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The structure of rarefied gas flows past simple aerodynamic shapes

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The direct-simulation Monte Carlo procedure for the modelling of rarefied gas flows on a digital computer has been used to generate representations of the simulated flows on a computer display unit. Photographs prepared from the displays illustrate the structure of the flows at the molecular level. The method has been applied to the steady hypersonic flow past circular cylinders, spheres, flat plates and blunt cones. These flows are represented either by several hundred typical molecular paths or by several thousand small arrows, each representing the position and velocity of a sample molecule at a particular instant. Colour was used to differentiate between undisturbed free-stream molecules, molecules that had struck the surface of the body and molecules that had been indirectly affected by the presence of the body. The method was also applied to the flow of a binary gas mixture past a circular cylinder, with colour used to differentiate between the components of the mixture.

1. Introduction

The value of flow visualization techniques is well established in almost all branches of fluid mechanics. In particular, the development of continuum gas-dynamics has been greatly assisted by the ease with which schlieren and shadowgraph techniques can be used to obtain clear and precise pictures of the strong and well-defined disturbances that typically occur in supersonic wind tunnels and shock tubes. However, the transition régime between continuum and free molecule flow is characterized by extremely low densities and comparatively diffuse disturbances. The conventional flow visualization techniques can no longer be applied and must be replaced by more difficult and less effective techniques, such as those employing glow discharges and electron beams. Since the transition régime requires a microscopic or kinetic theory approach rather than a continuum approach, the ideal flow visualization method would illustrate the flow at the molecular level. This would require a technique for the labelling and recording of individual molecules and cannot yet be envisaged.

On the other hand, recent studies (Vogenitz, Bird, Broadwell & Rungaldier 1968) have indicated that numerical experiments using the direct-simulation Monte Carlo method provide an accurate representation of rarefied gas flows. These experiments are carried out in simulated physical space within a digital computer, and several thousand simulated molecules are simultaneously followed

through representative collisions and boundary interactions. Computer display units are available for the monitoring of the motion of the individual molecules in the simulated flow, thus providing flow visualization at the molecular level.

For the calculation of two-dimensional steady flows, the molecules are initially set up as a uniform stream in Maxwellian equilibrium. The body is inserted at zero time and the steady flow is obtained as the large time solution of the resulting unsteady flow. The velocity components of the simulated molecules and their position co-ordinates in the simulated physical space are available in the store of the computer at all stages of the calculation, thus permitting a wide variety of simulation schemes.

Two types of flow visualization scheme have been developed. In the first, a two-dimensional flow is represented by several hundred typical molecular paths past the body. As the Knudsen number decreases, the number of collisions suffered by each molecule increases rapidly. The number of segments along each molecular path increases with the number of collisions and path representation becomes impracticable. The simplest alternative visualization scheme would be to display several thousand spots, each representing the position of a sample molecule at a particular instant. The information provided by this display is greatly enhanced if a vector is added to each spot indicating the magnitude and direction of the velocity of the molecule represented by the spot. Therefore, in the second scheme, each molecule is represented as a small arrow.

Colour may be used to differentiate between the various classes of molecules in a flow. In a simple gas consisting of only one type of molecule, distinct classes are established by reference to the molecular histories. The scheme that has been adopted is to divide the molecules into the following three classes: (i) free-stream molecules that have not been affected by the presence of the body; (ii) molecules that, at some time in their past history, have struck and been reflected from the surface of the body; (iii) molecules that have been indirectly affected by the presence of the body.

In the present work, these classes are distinguished by blue, red and yellow respectively. A blue molecule changes to yellow when it collides with a red or yellow molecule. Either a blue or yellow molecule changes to red when it interacts with the surface. A red molecule remains red irrespective of subsequent collisions and interactions. Therefore, for a near-continuum supersonic flow, an incipient shock wave shows as the transition from blue free-stream molecules to yellow molecules, and the merging of the red and yellow molecules defines a type of boundary layer. The method has also been applied to the flow of binary gas mixtures with colour used to differentiate between the molecules of the two species.

The work was carried out on the IBM 7040 computer and the Digital Equipment 338 Precision Display Unit in the Basser Computing Department, University of Sydney. The display unit was programmed to produce a separate black and white picture for the flow of each type of molecule, and the final photograph was obtained by making multiple exposures through appropriately coloured filters.

