$, . . . , which would replace Liouville's equation. Now we have seen that Boltzmann's single-particle distribution function provides us with the requisite macroscopic information about a gas flow. Clearly, to avoid considerable mathematical complexity, it is desirable to assume that only binary collisions are important so that only F_α, $F_{\alpha\beta}$ are retained and, further, that the colliding particles are statistically independent such that $F_{\alpha\beta} = F_\alpha F_\beta$ (molecular chaos). Then (12) becomes

$$\frac{\partial F_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \frac{\partial F_\alpha}{\partial \mathbf{x}_\alpha} + \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N} \frac{1}{m_\alpha} \frac{\partial F_\alpha}{\partial \boldsymbol{\xi}_\alpha} \cdot \int \mathbf{X}_{\alpha\beta} F_\beta \, d\mathbf{x}_\beta \, d\boldsymbol{\xi}_\beta = 0 \quad (33)$$

We will also introduce a truncated, single-particle distribution function which applies to a $6(N\text{-}1)$-dimensional domain D containing all states of particles $1, 2, \ldots, \alpha - 1, \alpha + 1, \ldots, N$ such that no particle is closer to the αth particle than d, a length specified by the molecular collision model adopted in a specific problem. For hard sphere molecules d is the diameter. Then the truncated, single-particle distribution function for the αth particle is defined as

$$F_\alpha{}^d(\mathbf{x}_\alpha, \boldsymbol{\xi}_\alpha, t) = \int_D F \, d\mathbf{x}_1 \ldots d\mathbf{x}_{\alpha-1} \, d\mathbf{x}_{\alpha+1} \ldots d\mathbf{x}_N \, d\boldsymbol{\xi}_1 \ldots d\boldsymbol{\xi}_{\alpha-1} \, d\boldsymbol{\xi}_{\alpha+1} \ldots d\boldsymbol{\xi}_N \quad (34)$$

If now we integrate Liouville's equation (9) over the domain D we obtain

$$\frac{\partial F_\alpha{}^d}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \frac{\partial F_\alpha{}^d}{\partial \mathbf{x}_\alpha} + (N-1) \int_{S_\beta} F_{\alpha\beta}{}^d (\boldsymbol{\xi}_\alpha - \boldsymbol{\xi}_\beta) \cdot d\mathbf{S}, \, d\boldsymbol{\xi}_\beta \quad (35)$$

which holds if the particles are identical and a finite cutoff is applied to the interparticle force. The integral is taken over a sphere of radius d. If we write $\mathbf{V} = \boldsymbol{\xi}_\beta - \boldsymbol{\xi}_\alpha$ and introduce polar coordinates in the diametral plane perpendicular to $\mathbf{V}$, then (35) becomes

$$\frac{\partial F_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha \cdot \frac{\partial F_\alpha}{\partial \mathbf{x}_\alpha} = (N-1) \int [F_{\alpha\beta}(\mathbf{x}_\alpha, \mathbf{x}_\beta{}^+, \boldsymbol{\xi}_\alpha, \boldsymbol{\xi}_\beta{}^+) - F_{\alpha\beta}(\mathbf{x}_\alpha, \mathbf{x}_\beta{}^-, \boldsymbol{\xi}_\alpha, \boldsymbol{\xi}_\beta{}^-)] V d\omega d\boldsymbol{\xi}_\beta \quad (36)$$

where we distinguish between approaching and receding particles by the superscripts minus sign and plus sign, respectively. Making use of the condition for molecular chaos and changing to Boltzmann's single-particle distribution function we have the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = -\frac{1}{m} \int [f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_1) - f(\boldsymbol{\xi}') f(\boldsymbol{\xi}_1')] V d\omega d\boldsymbol{\xi}_1 \quad (37)$$

where only binary collisions are considered and the primed velocities are the final values after encounter.

