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Shock collision at a molecular level

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The development of reflected waves are studied when two shocks of unequal strength collide and when a shock collides with a constant temperature wall. Both these problems are examined using the Monte Carlo technique developed by Bird (1967). Some limitations upon this technique are suggested and a modified time advance parameter used.

Introduction

The feasibility of studying gasdynamic problems from the particle viewpoint has been greatly increased by the advent of large high-speed computers. In fact it may not be unfair to state that the bulk of significant advances in this field over the last twenty years have been dependent upon the availability of computing devices. This has been largely due to the intractability of the Boltzmann equation. The analytically simpler BGK model has enabled the solution of many problems, but it requires the use of computers to obtain numerical solutions. The programming of the solution to steady plane shock wave problems, using the BGK model, appears to be a substantial task requiring a good knowledge of numerical techniques (Anderson 1966). The analysis of unsteady problems is naturally more complex and in one solution (Chu 1965) further approximations were necessary to obtain numerical results.

As resort must eventually be made to computer solutions, the use of Monte Carlo techniques, whereby the individual particle motions are simulated on the computer, appear very attractive. The programming time is much less than for the analytic techniques referred to above, as only simple mechanics are required. The approximations appear to be certainly no more severe than those necessary in analytic studies and in some cases less so. The greatest defect in Monte Carlo solutions is the computer time required. However, it is possible that the increase in computing costs can be offset by reduced programming costs. Two such Monte Carlo techniques are known to the author Bird (1965, p. 216, 1966, 1967, 1969), Vogenitz *et al.* (1968) and Denisik *et al.* (1967). In the present study a brief examination of both these techniques is made. As more information is available upon the method by Bird, a detailed examination of this technique is undertaken. The method of solution is a branch of 'experimental mathematics' and as in all experimental work many details must be evolved by the individual experimentalist. As all previous work has been set up either by Dr Bird or under

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his guidance, it appears useful to present the results of a study which was undertaken only using the published papers.

The main problem considered is the collision of two planar shock waves of unequal strength, generated in a gas composed of hard sphere molecules by two specularly reflecting pistons. The results may be compared with continuum theory and experimental results (Glass & Heuckroth 1959).† Also examined is the collision of a shock wave with a constant temperature wall. It appears from the abstract of Bird (1969) that a detailed study of the collision with an adiabatic wall will soon be available. Thus only a few results are presented here. As the shock structure was obtained in the course of these studies, these results are given and compared with those of Bird.

'Experimental' technique

As the Bird analysis will be used in the subsequent study, this will be described first and the differences with the Denisik *et al.* model will then be pointed out. Rather than repeat the description given by Bird (1967) a slightly different viewpoint on the technique will be taken. In addition, a modification is proposed and used in the present work.

Consider the gasdynamic system under study to be made up of a series of comparatively small, but nevertheless macroscopic subsystems. These macroscopic bodies "behave approximately like closed systems over not too great periods of time. In fact, the particles which take part in the interaction of a subsystem with neighbouring parts of the system, are mainly those near its surface. Their number in comparison with the total number of particles in the subsystem quickly falls with an increase in size of the latter" (Landau & Lifshitz 1958, p. 6). Now generate a number of particles with random velocity components to represent the interacting or information transferring particles. These are assigned to various parts of the system in a random fashion. Consider each particle to have two roles, one as a typical subsystem particle and the other as an information transferring particle. Only these of all the particles in the system can transfer information. The remainder collide between themselves and take up typical average subsystem conditions dictated by the information particles being studied. As the time considered is short, particles can only transfer information from one subsystem to the next and usually the particles can only come from the right-hand half of one zone and the left-hand side of the next. In fact by choosing the time under consideration, ΔT_m, such that the fastest particle in the zone will not travel more than 0·4–0·5 of a zone width in ΔT_m, this can be assured.

While in their role of transferring information, all the particles from each half of a subsystem may be considered to be at the boundary so that any particle may collide with any other particle. Further, each subsystem is considered to be statistically independent of the next during time ΔT_m. Consider the first zone interface and select a pair of molecules at random. These are retained or rejected proportionally to their relative velocity. Having chosen a pair, a collision vector

† I am indebted to Dr Glass for suggesting this problem.

can be chosen at random as the colliding pair are assumed to be from any part of the field. The number of such collisions which can occur in time ΔT_m in a given zone is calculated upon the probable time for each collision chosen. The incremental time ΔT_i for a given collision can reasonably be chosen to be inversely proportional to the relative velocity of the pair, V_{Ri}, the collision cross section, A, the number of colliding pairs of information particles, $N_c/2$, and the local number density, N. Therefore

$$\Delta T_m = \sum_{i=1}^{k} \Delta T_i = \sum_{i=1}^{k} \frac{1}{AN V_{R_i} N_c/2} \tag{1}$$

after k collisions, that is inversely proportional to the swept volume and number of particles.

After this process has been repeated for each subsystem interface, the particles are allowed to take up their new positions and the cycle repeated.