Apart from the addition of display routines, the programs are identical with those described by Vogenitz *et al.* (1968), and that paper may be referred to for

a fuller description of the simulation procedures. In all of the photographs, the flow is from the left to the right. The molecules are assumed to be hard spheres and the surface interaction is diffuse with perfect thermal accommodation.

2. Circular cylinder

Figure 1, plate 1, employs the path representation to illustrate the influence of Knudsen number on the flow past a circular cylinder with its axis normal to the flow direction. The Knudsen number K_n is defined as the ratio of the free-stream mean free path to cylinder diameter, and the speed ratio s is equal to the ratio of the stream speed to the most probable molecular speed in the free-stream gas. The speed ratio of the flows illustrated in figure 1 is 5, and the surface temperature of the cylinder is equal to the free-stream stagnation temperature. The upstream and downstream boundaries in the photograph correspond with the boundaries of the simulated region. However, the outer boundary of the simulated flow was outside the region shown in the photograph. The flow was actually simulated on only one side of the axis of symmetry, and the paths were assigned to the upper and lower regions of the display in a random manner.

Figure 1 (*a*) represents the flow at a Knudsen number of 10. While this flow is well within the transition régime, it is sufficiently close to the free molecule limit to show most of the features of free molecule flow. Very few free-stream (blue) molecules, other than those directly swept out by the cylinder, collide with the cylinder. The reflected (red) molecules do not in general suffer collisions until they have moved a considerable distance from the body. Under these conditions, the probabilities of a red molecule being deflected back to the surface or a yellow molecule colliding with the body are very small. However, the small sample of paths in figure 1 (*a*) includes one example of each of these events.

The Knudsen number is reduced by a factor of 3 between each case shown in figure 1. The first reduction to the $K_n = 3$ case shown in figure 1 (*b*) results in an increase in the number of yellow and red molecules striking the surface. However, the flow is generally similar to the $K_n = 10$ case. The next reduction in Knudsen number does lead to qualitative changes in the flow. Figure 1 (*c*) for $K_n = 1$ shows a large increase in the number of collisions and there is some sign of a collective disturbance. However, a significant number of undisturbed free-stream molecules continue to penetrate right through the flow field in the region immediately adjacent to the cylinder.

The critical change in the flow occurs in the next step in Knudsen number to 0·3, shown in figure 1 (*d*). The upstream disturbance is confined to a distance of the order of the diameter of the cylinder, and there is a well-defined transition from predominately blue to predominately yellow paths. Practically no blue molecules penetrate through the flow in the region adjacent to the cylinder. However, there are still regions in which all three classes of molecule are present, and it is not possible to distinguish an incipient shock wave from an incipient boundary layer. The number of collisions and path segments increases so rapidly with decreasing Knudsen number that it was not practicable to further extend this series of photographs.

3. Sphere

The alternative flow visualization scheme in which a large number of molecules are represented by arrows has been applied to the flow past a sphere and is illustrated in figure 2, plate 2. The photographs show a sample of the molecules within a thin two-dimensional 'slice' enclosing the centre of the sphere. The actual location of each molecule is shown by a dot, the length of the 'tail' is proportional to the speed of the molecule, and its slope corresponds to the direction of the projection of the molecular path in the plane of the slice. The speed ratio of the flow is 10 and the surface temperature is midway between the free-stream static and stagnation temperatures. There is again a sequence of four photographs with the Knudsen number changing by a factor of 3 between each, but this sequence starts at $K_n = 1$.

The flow at $K_n = 1$ shown in figure 2 (*a*) is of the 'highly rarefied' type with little sign of any collective phenomena. The reduction to $K_n = 0{\cdot}3$ in figure 2 (*b*) results in a qualitatively similar flow, although there is a noticeable reduction in the region of affected molecules upstream of the sphere. A significant number of the free-stream molecules near the sphere continue to penetrate right through the flow field.

In this case, the critical step in Knudsen number that causes the flow to change from the 'highly rarefied' to the 'quasi-continuum' state is that from $K_n = 0{\cdot}3$ to $K_n = 0{\cdot}1$. The latter flow is illustrated in figure 2 (*c*) and shows a clear transition from blue to yellow molecules and regions containing all three classes of molecule. This state corresponds closely with that shown for the cylinder in figure 1 (*d*). Although there are changes in the speed ratio and the ratio of surface to stagnation temperature, the change in geometry is probably the major factor in causing the reduction by a factor of three in the Knudsen number for the critical flow change.