We can write the Boltzmann equation in the form

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = -\nu f + g \quad (38)$$

where νf and g, both functions of ξ_i, x_i, t, are, respectively, the number of particles lost and gained in unit time from unit volume about $\mathbf{x}$, in a definite velocity range $d\boldsymbol{\xi}$ about $\boldsymbol{\xi}$, and $\nu(\xi_i, x_i, t)$ is the number of encounters for a molecule in unit time, or collision frequency.

2. BGK Kinetic Model for Collision Processes in Gases

The mathematical problem is to solve (38) for the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ subject to appropriate boundary conditions. The macroscopic properties of the gas flow are then obtained from (14), (15), and (16). The Boltzmann equation has been the subject of considerable investigation (Ref. 1). However, the complexity of the problem has been such that only simple molecular models have been considered and usually some form of expansion technique was used.

A model for collision processes in gases, proposed by Bhatnagar, Gross, and Krook (BGK),[36] is of special interest to the aerodynamicist since it gives promise not only of extending our understanding of transfer processes from the free-molecular into the transition regime, where both interparticle and wall collisions are significant, but also into the continuum regime where interparticle encounters are predominant. Rott[37] has shown that an inversion of the Boltzmann equation

Table 2 Accommodation coefficients for inert gases on nickel computed for one incident angle ($\theta_i = 45°$) (Ref. 35)

Gas particle	Incident energy (ev)	$\overline{E_l/E_i}$	σ'	σ
He	2.0	0.12	2.05	0.34
	8.0	0.13	2.07	0.48
Ne	2.0	0.40	1.89	0.22
	8.0	0.40	1.97	0.29
A	2.0	...[a]	...[a]	...[a]
	8.0	0.57	1.58	0.18

[a] Trapped condition.

given by Wild[38] can be used for an iterative solution, the first step of which leads to the BGK equation.

Wild's inversion expression relates the distribution function to $g(\xi_i, x_i - \xi_i\tau, t - \tau)$, i.e., g retarded by the time interval τ, and $h(\xi_i, x_i, t, \tau)$, which is the probability a molecule will not experience a collision between the positions $x_i - \xi_i\tau$ and x_i in the time interval between $t - \tau$ and t,

$$f = \int_0^\infty g_{\text{ret}}(\tau) h d\tau \tag{39}$$

This equation states that the distribution function is the result of a superposition of distribution functions g of molecules that experienced collision, retarded by the time interval τ, weighted by the probability h. Using the properties of h and retarded functions, it can be shown that (39) is another form of the Boltzmann equation (38). The first iteration of f according to (39) has the form

$$f^{(1)} = \int_0^\infty \nu_{\text{ret}}{}^{(0)}(\tau) f_{\text{ret}}{}^{(0)}(\tau) h^{(0)} d\tau \tag{40}$$

where $f^{(0)}$ is the local Maxwellian distribution function and in Maxwellian free-molecule motion $g^{(0)} = \nu^{(0)} f^{(0)}$. Reverting from (40) to the Boltzmann form (38), we have

$$\frac{\partial f^{(1)}}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f^{(1)}}{\partial \mathbf{x}} = \nu^{(0)}[f^{(0)} - f^{(1)}] \tag{41}$$

which is the BGK equation.

We see that the right-hand side or collision term in the Boltzmann equation has been altered. In fact, if we replace V by V_{av} in (37) for hard sphere molecules, we deduce (41) if, further, it is assumed that the distribution function for molecules coming from collisions is Maxwellian. Physically interpreted, (41) expresses explicitly the fact that particle collisions tend to relax the distribution function to that corresponding to local and ultimately absolute equilibrium.