There arise two problems with equation (1). Suppose $\Delta T_m = 2{\cdot}0$ and in one subsystem $\Delta T_1 = 1{\cdot}3$ and $\Delta T_2 = 1{\cdot}1$. If we only take $\Delta T_m = \Delta T_1$ a deficit of $0{\cdot}7$ in time exists, if $\Delta T_m = \Delta T_1 + \Delta T_2$ an excess of $0{\cdot}4$ in time is allowed. One possible solution is to consider that k must always be larger than 5, say, to keep the error relatively small. The second problem then arises where large density and temperature gradients exist in only part of the flow, such as through a shock wave. The value of a typical ΔT_k may be 50 times smaller behind a strong shock than in front so that to ensure that $k = 5$ in the pre-shock region, the post-shock $k = 250$. Thus during ΔT_m, on the average, every particle in each downstream subsystem will have collided at least once. This is unrealistic and contravenes restrictions upon statistical independence. Alternatively the subsystem may be kept large in width which will increase the number of particles in pre-shock zones and hence decrease ΔT_i there. Again, to maintain independence, large gradients of properties cannot be permitted in a closed subsystem. To keep gradients small the zone width must be fairly narrow with respect to the mean free path.

The solution proposed here is to calculate the probability of any collision occurring during a time δt. An estimate of the average collision time ΔT_A for a given subsystem is formed from equation (1) by substituting twice† the average absolute value of the peculiar velocities of the subsystem, for V_R. The average probability of a collision is taken to be $\delta t/T_A$. Thus when a stage is reached with the nth time step ΔT_k would make

$$\sum_{i=1}^{k} \Delta T_i > \Delta T_m$$

a random number R is chosen between 0 and $1{\cdot}0$ and if

$$\left(\Delta T_m - \sum_{i=1}^{k-1} \Delta T_i / \Delta T_A\right) < R$$

† A multiplication factor of two was chosen rather than the equilibrium value of $\sqrt{2}$ after running the program a number of times and examining the average collisional velocity through the shock.

the collision was assumed to occur and ΔT_m was taken to have elapsed exactly. If

$$R < \left(\Delta T_m - \sum_{i=1}^{k-1} \Delta T_i / \Delta T_A\right)$$

the collision was rejected and again ΔT_m was assumed to have elapsed. This settles the first problem raised. It also provides a solution to the second. If the time ΔT_m is adjusted for the dense regions, the rarefied upstream regions will all have $\Delta T_1 > \Delta T_m$ so the above selection principle can be invoked. It should be particularly important in defining the front foot of the shock as small errors from here may be transmitted downstream. In a problem with moving boundaries such as shock generation by a moving piston, the piston only transmits information about its motion while the particles are moving. Thus the sequence consists of an input of information from the piston and this is then transmitted to other parts of the system for a small time ΔT_m before further input is generated.

The technique by Denisik *et al.* (1967) has not been applied to problems with moving boundaries. It has been applied to situations undergoing chemical change. In this solution spatial correlation is neglected and only particle velocities and time are used as arguments. However, this does not appear to be a necessary restriction and the moving boundaries and zones could be used as before. A total interaction cross section for each particle with the other particles is calculated as

$$\sigma_i = \sum_{j=1}^{N} \frac{|V_i - V_j|}{|V_i|} \sigma_{0ij} \quad (i = 1, \ldots, N), \tag{2}$$

where V_i = velocity of the ith particle, σ_{0ij} is the interaction cross-section of the ith and jth particles. As σ_{0ij} is constant for hard sphere molecules

$$\sigma_i = \frac{\sigma_{0ij}}{|V_i|} \Sigma |V_i - V_j|. \tag{3}$$

The probability of no collisions occurring in a distance x is

$$P(x) = \exp\{-x/\lambda\} = \exp\{-n\sigma|v|t\} = P(t), \tag{4}$$

where $P(t)$ is the probability of a time of flight t before a collision occurs.

Thus the time of flight of the ith particle before a collision is

$$t_i = -\frac{\ln P(t) N}{n\sigma_i |V_i|} = -\frac{\ln \xi_i N}{n\sigma_{0ij} \Sigma |V_i - V_j|}, \tag{5}$$

where ξ is a random number between 0 and 1·0. Now $\Sigma|V_i - V_j|/N$ may be considered as an average value of the collision velocity between the ith particle and all others in the system. When this is divided by $\ln \xi_i$ a value equivalent to Bird's V_R is obtained. If t_i is now calculated for all N particles and the minimum chosen, the first particle k to collide in time will be found. The collision of partner j to i is selected at random with probability

$$W_j = \frac{|V_i - V_j|}{\sum_{j=1}^{N} |V_i - V_j|}. \tag{6}$$

In the original paper the lower limit on the summation is $j = i$. It is hard to see any reason for this as the particles are not ordered. Velocities are then calculated and the whole cycle repeated. If this is repeated $\frac{1}{2}N$ times the time for a mean free path to be covered will be obtained. Thus in the Bird solution when only a random pair of particles is chosen the factor $\frac{1}{2}N$ must be used. It is obvious that the two techniques should produce the same result with the latter not requiring the proposed alteration to the Bird method. However, the technique of Denisik *et al.* would require very much greater computation time as the collision cross-sections must be repeated for each collision and t_i min found.

