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The structure of normal shock waves in a binary gas mixture

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A previous study of normal shock waves through numerical experiments with a simulated gas on a digital computer is extended to binary gas mixtures. The mixture is simulated by two sets of rigid elastic sphere molecules with the appropriate mass and diameter ratios. Velocity profile results for medium strength waves in a mixture of equal parts argon and helium are in qualitative agreement with the continuum calculations of Sherman (1960), but there is no initial acceleration of the argon in mixtures containing a very small initial mole fraction of this gas. The temperature profiles are similar to those for the velocity in that the argon profile lags behind the helium profile. However, when there is a small proportion of heavy gas, the profiles cross-over and the temperature of the heavy gas overshoots the Rankine–Hugoniot downstream value. For very strong shock waves, the overall shock thickness expressed in upstream mean free paths becomes larger, but the profiles are generally similar to those for the medium strength waves.

1. Introduction

The structure of a normal shock wave in a binary mixture of non-reacting perfect gases has been the subject of a number of theoretical studies. These depend on a variety of assumptions and approximations and some conflicting results have been produced. While clarification is now being provided by experimental studies, reliable results have been obtained only for the density profile over a restricted range of shock Mach number. This paper presents results from numerical experiments using an extension of the direct simulation Monte Carlo method that has recently been applied (Bird 1967) to the corresponding problem in a simple gas.

Probably the major theoretical contribution has been made by Sherman (1960), and reference may also be made to this paper for a discussion of earlier work. Sherman obtained a solution through numerical integration of the Navier–Stokes equations together with the Chapman–Enskog result for the diffusion velocities in a binary mixture. Quite apart from the implicit assumption of the validity of a continuum approach, the method assumes that the species are in thermal equilibrium with one another through the shock, since this is an intrinsic feature of the Chapman–Enskog procedure. Sherman pointed out that these assumptions are of doubtful validity when considering medium to strong shock waves, or mixtures of large molecular mass ratio. His analysis of these cases produced some unexpected results, notably the prediction that the heavy component in a mixture with a small initial mole fraction of this component first accelerates before being slowed down in the wave. This finding has been critically examined by Liu (1965) who questioned the validity of Fick's law of diffusion under these conditions. Oberai (1965, 1966) has extended the Mott–Smith method to binary mixtures and did not find an initial acceleration of the heavy component.

An electron beam technique has recently been used by Center (1967) to measure the density profile of each component in a Mach 2 shock wave in argon–helium mixtures. While Center also found no evidence of the so-called 'Sherman anomaly', the observed broadening of the shock profile due to diffusion effects was in qualitative agreement with the predictions of Sherman's continuum theory.

Numerical experiments of the type reported in this paper have the advantage that all flow properties are accessible for sampling. It has therefore been possible to obtain information on the temperature non-equilibrium between the components of the gas mixture within the wave. The major disadvantage of the approach is the statistical scatter introduced into the results by the finite sample size in any computer run of acceptable length.

2. Extension of method to gas mixtures

The steady shock wave profile is obtained as the large time solution of the unsteady flow produced by the insertion of a moving piston into a steady flow. The general approach is identical to that applied to the shock wave in a simple gas (Bird 1967) and reference may be made to this paper for the details of the method. Only the extensions that are necessary for treating binary gas mixtures are described here.

All molecules are represented by smooth rigid elastic spheres and the mass m and diameter σ of each species is specified. Both species are set up in equilibrium at the same temperature upstream of the wave. Distances are made non-dimensional by relating them to the mean free path in this region. This is given by Chapman & Cowling (1939) as

$$\lambda_0 = \frac{1}{\pi(N_{01}+N_{02})}\left[\frac{N_{01}}{2^{\frac{1}{2}}N_{01}\sigma_1^2+N_{02}\{(\sigma_1+\sigma_2)^2/4\}\{1+(m_1/m_2)\}^{\frac{1}{2}}} + \frac{N_{02}}{2^{\frac{1}{2}}N_{02}\sigma_2^2+N_{01}\{(\sigma_1+\sigma_2)^2/4\}\{1+(m_2/m_1)\}^{\frac{1}{2}}}\right],$$

where N_0 is the upstream number density and the subscripts 1 and 2 have been used to distinguish the two species. The corresponding expression for a simple gas is

$$\lambda_0 = (2^{\frac{1}{2}}\pi\sigma^2 N_0)^{-1}$$

and this example illustrates the degree of detail complication introduced by the consideration of a second gas. The required expressions for the gas constant, the speed of sound and the most probable molecular speeds of the two species may also be found in Chapman & Cowling.