The modified collision terms in (41) are such that particle number, momentum, and energy are conserved in each collision. If $Q(\xi)$ is a summational invariant with respect to a collision, then

$$\int Q(\xi)[f^{(0)} - f^{(1)}] \mathbf{d}\xi = 0 \tag{42}$$

if ν is independent of ξ. Thus if $Q = m$, we obtain (14) by actual integration of $\int f^{(0)} \mathbf{d}\xi$, and substitution in (42). Similarly, if $Q = m\xi_i$, $m\xi_i\xi_j$, and $m\xi_i\xi_j\xi$, we obtain (15) and (16), respectively. Furthermore, if $Q = \log f$, then

$$\int [f^{(0)} - f^{(1)}] \log f^{(1)} \mathbf{d}\xi = \int [f^{(0)} - f^{(1)}] \log f^{(1)}/f^{(0)} \mathbf{d}\xi \leq 0 \tag{43}$$

and we see that the H theorem is also valid.

The application of the BGK equation to a particular problem will involve a selection of the collision frequency ν, which depends on appropriate physical quantities that characterize the problem. For example, it could be identified with the reciprocal of the freestream, Maxwellian relaxation time.

3. Hypersonic Aerodynamics in Nearly Free-Molecular Flow

We will now consider two methods of treating the Boltzmann equation using the BGK kinetic model in some form to simplify the mathematical method. The following examples are concerned with the perturbation of the free-molecular distribution function produced by interparticle collisions that, although few in number, are not negligible. The associated flow is called nearly free-molecular motion.

In nearly free-molecular flow, the distribution function at a point will depend very much on whether or not the particle velocity vector lies within the solid angle Ω_B subtended by the body at the point and is directed away from the surface. Willis[39-41] divides the particles into two classes: class B, which includes those whose velocities lie within Ω_B; and class C for all others. Thus the contribution to the collision term by class B particles is (η const):

$$-\eta f_B(n_B w_{BB} + n_C w_{BC}) + \eta(n_B{}^2 w_{BB} \Phi_{BB} + 2n_B n_C w_{BC} \Phi_{BC} + n_C{}^2 w_{CC} \Phi_{CC}) \tag{44}$$

where

$$\Phi_{ij} = \left(\frac{m}{2\pi k T_{ij}}\right)^{3/2} \exp\left[-\frac{m}{2kT_{ij}}(\boldsymbol{\xi} - \mathbf{u}_{ij})^2\right] \tag{45}$$

A corresponding expression for C particles is obtained by interchanging B and C. The macroscopic properties of the flow at the point in question are given by the following relations based on net conservation:

$$n_i = \int_{\Omega i} f \mathbf{d}\xi \qquad 2\mathbf{u}_{ij} = \frac{1}{n_i}\int_{\Omega_i} \xi f \mathbf{d}\xi + \frac{1}{n_j}\int_{\Omega j} \xi f \mathbf{d}\xi$$

$$\frac{6kT_{ij}}{m} = \frac{1}{n_i}\int_{\Omega i} (\xi - \mathbf{u}_{ij})^2 f \mathbf{d}\xi + \frac{1}{n_j}\int_{\Omega j} (\xi - \mathbf{u}_{ij})^2 f \mathbf{d}\xi \tag{46}$$

Willis then wrote the Boltzmann equation (with the modified BGK term indicated previously replacing the collision term) in the form of an integral equation and applied a method of successive approximations.

An alternative method was proposed by Grad[42] and developed by Sirovich[43] and Rose,[44] the latter's work being based on the assumption that $a \leq s \leq \lambda_1$, where a is a characteristic body dimension; s is the position at which f is to be determined, measured from an origin of coordinates in the body; and λ is the mean free path. Then the action of the body on the gas may be represented by a point source function that can be added to (41) to represent the effect of the body, i.e., we can write for steady motion

$$\boldsymbol{\xi} \cdot \frac{\partial f^{(1)}}{\partial \mathbf{x}} = \nu^{(0)}[f^{(0)} - f^{(1)}] + \zeta(\boldsymbol{\xi})\delta(\mathbf{x}) \tag{47}$$

where $\delta(\mathbf{x})$ is the Dirac delta function and $\zeta(\boldsymbol{\xi})$ is identified with the net mass radial flow from the origin. Furthermore, this assumption permits the linearization of the preceding equation about values at infinity where the motion is Maxwellian.