Experimental details

As pointed out by Vogenitz *et al.* (1968), if the time steps are normalized to the mean time between collisions in front of the shocks, the size of molecules need not be specified. However, it seemed worthwhile to use firm numbers to obtain readily an indication of actual dimensions and times although the actual selection is unimportant. A molecular radius of 1 Å and a number density of $0{\cdot}4 \times 10^{19}$ or 0·15 atmospheres were chosen to study the shock collision problem. Mach numbers of 10·0 and 4·0 were used for shock strength. The reflexion from a cold wall again used a molecular radius of 1 Å but a number density of $1{\cdot}08 \times 10^{19}$ or 0·37 atmosphere. Shock strength was that of a Mach 10·0 wave. An initial temperature was not chosen and the particle velocities were normalized to the most probable particle velocity V_m at 273 °K. To aid in interpreting the figures V_m typically equals $1{\cdot}5 \times 10^5$ cm/s for H_2, which has the required molecular radius. The number of particles used ranged from 3600 to 6000 and run time maximum was $1\frac{1}{2}$ h on an IBM 360/65. The initial number of particles per zone was 60–70. This was chosen so that the number of collisions in ΔT_m would only involve a small percentage of those in the zone. As stated before, the time between the movement of molecules, ΔT_m, was usually chosen so that the fastest particle in the system would not move more than 0·4 of a zone in ΔT_m. The initial zone width was 1·2 times the mean free path λ_∞ in the undisturbed gas. As ΔT_m was related to the zone width it was found that zone widths less than $0{\cdot}18\ \lambda_\infty$ produced such a small number of collisions in ΔT_m that the whole process would be controlled by the average probability of collision principle suggested above. It appears in retrospect that it would be better to raise the restriction of 0·4 of the zone width for the fastest particle to say 0·7 as very few particles would be involved. This would allow the minimum zone width to be reduced below $0{\cdot}18\ \lambda_\infty$.

The piston velocity was set as in Bird (1965) as

$$V/V_m = \sqrt{(2\gamma)}[M^2 - 1]/(\gamma + 1)M,$$

where M is the desired Mach number. It was found necessary to start the $M = 4{\cdot}0$ piston before the $M = 10{\cdot}0$ piston to arrange for both reflected shocks to move out of the region at the same time.

In deciding whether to retain or reject a pair of particles for collision the probability is set proportional to the relative velocity. This means that a maximum possible relative velocity must be found to calculate an actual probability.

This was taken to be twice the maximum velocity of any particle in each zone. Finally it is worth mentioning that in setting up a Monte Carlo system for such large runs provision should be made to dump the relevant core after a given time so that restart may be effected later.

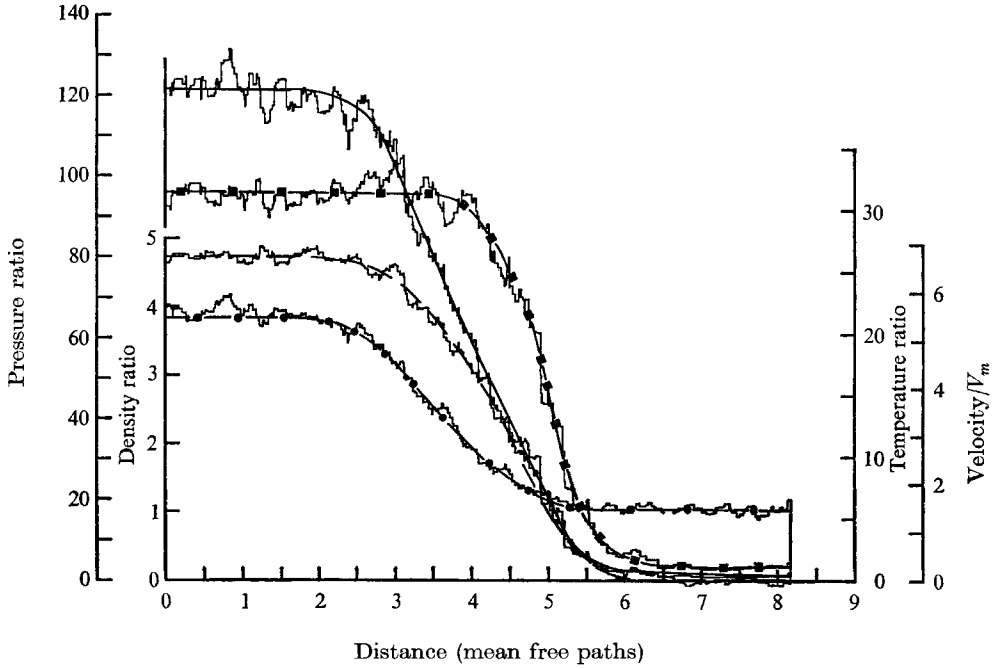

FIGURE 1. Variation of density, pressure, temperature and velocity through a Mach number 10 shock wave. Result shown for $2{\cdot}2\tau$ after start of motion of generating piston. $\tau = 0{\cdot}5 \times 10^{-3}/V_m$ sec, $\lambda = 0{\cdot}562 \times 10^{-3}$ cm. ■—■—, temperature ratio; ●—●—, density ratio; ——, pressure ratio; — — —, velocity.