The major additional problem to be faced in the simulation is the maintenance of the correct balance between the various types of collision. This is achieved by keeping four time counters t_{nm} $(n, m = 1, 2)$ for each cell. These counters are kept approximately equal by always computing the collision of the type corresponding to the counter currently having the least value. For example, if the value of t_{11} is the least of the four counters, the next collision to be computed will be a collision between two type 1 molecules. The choice of the molecules for the collision pair from those within the cell under consideration is again such that the collision probability is proportional to the relative velocity v_r. The collision dynamics for rigid sphere molecules of unequal mass and size may be obtained from Chapman & Cowling. The correct distribution of impact parameters is easily generated since all directions are equally likely for the velocities after impact relative to the centre of mass.

Each time a collision is computed, the appropriate time counter is advanced by

$$\Delta t_{nm} = \frac{4}{\pi(\sigma_n + \sigma_m)^2 v_r}\left[\frac{1}{N_{c_n} N_m} + \frac{1}{N_{c_m} N_n}\right],$$

where N_c is the actual number of simulated molecules.

When sampling the flow properties of the binary mixture, the density is given by

$$\rho = \sum_n N_n m_n,$$

where $n = 1, 2$.

The mass velocity is given by

$$u = (\sum_n N_n m_n \bar{u}_n)/\rho,$$

where $\bar{u}_n$ is the average velocity of species n.

The peculiar velocity of a particular molecule is given by $U_n = u_n - u$ and the temperature of the mixture is defined in the usual way by

$$T = (1/3k) \times \sum_n \overline{m_n U_n},$$

where k is the Boltzmann constant. However, when sampling the temperatures of the individual species, the peculiar velocities are measured relative to the mean velocity of that species. These temperatures are then independent of the diffusion velocities.

The above discussion assumes that the number ratio of simulated molecules in the computer is equal to the real gas number density ratio. This procedure leads to difficulties when the number density ratio is very different from unity, since the consequent small number of simulated molecules of the rarer species would lead to unsatisfactory simulation and a quite unacceptable level of statistical scatter in the results for this species. This problem may be overcome by setting up an equal initial number N_{c_0} of simulated molecules of each species and by altering the collision procedures so that the number of actual molecules represented by each simulated molecule is proportional to the number density of the species to which it belongs. For example, if the undisturbed number density ratio is $N_r = N_{02}/N_{01}$ (with $N_{02} > N_{01}$) and each simulated type 1 molecule represents k actual molecules, then each simulated type 2 molecule represents $N_r \times k$ actual molecules. The velocity components of type 1 molecules are replaced each time a cross-collision is computed, but the velocity components of the type 2 molecules are replaced only once in every N_r cross-collision. In addition, the term which represents the contribution of the type 2 molecule to the appropriate time counter is set to zero when the velocity components are not replaced.

The computations were carried out on an English Electric KDF-9 computer and a typical case required a run of 30 min.

3. Results and discussion

3.1. *Comparison with Sherman's results*

As noted in § 1, Sherman (1960) has provided the most comprehensive set of analytical results. His most detailed results were for a shock wave of Mach number 2·05 in an argon–helium mixture, and Center (1967) chose this combination for his experiments. The first application of the simulation method was therefore to this case.

The argon–helium mixture was simulated by two sets of rigid sphere molecules with mass and diameter ratios of 10:1 and 1·5:1 respectively. The velocity profile for a shock of Mach number 2·05 in a mixture of equal parts by mole is shown in figure 1. The velocity and distance are made non-dimensional through division by the upstream speed of sound a_0 and mean free path λ_0 respectively. The origin is the point at which the moving piston is inserted into the flow to initiate the steady shock wave. Sherman's results use the point of inflexion of the mixture profile as the origin and are expressed in terms of a non-dimensional distance involving the viscosity of the mixture. In order to make a direct comparison, Chapman & Cowling's first approximation to the coefficient of viscosity in a mixture of rigid sphere molecules was computed. This has been used to relate the units and Sherman's results are also plotted in figure 1.