Figure 1 (*d*) shows the flow past the sphere at a Knudsen number of 0·03. The flow in the stagnation region is almost continuum in nature. The shock wave is distinct from the boundary layer and the shock detachment distance is in agreement with the continuum value. The wake is still in a highly rarefied state, although the small sample size can give a false impression of the degree of rarefaction.

4. Leading-edge problem

Both the 'path' and 'arrow' representations have been applied to the flow past a perfectly thin flat plate parallel to the stream, resulting in figures 3 (*a*) and (*b*), plate 3, respectively. The speed ratio is 10 and the surface temperature is midway between the free-stream static and stagnation temperatures. The rear boundary in figure 3 (*a*) is 25 free-stream mean free paths from the leading edge of the plate. The sample size is extremely small in this type of presentation, and only one red reflected molecule illustrates the influence upstream of the leading edge that has been discussed previously by the author (Bird 1967). The flow region represented by this photograph covers the transition from predominantly

blue to predominantly yellow and red molecules, but all three classes are well mixed.

Figure 3(*b*) extends back further to 50 freestream mean free paths from the leading edge. The upstream influence is more clearly shown by the larger sample size. As the downstream boundary of the simulated region is approached, the incipient shock wave is almost distinct from the 'boundary layer' defined by the merging of the red and yellow molecules. An interesting feature is that, while some yellow molecules would always be expected to diffuse through the boundary layer, the molecules near the downstream region of the surface are predominantly red. It should be noted that the flat plate flow is much more sensitive than the cylinder and sphere flows to changes in the surface interaction model.

5. Blunt cone

The flow visualization method may be readily applied to bodies of more complex geometry. Figure 4, plate 4, illustrates the flow past a blunt cone. The speed ratio is 10, the Knudsen number based on the overall length of the body is 0·05, and the surface temperature is midway between the free-stream static and stagnation temperatures.

6. Binary gas mixture past cylinder

For a binary gas mixture, colour must be used to differentiate between the two species, and it would be difficult also to differentiate between the various classes of molecule in each gas. Figure 5, plate 5, shows the flow past a circular cylinder of a mixture of equal parts by mole of molecules with a mass ratio of 25:1. The Knudsen number is 0·05, the Mach number is 10, and the surface temperature is 20 times the free-stream static temperature. The 'arrow' type of representation has been used with the heavy molecules shown as yellow, and the light molecules as green.

The two components of the mixture are in thermal equilibrium in the free stream and the higher thermal speeds of the light molecules result in the green arrows near the upstream boundary being inclined at larger angles to the free-stream direction. The Mach number is defined by the speed of sound in the mixture and the speed ratio is different for each species. In keeping with this, there is a definite suggestion of a light gas shock layer located upstream of the heavy gas shock layer. Since the gases are not in equilibrium in a frame of reference fixed to the cylinder, the light gas temperature in the stagnation region is much higher than the heavy gas temperature in that region. The difference in length of the yellow and green velocity vectors is most marked in the stagnation region, and the high speed of the light molecules persists around to the rear of the cylinder. Since a molecule is located at the head of the arrow, the extension of the tail into the cylinder does not mean that a molecule has penetrated the surface. The sample size is not sufficient to show clearly either the separation that occurs in front of the cylinder or the more complete separation that occurs behind it. The gas immediately behind the cylinder is composed almost entirely of the light species.

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Mr D. S. Richardson was responsible for the operation of the display unit and for the photography.