Results

The mean free path was $0{\cdot}562 \times 10^{-3}$ cm and the mean time between collisions τ, $0{\cdot}5 \times 10^{-3}/V_m$ sec. Figure 1 shows the variation of density, pressure, temperature and velocity through a Mach 10·0 shock wave at a time $2{\cdot}2\ \tau$ after the piston was impulsively set in motion. This graph has been produced by averaging 11 sets of results simulating approximately a total of 4×10^4 molecules. The zone widths were approximately the same width in all cases. A thick mean line has been inserted to assist in the discrimination between curves and to show general trends. This has not been statistically fitted as the possible statistical fluctuations in the results makes such an exercise meaningless. The number of collisions during ΔT_m in a typical dense region was 19 and the undisturbed region either 0 or 1. It can be seen that the pressure and density profiles commence decreasing at about the same point but the temperature front lies considerably further from the piston. This is due to a few high-speed molecules raising the mean peculiar velocity (Chapman & Cowling 1968) without changing the local number density. The maximum slope thickness χ of a quantity K is defined as $(K - K_0)/(dK/dX)_{\max}$

and the reciprocal shock thickness R, as λ_∞/χ. Using these definitions $R_\rho = 0{\cdot}41$, $R_p = 0{\cdot}32$, $R_T = 0{\cdot}83$, and $R_V = 0{\cdot}38$ where subscripts ρ, p, T and V indicate density, pressure, temperature and velocity. In Bird (1969) it was found that the shock density did not reach its Hugoniot value at the piston face until time 2τ, which is substantiated by the present work. Also the values of R_ρ agree well with the results of Bird (1969).

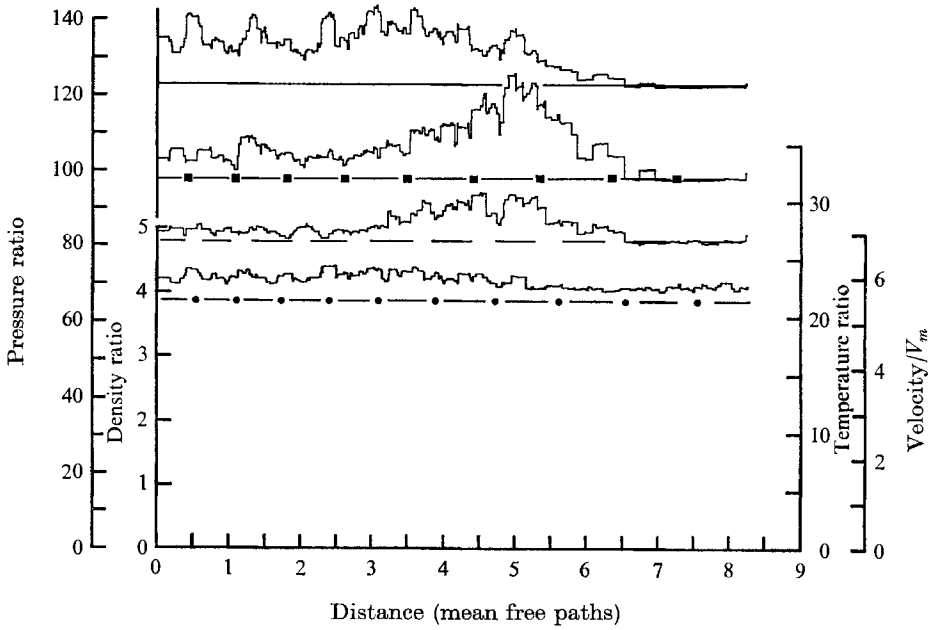

FIGURE 2. Standard deviation of results in figure 2 shown as 1 standard deviation above post-shock conditions. $\tau = 0{\cdot}5 \times 10^{-3}/V_m$ sec, $\lambda = 0{\cdot}562 \times 10^{-3}$ cm. ■——■—, temperature ratio; ●—●—, density ratio; ——, pressure ratio; — —, velocity.

The slope of the temperature profile is much greater at the leading edge of the shock than at the top. This may be a peculiarity of the present set of results although it could be a result of the modified time advance measure. A study of the longitudinal temperature profile (Bird 1967) gave a maximum temperature ratio of 43·0. This, as in Bird (1967), agreed well with the value of 42·1 predicted by Yen (1966). Finally, a sample of six results for number density $1{\cdot}07 \times 10^{19}$ at time $7{\cdot}4\,\tau$ after the piston started moving gave shock thicknesses which agreed with the above.

The standard deviation was calculated at each point and the results are shown in figure 2 as one standard deviation above a line at post shock conditions. If each point was statistically independent of the next, the standard deviation of the mean could be found. However, some correlation does exist and the errors are probably not as great as suggested here. Derzko (private communication) has shown that in the steady state regions the statistical fluctuations decrease inversely as the square root of the number of observations, when using this technique.