The results from the two approaches for this mixture are in qualitative agreement as far as the overall separation and the ratio of the helium to argon maximum slope thickness are concerned. The major difference is that the Monte Carlo profile is thinner than the continuum profile. This might be due to the approximate relation of mean free path to viscosity or to the representation of the real atoms as rigid spheres. Center's experimental results agree with Sherman's in this case with regard to both the degree of separation and the overall width.

Figure 2 shows the corresponding results for a mixture with 10% helium. The continuum profile almost lies within the statistical scatter of the Monte Carlo result, although there is clear indication that the latter profile is again thinner. The maximum slope thickness of the argon profile is again rather less than that of the helium profile, in agreement with both the continuum and experimental results.

On the other hand, in a mixture with a very small mole fraction of argon for which results are shown in figure 3, there are qualitative as well as quantitative differences between the Monte Carlo and continuum profiles. There is no sign in the Monte Carlo profile of an initial acceleration of the argon, and the maximum slope thickness of the argon profile is greater than that of the helium profile. Both these findings are in agreement with Center's measurements, and figure 4

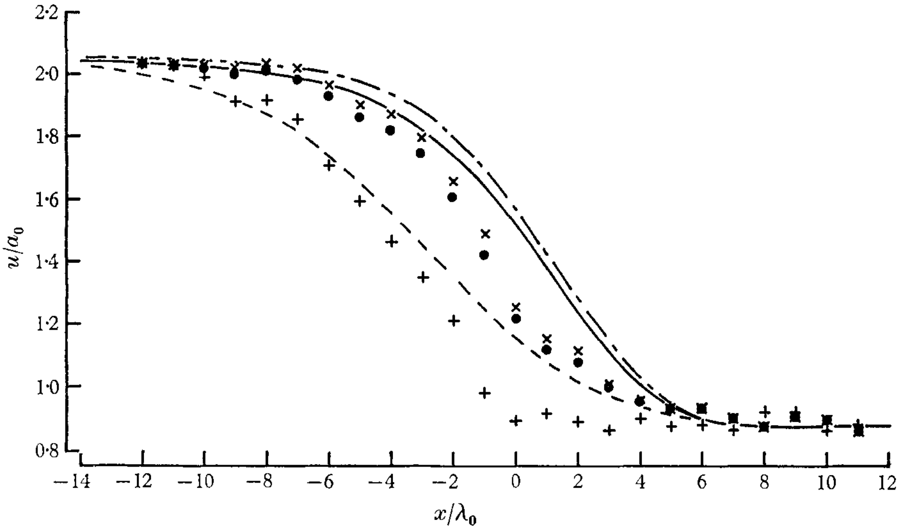

FIGURE 1. Velocity profile through a shock of Mach number 2·05 in a mixture of equal parts argon and helium. ●, model gas results for mixture; ×, argon; +, helium. ——, continuum results (Sherman 1960) for mixture; —·—, argon; — —, helium.

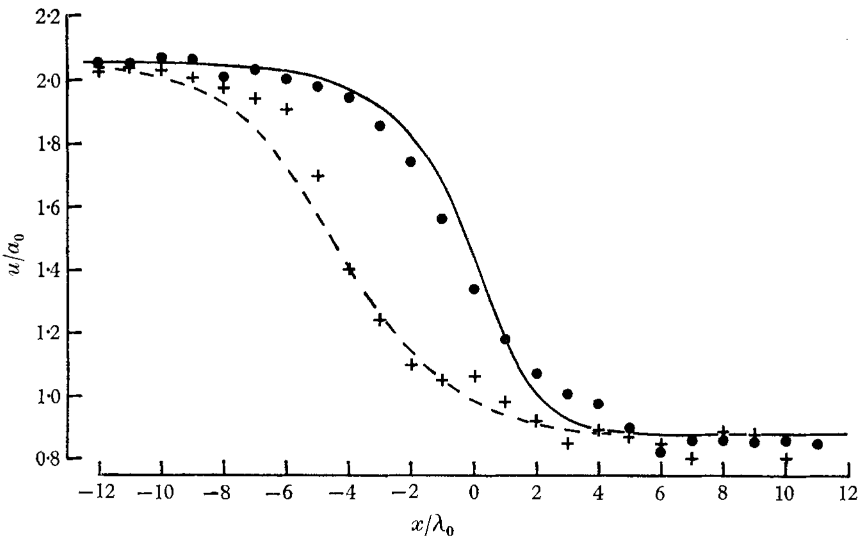

FIGURE 2. Velocity profile through a shock of Mach number 2·05 in a 10% helium–90% argon mixture. ●, model gas results for mixture and argon; +, helium. —, continuum results (Sherman 1960) for mixture and argon; — —, helium.