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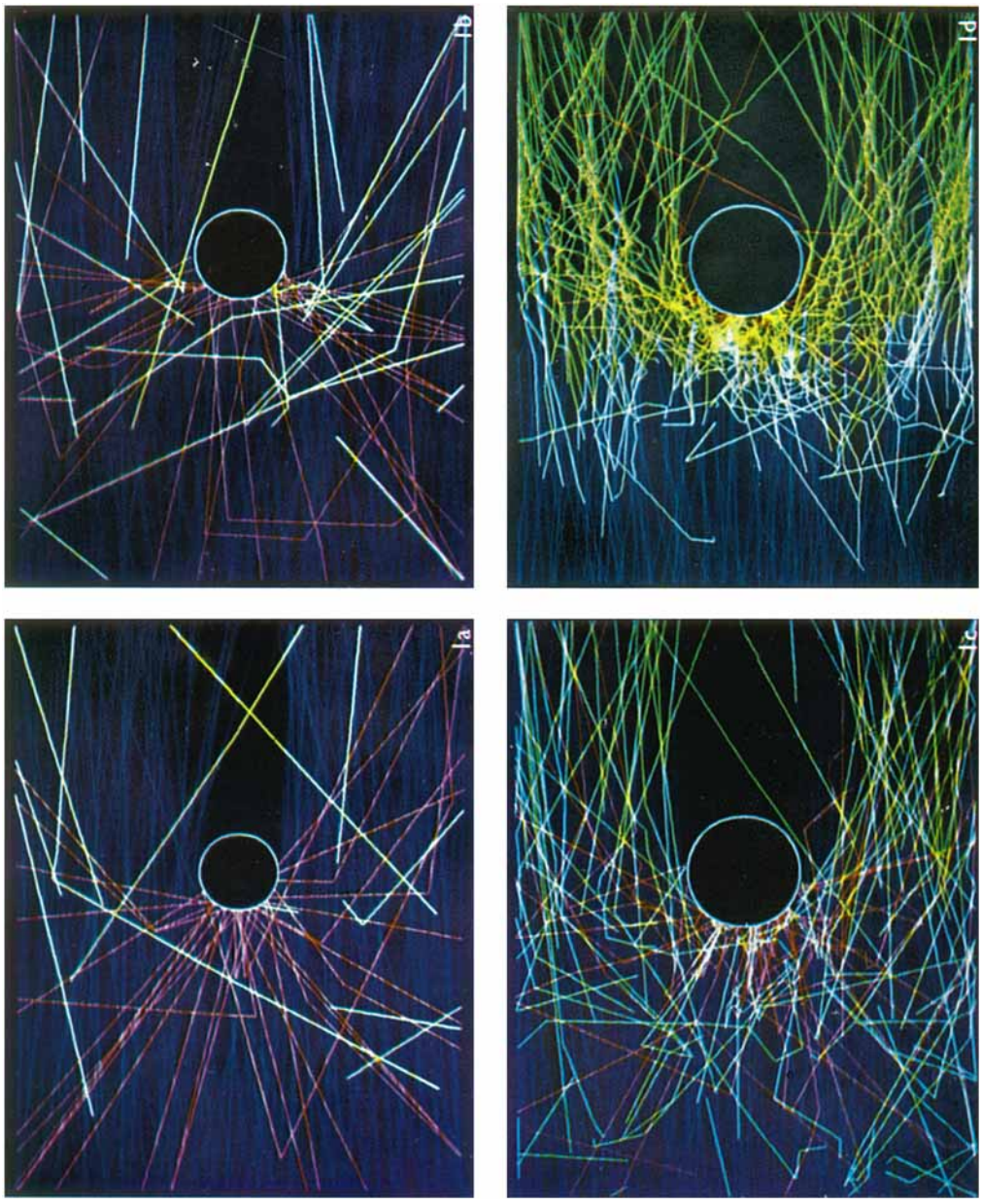


FIGURE 1. Typical molecular paths past a circular cylinder at a speed ratio of 5. (*a*) Knudsen number = 10, (*b*) Knudsen number = 3, (*c*) Knudsen number = 1, (*d*) Knudsen number = 0·3.