Using the previous methods, the hypersonic drag of a sphere has been determined by Willis and Rose. It was assumed that the particles reflected perfectly diffusely from the surface of the sphere ($T_r = T_B$, $\alpha = 1$). They obtained,

Willis ($S_B \geq 2$)

$$C_D(\text{sphere}) = C_{D_{FM}} - \frac{(0.165\, S_B + 1.44 - 1.13/S_B)}{(S_\infty K n_\infty)} \tag{48}$$

Rose

$$C_D(\text{sphere}) = C_{D_{FM}} - (0.33 S_B - 0.12)/S_\infty K n_\infty \tag{49}$$

where $C_{D_{FM}}$ is the free molecule drag of the sphere for $\alpha = 1$, and

$$S_B{}^2 = \frac{m u_\infty{}^2}{2kT_B} \qquad S_\infty{}^2 = \frac{m u_\infty{}^2}{2kT_\infty} \qquad K n_\infty = \frac{\lambda_\infty}{D} \tag{50}$$

Willis' relation was obtained by fitting numerical results. These results have been compared[41] with experimental observations made by Kinslow and Potter.[45] Figure 11 shows that both statistical models discussed previously give values of $C_{D_{FM}} - C_D$, which are relatively close to the measured values.

The hypersonic drag of a cylinder is an interesting case since it introduces the effect of body shape. This has also

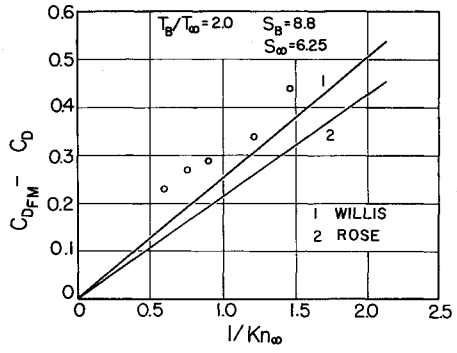


Fig. 11 Variation of the hypersonic drag of a sphere with the Knudsen number.

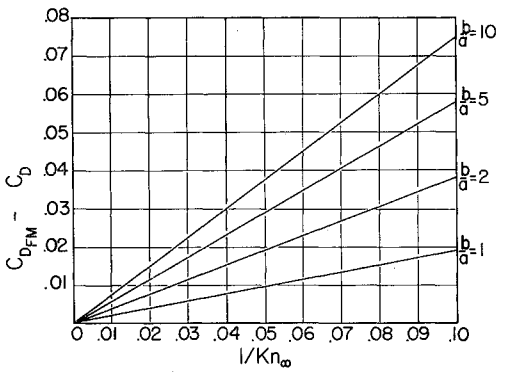


Fig. 13 Effect of the length/radius ratio on hypersonic cylinder drag at large Knudsen numbers.

been considered theoretically by Taub[46] and Rose,[47] their results being restricted still to nearly free-molecular motion. Willis[48] had obtained an hypersonic drag relation for a two-dimensional strip oriented perpendicular to the macroscopic motion in the form

$$C_D(\text{cylinder}) = C_{D_{FM}} - H(S_\infty, S_B)[\beta \log(\beta/S_B)] \quad (51)$$

where H is a tabulated function[41] and

$$\beta = \frac{1}{4}\left(\frac{\pi T_\infty}{T_B}\right)^{1/2} \frac{1}{Kn_\infty} \quad (52)$$

This form was also confirmed for the infinite cylinder. Terms of order β have been assumed to be negligibly small compared with $\beta \log\beta$, a restriction that will limit the validity of the theory. A detailed experimental investigation over a wide range of Knudsen and Mach numbers was carried out by Maslach and Schaaf[49] and later with improved techniques by Tang[50]. A comparison of the Willis-Taub theory with experiment for nearly free-molecular flow for $1.0 < Kn_\infty < 100$, $M \cong 10$ is shown in Fig. 12 (see Ref. 41). The agreement is reasonably good down to $Kn_\infty = 2$ with a steady divergence at $Kn_\infty < 2$ as would be expected. It is important to note, however, that both theory and experiment were done for the case of diffuse reflection which probably deviates from the true situation in hypersonic flight.