shows a direct comparison between these and the Monte Carlo result. The experimental density profiles are based on those shown in figure 6 of Center's paper, but no attempt has been made to reproduce minor irregularities. The length coordinates have been related through the conversion to Sherman's units described above and the relation between these and the experimental units that is implied in figure 7 of Center's paper. The lengthwise positioning of the experimental profile relative to the Monte Carlo profile is quite arbitrary. The Monte Carlo results in figures 3 and 4 are from separate computer runs.

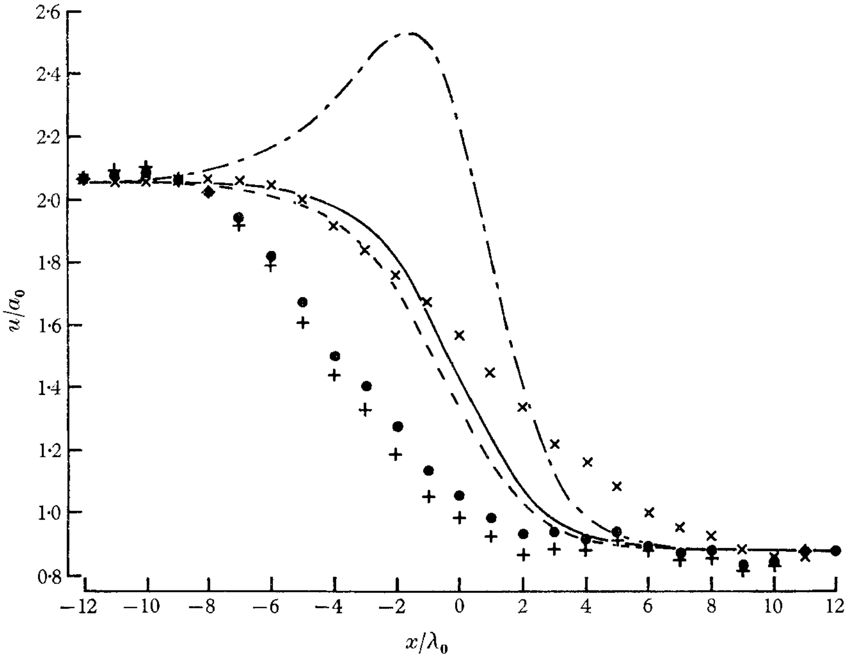

FIGURE 3. Velocity profile through a shock of Mach number 2·05 in a 2% argon–98% helium mixture. ●, model gas results for mixture; ×, argon; +, helium. —, continuum results (Sherman 1960) for mixture; —·—, argon; — —, helium.

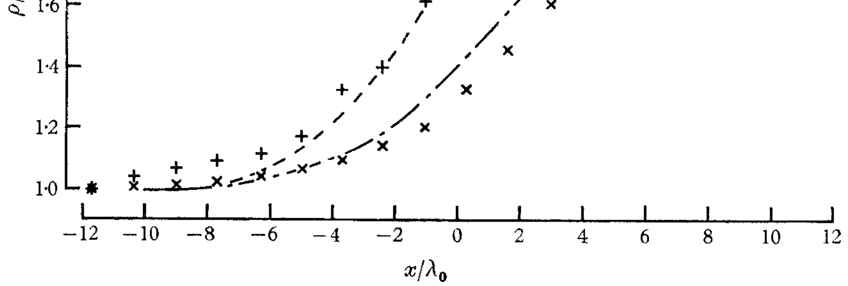

FIGURE 4. Density profile through a shock of Mach number 2·05 in a 2% argon–98% helium mixture. ×, model gas result for argon; +, helium. —·—, smoothed experimental result (Center 1967) for argon; — —, helium. ⊖, Rankine–Hugoniot downstream value.