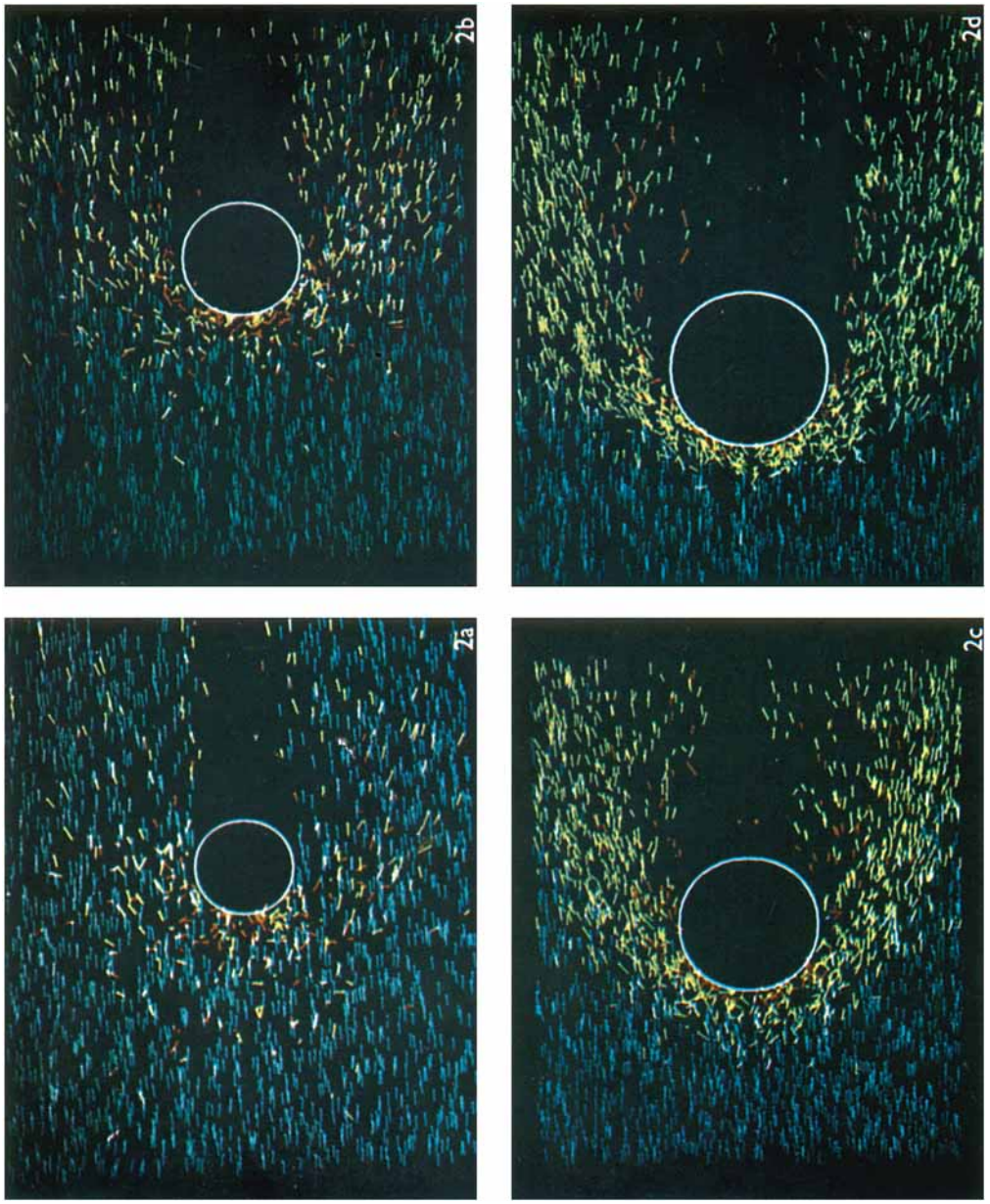
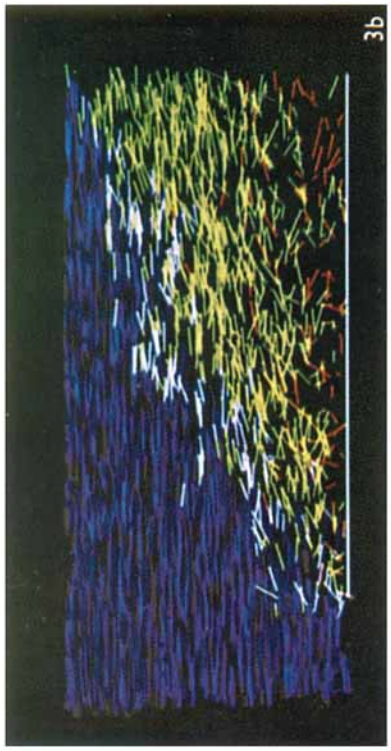
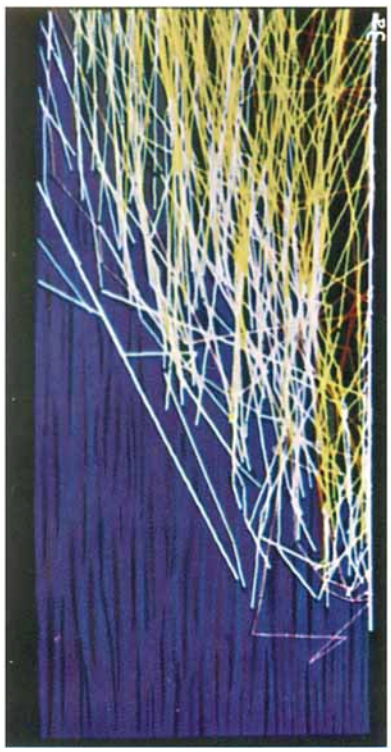
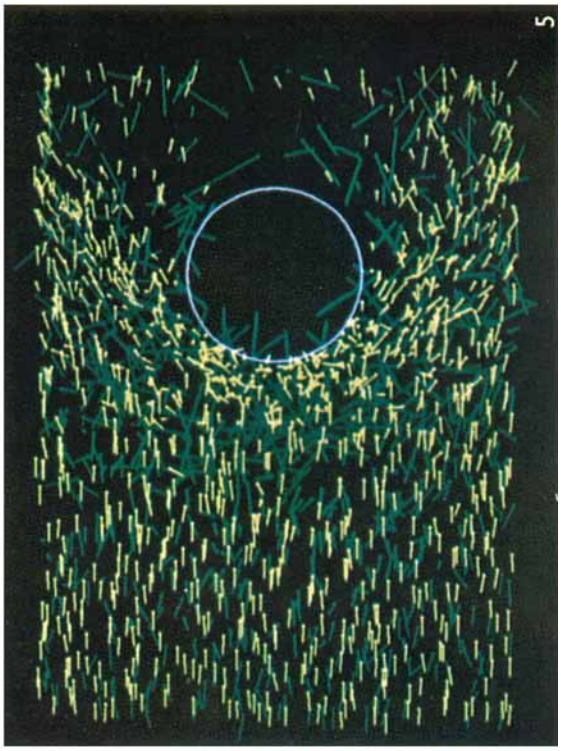