The cylinder drag formula obtained by Rose for hypersonic, nearly free-molecular motion with diffuse reflection has the form

$$C_D(\text{cylinder}) = C_{D_{FM}} - \frac{0.25}{Kn_\infty}\left(\frac{T_\infty}{T_B}\right)^{1/2} \log_e\left[\frac{b}{a} + (1 + b^2/a^2)^{1/2}\right] \quad (53)$$

with the restriction that b/a (i.e., length/radius) $\ll Kn_\infty^2$. Since we are interested in the possible effect of body shape, Fig. 13 has been prepared to show the effect of cylinder length/radius ratio. We see that the drag coefficient of a cylinder departs more and more from the free-molecule value as the length/radius ratio is increased and the Knudsen number decreased. Both effects lead to a C_D less than $C_{D_{FM}}$. For further studies of the effect of body shape the reader's attention is directed to Ref. 51.

The equilibrium temperature of the cylinder has been determined by Willis et al.[41] using Taub's results.[46] Following along lines similar to those outlined previously, the normalized equilibrium temperature was found to be given by

$$\frac{T_{eq} - T_{eq}(Kn_\infty = 0)}{T_{eq}(Kn_\infty \to \infty) - T_{eq}(Kn_\infty = 0)} = 1 + G(S_\infty, S_B)\beta \log\beta \quad (54)$$

A comparison with experimental results obtained by Dewey[52] shows that the theoretical results fall within the range of scatter for $Kn_\infty > 5$. The theory succeeds only in indicating the trend of the variation of the normalized equilibrium temperature with $1/Kn_\infty$ for nearly free-molecular motion.

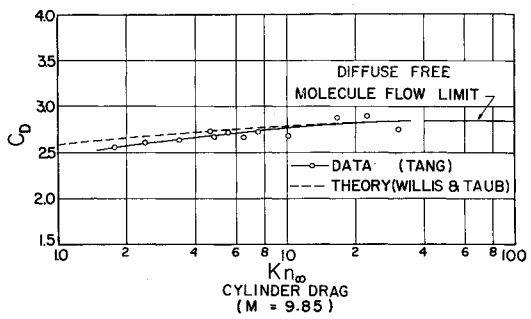


Fig. 12 Hypersonic drag of a cylinder over a range of Knudsen numbers.

4. Expansion Flows in the Transition Regime

The aerodynamic problems in Sec. 3 involved only a small departure from free-molecule motion. We now investigate the application of the BGK equation (41) to the study of flows in the transition range between continuum and free-molecule flow. As an example we shall consider the free, spherically symmetrical, steady expansion of a monatomic gas from an inviscid, equilibrium flow to a free-molecular, nonequilibrium motion. An important simplifying feature of this example is that particle-surface interactions are not involved in the theory and that the assumption of spherical symmetry is an acceptable approximation, which makes the problem reasonably tractable[53] and retains the essential physical characteristics of the motion. A knowledge of the free expansion of jets into a vacuum is important in the design of rocket exhaust systems and molecular beam facilities. In the past the expansion flow has been calculated using continuum theory.

We will present here a method given by Brook and Oman.[54] They have considered the BGK equation in the dimensionless form

$$\kappa v(d\varphi/dx) = \Phi - \varphi \quad (55)$$

where for spherical symmetry

$$\varphi = r^2 f^{(0)} \qquad \Phi = r^2 f^{(1)} \quad (56)$$

$$v = \xi_r/u \qquad x = r/L \quad (57)$$

where u is the local mass velocity, and L is a characteristic length defined in terms of the local temperature gradient

$$L = T/(dT/dx) \quad (58)$$

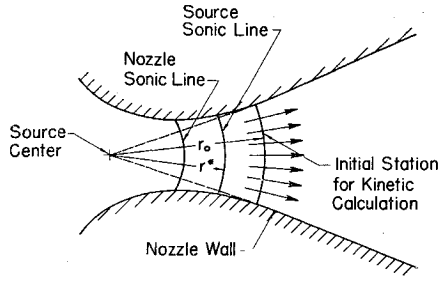


Fig. 14 Theoretical model of the transition expansion flow in a nozzle.