As mentioned earlier, Sherman assumed the temperatures of the two species to be equal to the mixture temperature at every point in the wave. However, the velocity change in the argon lags behind that in the helium and one would expect a similar effect in the temperature profile. Figure 5 shows the temperature profile given by the Monte Carlo method for a mixture of equal parts and a temperature lag is, in fact, observed. The temperature non-equilibrium is greatest near the front of the wave and two species attain temperature equilibrium at approximately the point in the wave where the velocity distribution functions return to their equilibrium shape. The corresponding profiles for the mixture with only 2 % of argon are presented in figure 6. There is again a lag in the argon temperature rise at the front of the wave and instead of the individual species temperatures drawing progressively closer to the mixture temperature, they cross-over near the centre of the wave and there is a marked overshoot of the argon temperature. Furthermore, it appears that the temperature non-equilibrium between the species persists for a considerable distance downstream of the wave.

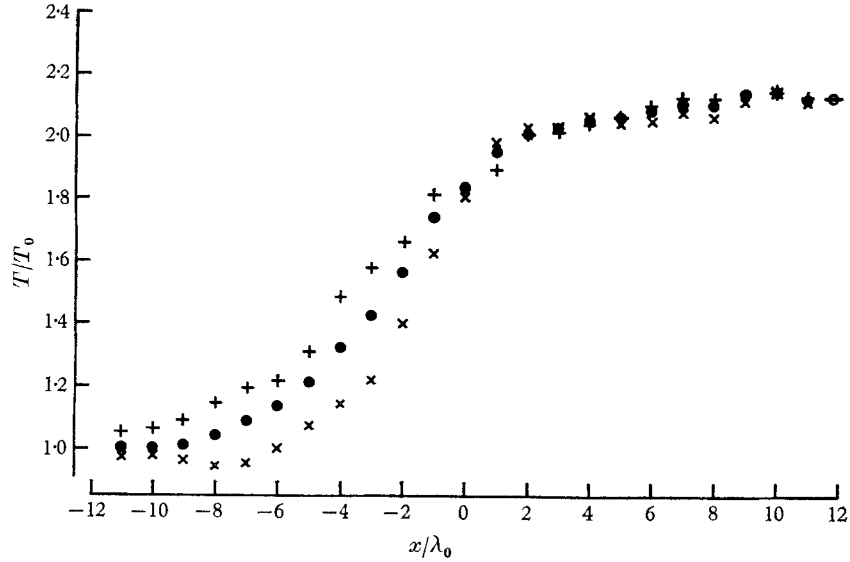

FIGURE 5. Temperature profile through a shock of Mach number 2·05 in a mixture of equal parts argon and helium. ●, mixture; ×, argon; +, helium. ⊖, Rankine–Hugoniot downstream value.

There are several detailed points about the temperature profiles which require comment. First, the upstream temperature ratios are consistently some 5–10 % below unity. The reason for this is that the peculiar velocities are measured relative to the instantaneous stream velocity in each cell. There is a statistical scatter in the stream velocity and, while the positive and negative fluctuations counteract one another as far as the average stream velocity is concerned, the temperature is always reduced. The second concerns the fact that near the front of the profile shown in figure 6, both species temperatures are below the mixture temperature. This is due to the peculiar velocities for the mixture temperature being taken relative to the mass average velocity, while those for an individual component gas are measured relative to the average velocity of the molecules representing that gas. This effect disappears downstream of the wave where the diffusion velocities are zero, and the argon temperature overshoot is independent of this effect.