FIGURE 2. Molecular representation of the flow past a sphere at a speed ratio of 10. (*a*) Knudsen number = 1, (*b*) Knudsen number = 0·3, (*c*) Knudsen number = 0·1, (*d*) Knudsen number = 0·03.







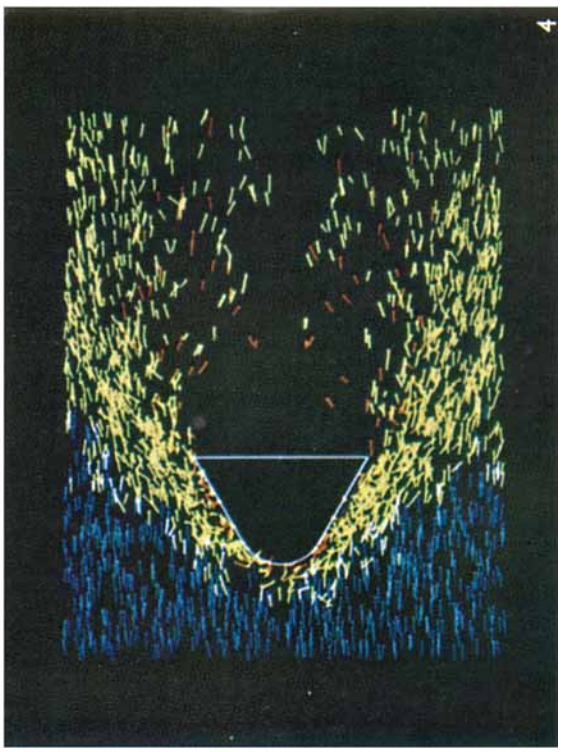


FIGURE 3. Molecular representation of the flow past a flat plate at a speed ratio of 10. (*a*) Knudsen number = 0·04, (*b*) Knudsen number = 0·02.

FIGURE 4. Molecular representation of the flow past a blunt cone at a speed ratio of 10 and a Knudsen number of 0·05.

FIGURE 5. Molecular representation of the flow of a mixture of equal parts of gases with a mass ratio of 25 past a circular cylinder at a Mach number of 10 and a Knudsen number of 0·05.