Two shock waves, one of Mach number 10·0 and the other of Mach number 4·0 were generated in a hard sphere gas by two opposing pistons. Sufficient distance (between 60 and 100 zones of length $1{\cdot}2\lambda$) was allowed between the pistons to ensure that both shocks were fully formed before collision. At a time $0{\cdot}112\tau$ after first collision between the temperature profiles, the conditions are as shown in figure 3(*a*). The figure is a composite of 11 results and as would be expected, the fluctuations are larger than previously. The only remnant of the precollision conditions is seen in the density profile. Pressure, temperature and velocity profiles show no trace and are smoothly curving. The average velocity of the zero velocity point, $4{\cdot}8 \times V_m$, is less than that of the final reflected wave velocity $5{\cdot}7 \times V_m$.

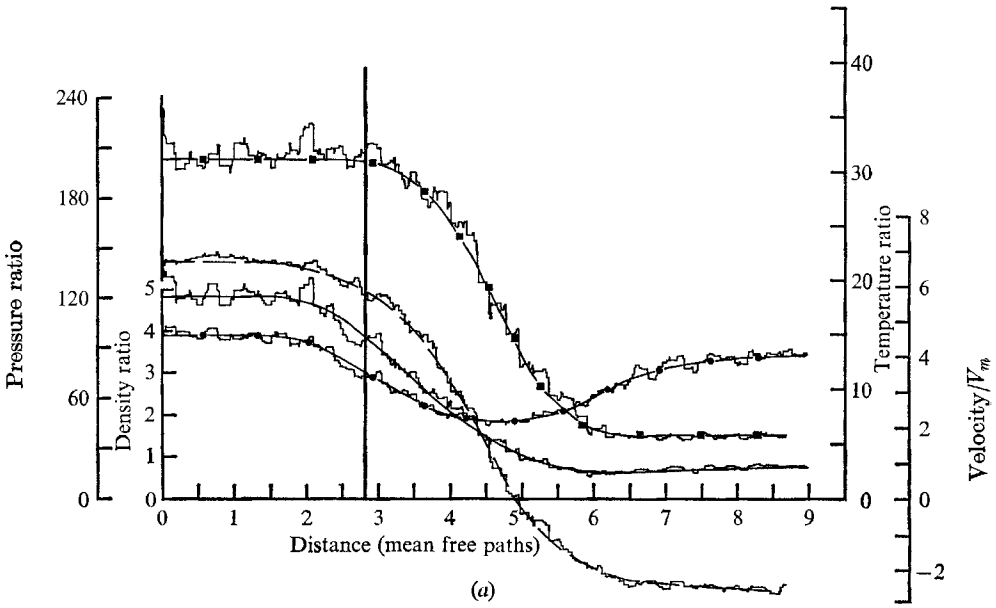

FIGURE 3. For legend see p. 858

At a time $0{\cdot}288\tau$ after collision, the density profile has become almost smooth although the slope on the Mach 4·0 side is steeper than the Mach 10·0, as shown in figure 3(*b*). These curves are the average of 13 sets of results. The pressure and velocity are still smoothly curving but the temperature has started to increase above the Mach 10·0 post shock value. The temperature is often the most sensitive parameter (see Bird 1967). The average velocity of the zero velocity point was $4{\cdot}3 \times V_m$, a decrease from the initial stage.

Nine sets of results were used to produce the curves for time $0{\cdot}548\tau$ after collision, shown in figure 3(*c*). In this case, temperature, pressure and density are all sharply peaked. However, there is no sign of a contact discontinuity developing or of the constant velocity region. The zero velocity point had an average velocity of $4{\cdot}2 \times V_m$.

The first appearance of the contact discontinuity occurred at $0{\cdot}576\tau$ after

collision. This is shown in figure 3(*d*), which is the average of 7 results. The particle velocity was about $3{\cdot}2 \times V_m$ which compares favourably with the continuum result of $3{\cdot}13 \times V_m$. Neither the pressure, temperature, nor the density reached their maximum values of 339,498 and 11·1 respectively. The discontinuity in density was not apparent at this stage, either. Thus in this case the particle velocity was