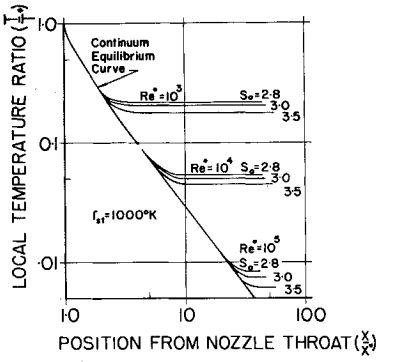


Fig. 15 Calculated transition of temperature in a nozzle from continuum, equilibrium motion to "frozen," nonequilibrium flow.

The convective terms on the left-hand side of (55) represent an approximation which the authors have shown to be reasonable for moderately high Mach numbers. Also κ has the form $u/\nu L$. The parameter ν has been investigated by Narasimha[55] who determined the Chapman-Enskog expansion[1] for the BGK model and suggested that an appropriate, low-density form for ν is $\frac{5}{4}p/\mu$, where p is the pressure and μ the viscosity. Thus

$$\kappa = \frac{4}{5}\frac{\mu}{p}\frac{u}{T}\frac{dT}{dx} \tag{59}$$

It will be seen from (55) and (59) that nonequilibrium flow arises from two sources: 1) large dT/dx and 2) large μ/p (or low collision frequency).

The conditions under which the problem was solved are indicated in Fig. 14. We consider that the kinetic theory applies to the radial flow downstream from the throat of an ideal supersonic nozzle. The flow is assumed to be inviscid (equilibrium), continuum motion up to an arbitrarily selected initial station x_0, i.e., up to this point the continuum relation

$$\left(1 - \frac{u^2}{a^2}\right)\frac{du}{dr} + \frac{2u}{r} = 0 \tag{60}$$

is taken to be valid. The nozzle is "ideal" in the sense that the postulated physical conditions could only be achieved in practice if the particles reflect specularly from the walls. It will be noted further that at the sonic line (Fig. 14), $dT/dx \rightarrow \infty$ and, hence, the initial station must be downstream of the sonic line ($x_0 > x^*$ where the starred quantity is evaluated at $u = a$).

Brook and Oman used an iterative procedure on a digital computer with argon as the test gas. Their results showed that, despite the local decreasing collision frequency that accompanies the expansion, the variation of density and macroscopic velocity with radial position are still essentially the same as that calculated by the continuum theory. On the other hand, the computations showed that the temperature deviated from the continuum value. It approached an asymptotic value as the collision frequency decreased, departing from the continuously decreasing temperature of continuum flow and from equilibrium. The transition from continuum, equilibrium motion to free-molecular, "frozen" flow was sudden as is indicated in Fig. 15 for a stagnation temperature of $T_{st} = 1000°K$ for three sonic Reynolds numbers. It will be noted that these calculations leave some uncertainty as to the final (asymptotic) downstream temperature depending on the choice of x_0 (see S_0, Fig. 15).

We see that much of the expansion occurs in the continuum regime and that subsequent changes in stream velocity are small. Furthermore the conservation of mass relates macroscopic velocity and density and, hence, the ultimate density is close to the value calculated by continuum theory. But the kinetic effect due to a decreasing collision frequency does lead to a frozen (constant-temperature) state. The final asymptotic temperature is primarily dependent on the sonic Reynolds number. The calculations also showed a smaller dependence on stagnation temperature and some influence of the selected position of the initial station (Fig. 14) on the final asymptotic temperature.