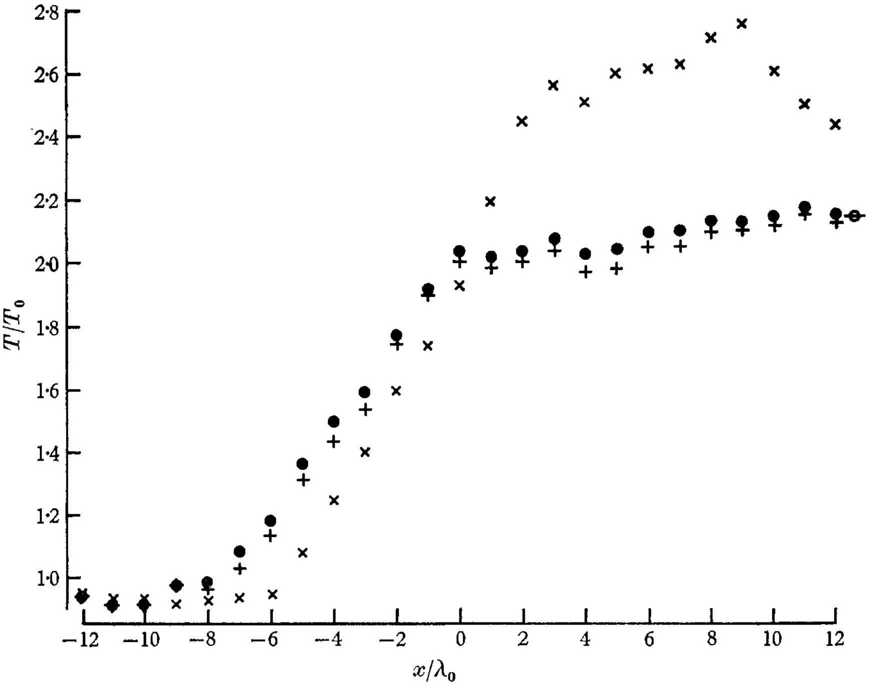

FIGURE 6. Temperature profile through a shock of Mach number 2·05 in a 2% argon–98% helium mixture. ●, mixture; ×, argon; +, helium. ⊖, Rankine–Hugoniot downstream value.

3.2. *Strong shock waves*

Similar computations were performed for strong waves with a shock Mach number of 10. The velocity and temperature profiles in a mixture of equal parts by mole argon and helium are shown in figures 7 and 8 respectively. A result of major interest is that the shock profile is now slightly thicker in terms of upstream mean free paths than at $M_s = 2{\cdot}05$. This is in direct contrast to the simple gas case and the computations were repeated for even stronger shock waves. It was found that the effect continues to at least a shock Mach number of 50. In fact, the profile becomes so wide that the computer storage capacity was inadequate for the proper simulation of extremely strong shocks. As far as the temperature profiles are concerned, there is an indication of an argon temperature cross-over and overshoot. However, this effect is of the same order as the statistical scatter and may not be significant. This point was investigated further by carrying out the corresponding computation for a mixture of helium and xenon, but there was no significant overshoot in the temperature of the heavy component.

Figures 9 and 10 show the velocity and temperature profiles for a shock of Mach number 10 in an argon–helium mixture containing 2% argon. The overall thickness of this wave also shows a slight increase over that of the corresponding wave at the lower shock Mach number. The argon temperature cross-over and overshoot effect is again apparent and an investigation was made into the

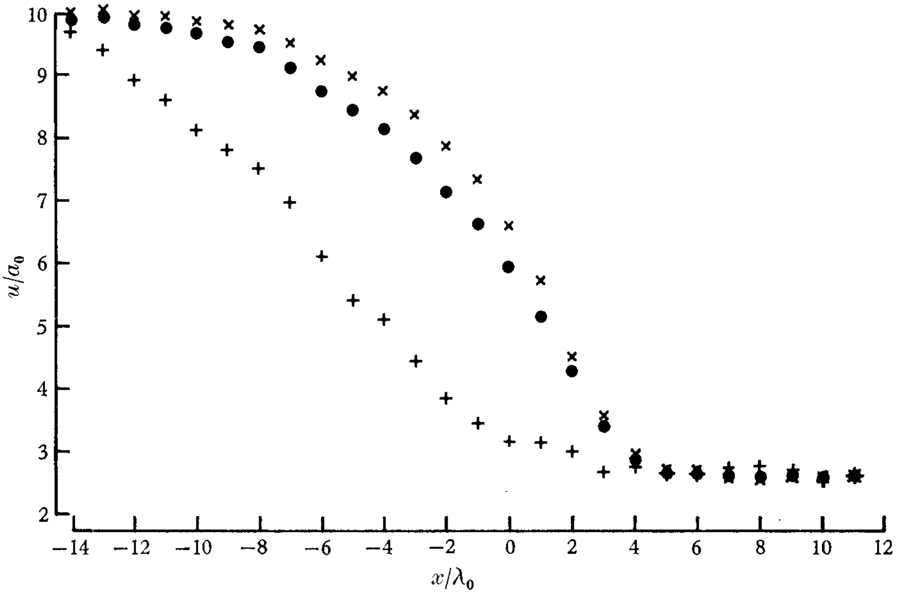

FIGURE 7. Velocity profile through a shock of Mach number 10 in a mixture of equal parts argon and helium. ●, mixture; ×, argon; +, helium.