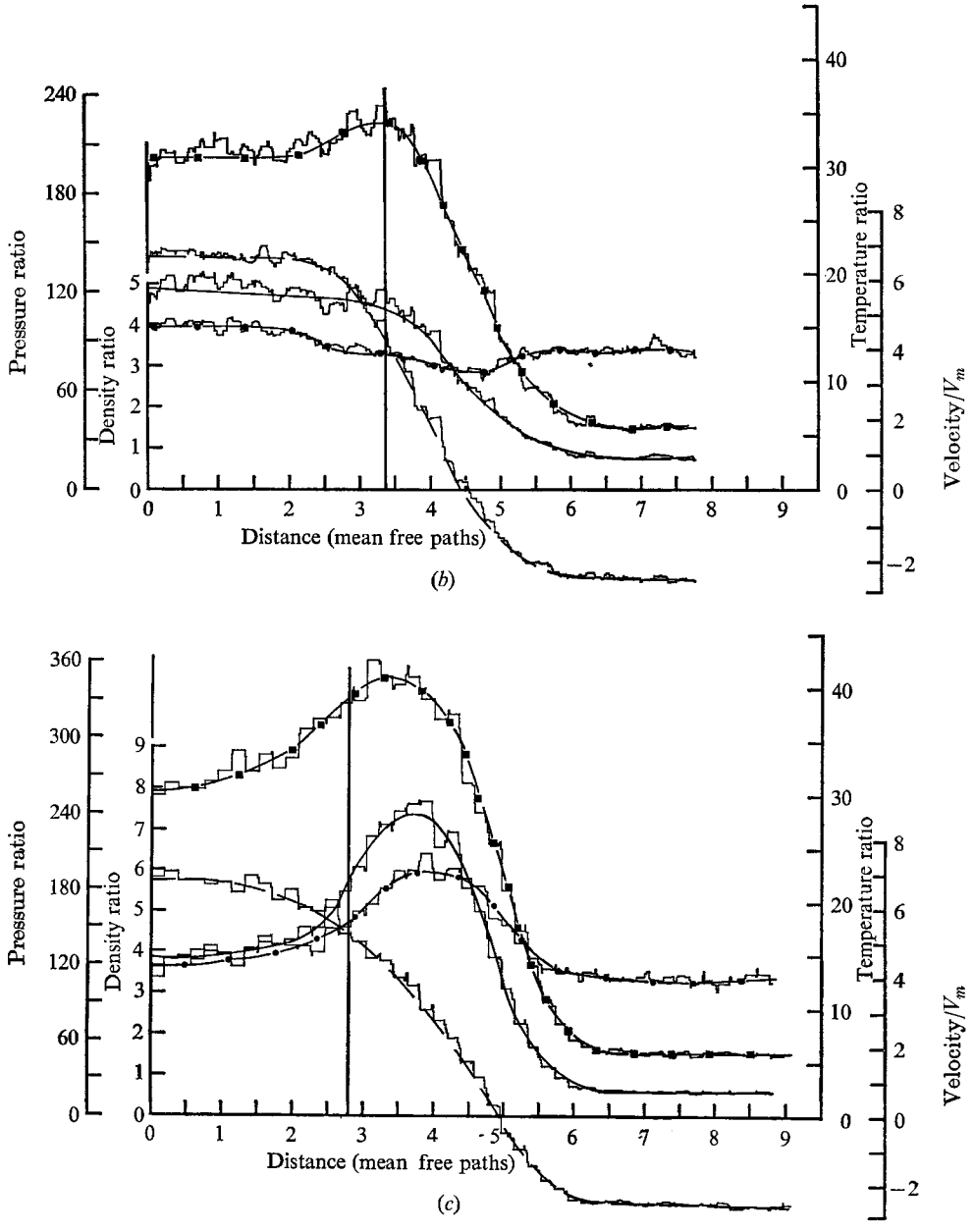

FIGURE 3. For legend see p. 858

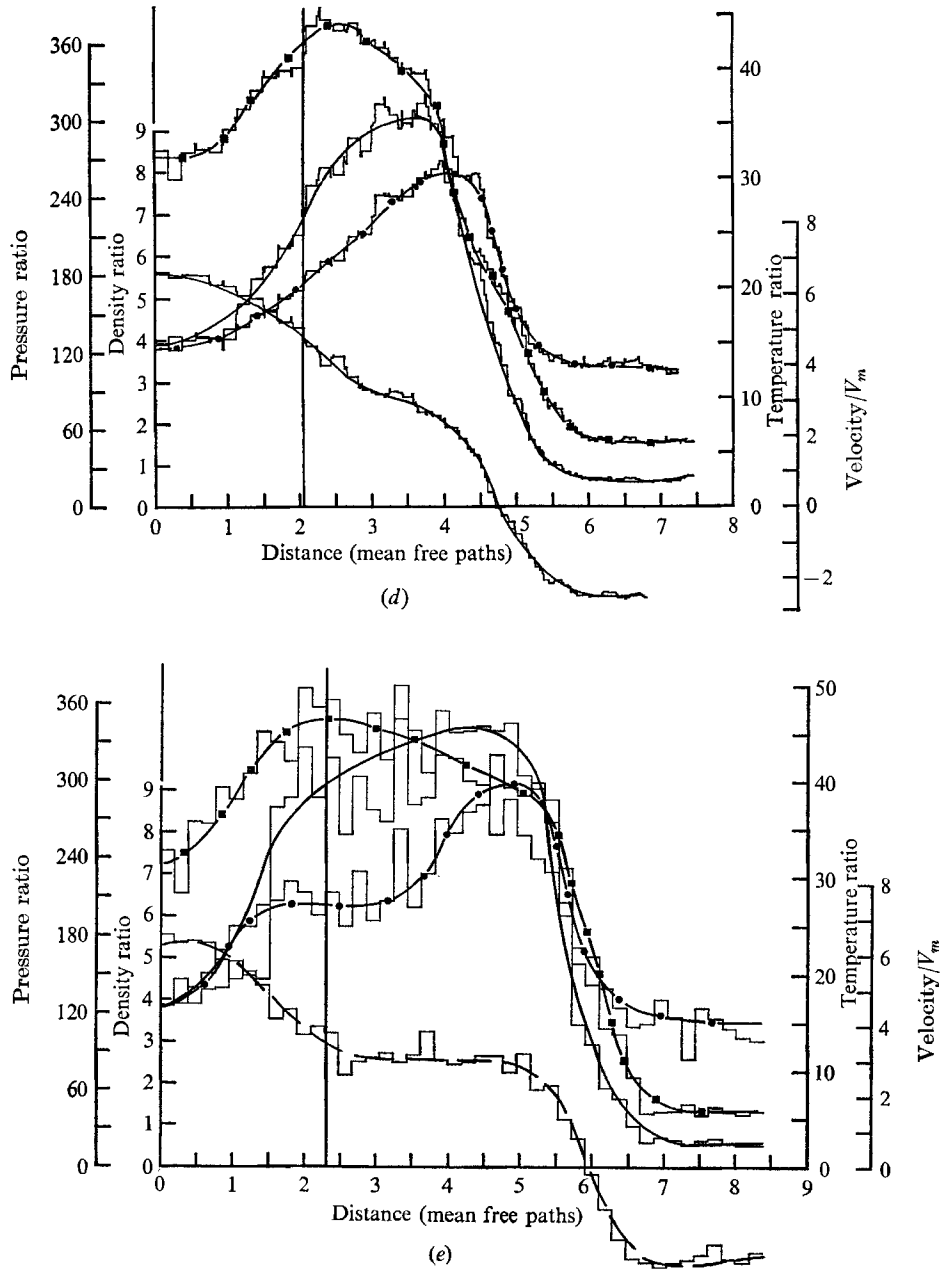

FIGURE 3. Variation of density, pressure, temperature and velocity at various times are a Mach number 10 shock collided head on with a Mach number 4 shock. Vertical line is the point of collision. Initial number density $0{\cdot}4 \times 10^{19}$. $\tau = 0{\cdot}5 \times 10^{-3}/V_m$ sec, $\lambda = 0{\cdot}562 \times 10^{-3}$ cm. ■—■—, temperature ratio; ●—●—, density ratio; ——, pressure ratio; — —, velocity.

(*a*) $0{\cdot}112\ \tau$ after collision; (*b*) $0{\cdot}288\ \tau$ after collision; (*c*) $0{\cdot}548\ \tau$ after collison; (*d*) $0{\cdot}576\ \tau$ after collision; (*e*) $0{\cdot}951\ \tau$ after collision.

the most sensitive indicator of the final state. The velocity of the zero velocity point was $4{\cdot}7 \times V_m$, thus increasing towards the final value.

One result at $0{\cdot}951\,\tau$ after collision has been produced which required two hours computing. This could only be performed once due to restrictions upon maximum continuous running times at the University of Toronto. The results are shown in figure 3(*e*) and it can be seen that a distinct discontinuity exists in the density profile. The particle velocity has a long constant value region roughly equally spaced about the density discontinuity. The pressure has reached a plateau at 339. However, there is no sign of a discontinuity in temperature. This could be expected as the reflected shocks have not developed sufficiently and a sharp discontinuity in temperature would not be normally found. The velocity of the zero velocity point when comparing the positions of the point at time $0{\cdot}567\,\tau$ and $0{\cdot}951\,\tau$ for this result was $5{\cdot}7 \times V_m$, the exactly predicted value.

It is clear that if sufficient computer time was available, and this would mean an additional 30 h, the motion of the reflected shocks could be followed and would produce Hugoniot values.