Experimental evidence that the temperature and Mach number freeze in a free supersonic jet has been given by Anderson, Andres, Fenn, and Maise.[56] They investigated the flow of a jet of argon from a sonic nozzle (outlet diameter 0.77 mm, stagnation pressure 10 Torr) using a time-of-flight system developed by Becker and Henkes.[57] The resulting velocity distributions were found to be unchanged over the range from 13 to 40 nozzle diameters downstream from the outlet. It was concluded that Mach number and static temperature had frozen somewhere upstream of 13 nozzle diameters. A review of a series of results led Anderson et al. to a correlation of the asymptotic Mach number with a Knudsen number (Kn_{st}) based on the stagnation mean free path and nozzle diameter. This correlation is illustrated in Fig. 16. The theoretical results of Brook and Oman and the preceding experimental studies were presented recently at the Fourth International Symposium on Rarefied Gas Dynamics and a direct quantitative comparison is not yet available.

Information such as that just described has opened the way for new developments in the design of molecular beam facilities. Surveys of this subject have been prepared.[58–60]

5. Transition through a Plane Shock Wave

The variation of the macroscopic quantities through a plane shock layer has been the subject of considerable study.[61, 62] The simplification introduced by one-dimensionality permits the retention of much of the physics of the problem. Furthermore the absence of solid boundaries eliminates diffi-

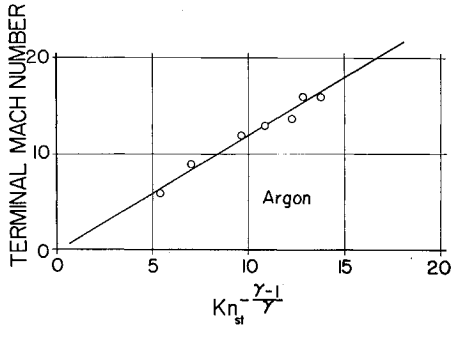


Fig. 16 Correlation of "frozen" (asymptotic) Mach number with the Knudsen number based on the stagnation mean free path and the minimum nozzle diameter.

culties arising from an incomplete knowledge of particle-surface interactions. On the other hand, since there is no geometrical dimension for reference purposes, no simple condition is available to establish limiting regimes, such as free-molecule flow or continuum motion. The results must be judged according to mathematical consistency or by comparison with experimental results. The shock transition problem has been of considerable interest to specialists in rarefied gas flows because the physical properties of the motion can best be investigated in a low-density tunnel where the large thickness of the shock facilitates probing techniques.

The structure of the plane shock layer has been investigated by Liepmann, Narasimha, and Chahine[63–65] using the BGK model for Boltzmann's equation and comparing their results with those derived from the Navier-Stokes equation of continuum theory. The transition problem involves the connection of one Maxwellian flow state with another by a nonequilibrium process. These authors represented the transition by 1) the Navier-Stokes equation, which applies

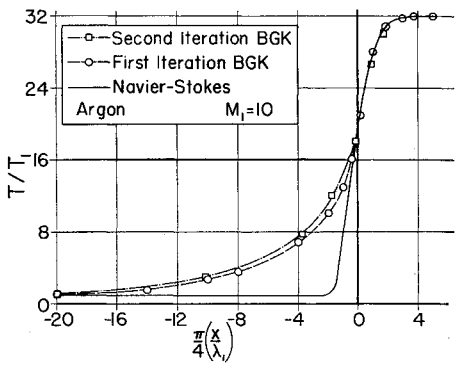


Fig. 17 Calculated temperature transition through a plane shock wave.

only if the ratio shearing stress/pressure is small, and 2) by the BGK equation in which ν is chosen equal to p/μ. Navier-Stokes profiles were obtained by the method of Gilbarg and Paolucci[66] starting with the saddle-point singularity on the downstream, high-pressure side of the layer and proceeding to the final state on the upstream side. Then BGK profiles were determined by an iterative method (that was adapted later by Brook and Oman for their expansion problem[54]), starting with the known Navier-Stokes solution and proceeding upstream as before to lower pressures.