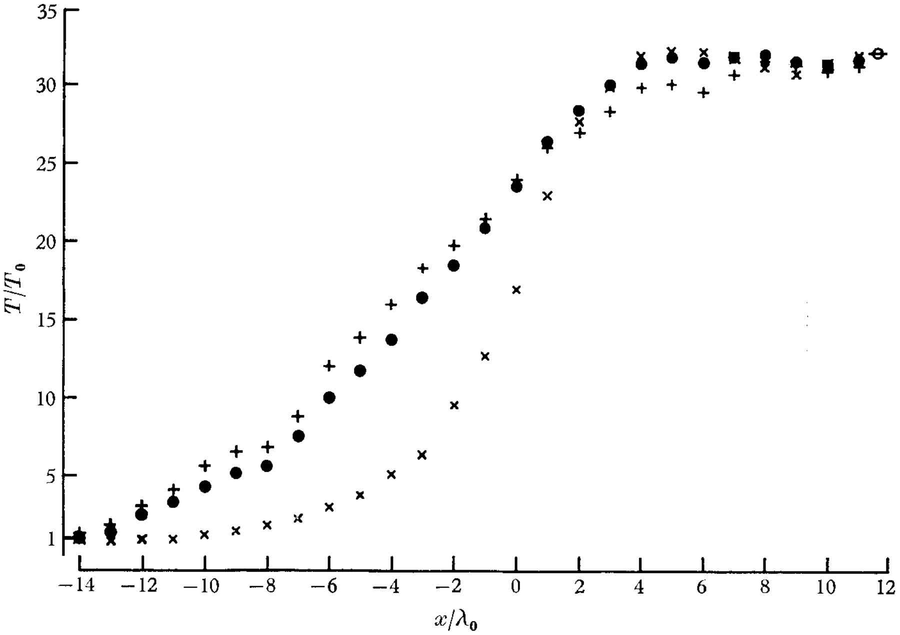

FIGURE 8. Temperature profile through a shock of Mach number 10 in a mixture of equal parts argon and helium. ●, mixture; ×, argon; +, helium. ⊖, Rankine–Hugoniot downstream value.

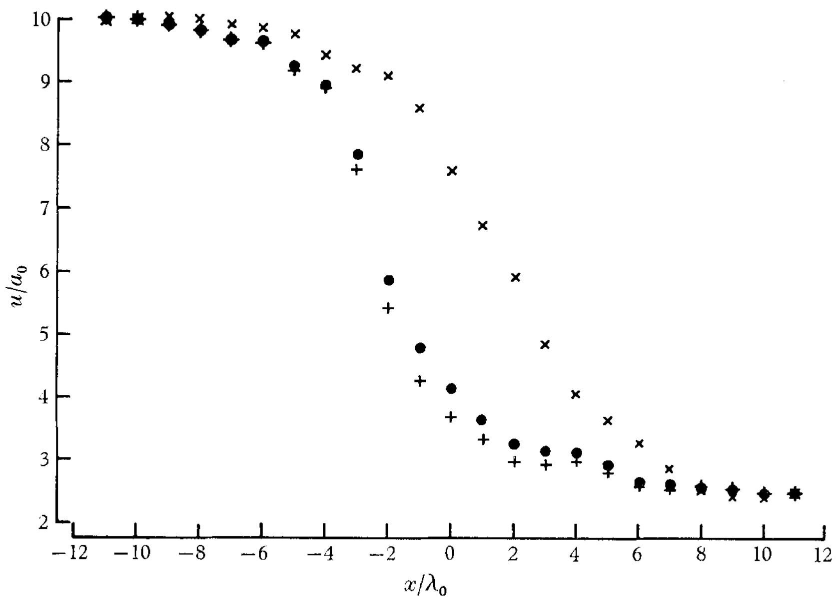

FIGURE 9. Velocity profile through a shock of Mach number 10 in a 2% argon–98% helium mixture. ●, mixture; ×, argon; +, helium.