The other problem which was considered very briefly was the collision of a Mach 10·0 shock wave with a cold wall. The cold wall was simulated by a diffuse reflective surface. This exercise was performed in a denser gas, number density $1{\cdot}07 \times 10^{19}$. As Bird (1969) examines the adiabatic wall case, it appeared interesting to find the rate of growth of the thermal boundary layer. The results for two stages, $0{\cdot}53\,\tau$ after collision, (figure 4(*a*)) and $0{\cdot}95\,\tau$ sec after collision (figure 4(*b*)), are shown. The figures were produced from 5 and 6 sets of results respectively. In figure 4(*a*) it can be seen that the boundary layer is only about $0{\cdot}4\,\lambda_\infty$ wide in the temperature profile. By $0{\cdot}95\,\tau$ this has grown to $1{\cdot}0\lambda_\infty$. The remaining parameters, pressure, velocity and density are not sufficiently sensitive to show the different effects of the boundary layer and the reflected shock. As would be expected, the stable downstream values were not attained. However, it can be seen that the thermal boundary layer has been formed and it could be followed to later times if so desired. Again considerable computer time would be required.

Concluding remarks

The examination of shock structure which has been briefly examined here agrees well with the more extensive results by Bird (1969). The solution to the shock collision problem has demonstrated the power of this technique. In fact this problem probably could not be solved to this degree of accuracy by any other method presently available. It was found that the reflected waves were not formed in a recognizable fashion until about $0{\cdot}8\,\tau$ after the collision. If the mean density ratio throughout this time is 7·5, this represents about 6 mean collisional times. Although it would have been desirable to follow the reflexion process further to show the development of the thermal contact surface, the increase in computer time was not warranted. The experimental results by Gould (1952) suggest that the reflexion process is completed substantially by the stage obtained here, the remaining process would be simple diffusion between the two hot gases.