Liepmann et al. found that at a Mach number of 1.5 the Navier-Stokes and BGK transitions are almost exactly the same. However, at higher Mach numbers a noticeable difference occurs on the low-pressure, upstream side of the point of maximum slope, the two calculated transitions on the high-pressure, downstream side being essentially the same. This effect is illustrated in Fig. 17 for the temperature transitions through the shock layer in argon at $M_1 = 10$. The subscript 1 refers to the initial upstream state. On the other hand, the maximum slope of the transition profile remains sensibly the same for both methods. If the thickness of the shock layer is defined in terms of this maximum slope, then both methods give essentially the same value. It seems more reasonable to base the shock thickness on the area under the profile as was suggested by Grad and, in this case, the more accurate BGK method for the higher Mach numbers gives a greater shock thickness. The authors noted that the profiles showed smaller deviations due to kinetic effects for velocity (and density, therefore) than for temperature.

Although useful experimental information has been reported by Sherman,[67] who measured the temperature transition at $M_1 = 3.7$, his results can be said to provide only qualitative confirmation of the computations described previously. Recently Schultz-Grunow and Frohn[68] measured the density distribution through a shock wave traveling through rarefied argon in a shock tube for $1.65 \leq M_1 \leq 9.5$. Satisfactory agreement with the previously described computations was apparently not obtained. However, density measurements present difficulties since they must be measured very accurately (to a few percent). Also, the experimental results were compared with density profiles obtained from the BGK velocity distributions using a continuum equation. It is evident that experimental measurements of temperature are preferred since here the computed deviation due to kinetic effects was largest.

IV. Conclusions

The view of the mechanics of rarefied gases presented here has outlined a procedure for solving problems in this field which emphasizes a direct solution of the Boltzmann equation for the single-particle distribution function in accordance with prescribed boundary conditions and the subsequent evaluation of the macroscopic properties of the flow from the various integral moments of f taken with respect to the particle velocity [see Eqs. (14–16)]. The gas has been assumed to be highly rarefied, and extensions of the Navier-Stokes equations of continuum fluid mechanics to the slip flow regime have not been reviewed. Also applications of Grad's thirteen-moment method or the Burnett expansion are not considered.[1, 69, 70] The emphasis placed here on the BGK model of the Boltzmann relation is not intended to detract from other useful methods such as the Monte Carlo system.[16]

Glancing back over what has been said previously, it is apparent that our study of free-molecule motion has pointed up the importance of the particle-surface interaction. The time has come for a courageous study of the complex gas-solid interface from which aerodynamic boundary conditions (f_B) can be derived. Theoretical work, such as that of Oman et al. and Goodman, should be extended. It is also important that laboratory simulation of the hypersonic interaction be achieved. A molecular-beam technique for doing this is already well developed and work of considerable interest is now in progress.[58–60] In particular the body surface condition must be as well understood and reproducible as the flow characteristics.

Although, from the point of view of flight in the upper atmosphere, free-molecular motion may not appear to be very significant, yet it forms the starting point for an understanding of the aerodynamics of the transition regime where iterative procedures depend on a knowledge of the free-molecular state. It is the writer's view that a knowledge of free-molecule flow in and around a wide range of geometrical configurations is just as essential as for the case of continuum motion. In particular, internal flow systems probably involve adsorbed gases and "dirty" surfaces so that the assumption of diffuse reflection is likely to be justified.

It is clear that the BGK equation has opened the way to tractable methods of investigating transition flows which yield valuable physical information. Despite our uncertain knowledge of particle-surface interactions, much can be learned by further studies of this equation, assuming diffuse reflection in the interim. However, it is not the author's intention to overrate the importance of the BGK model of the Boltzmann equation. The latter is still nonlinear and contains much of the difficulty inherent in the original Boltzmann equation, the solution of which is the ultimate requirement.

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