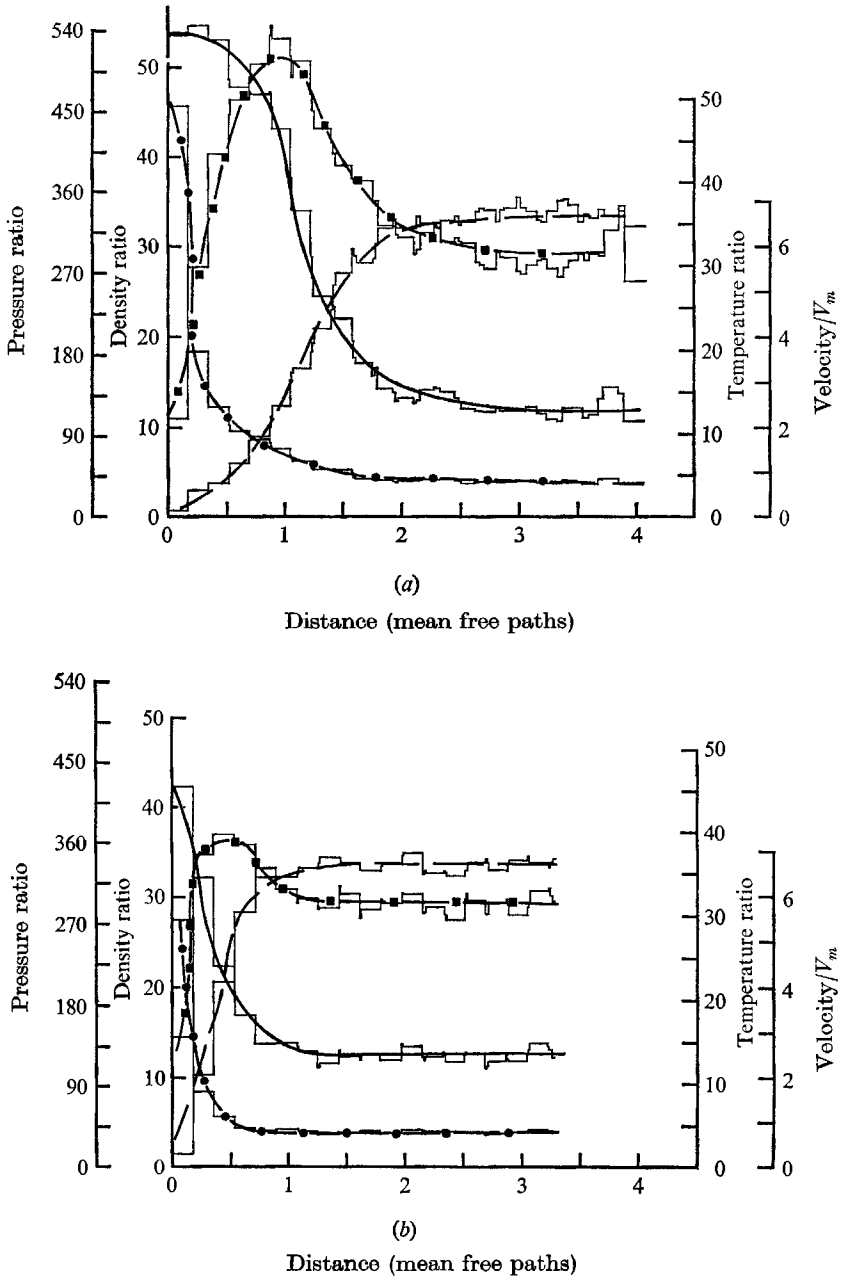

FIGURE 4. Variation of density, pressure, temperature and velocity at various times after collision of a Mach number 10 shock wave with a cold wall. Initial number density $1{\cdot}07 \times 10^{19}$. $\tau = 0{\cdot}5 \times 10^{-3}/V_m$ sec, $\lambda = 0{\cdot}562 \times 10^{-3}$ cm. ■—■—, temperature ratio; ●—●—, density ratio; ——, pressure ratio; — —, velocity. (*a*) 0·53 τ after reflexion. (*b*) 0·95 τ after reflexion.

Thus until analytic techniques become less dependent upon complex numerical calculations, this Monte Carlo technique by Bird appears to provide one of the quickest methods of setting out to solve unsteady flow problems where changes occur over small regions relative to the mean free path.

I would like to express my appreciation of the interest and encouragement I have received from Dr G. N. Patterson and Dr I. I. Glass. I would also like to acknowledge the many helpful discussions I had with Dr J. H. deLeeuw and Dr N. A. Derzko in the course of this work. Financial assistance received from the National Research Council of Canada and the Aerospace Research Laboratory of the USAF under contract no. AF-33(615)-5313 is acknowledged with thanks.

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