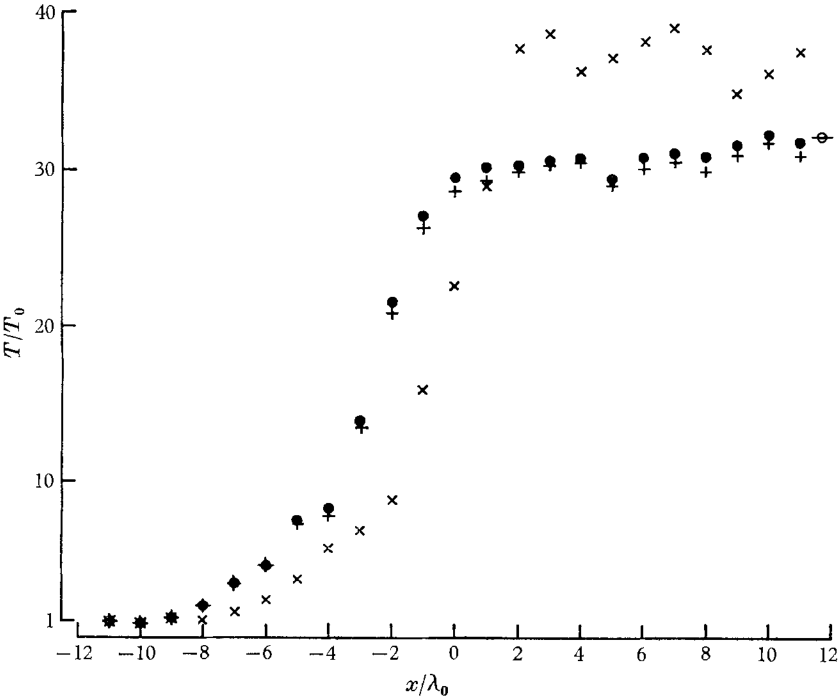

FIGURE 10. Temperature profile through a shock of Mach number 10 in a 2% argon–98% helium mixture. ●, mixture; ×, argon; +, helium. ⊖, Rankine–Hugoniot downstream value.

velocity distribution functions of the species. The temperatures based on the longitudinal and lateral velocity components exhibited the normal behaviour of an overshoot in the longitudinal temperature in the centre of the wave. These two temperatures became equal and the velocity distribution functions for each species returned to the Maxwellian distribution before the velocity and the mixture temperature reached their Rankine–Hugoniot downstream values.

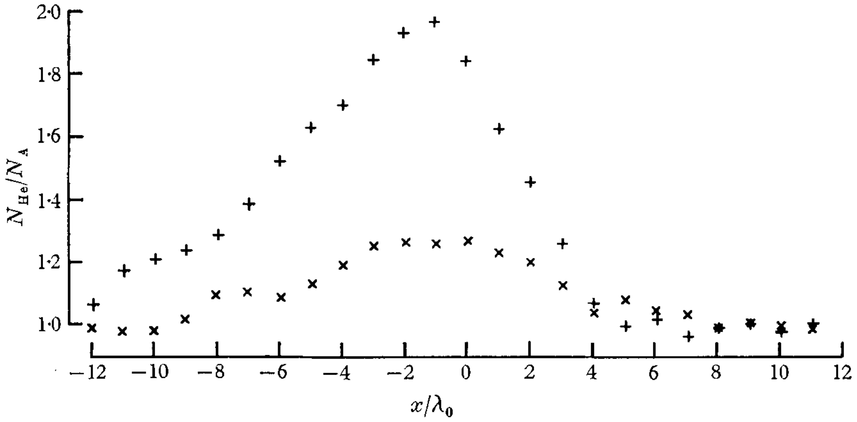

FIGURE 11. Degree of separation within shock waves in a mixture of equal parts helium and argon. ×, shock Mach number $M_s = 2{\cdot}05$; +, $M_s = 10$.

Sherman applied the continuum analysis to very strong shock waves and predicted that the degree of species separation within the wave should increase with shock Mach number. Figure 11 shows the ratio of helium to argon number density in a mixture of equal parts by mole of these gases at shock Mach numbers of 2·05 and 10. The results are in qualitative agreement with continuum theory which predicts maximum number density ratios of 1·36 and 2·2 for shock Mach numbers of 2·05 and ∞, respectively. Sherman discussed the implications of the concentration of helium within the wave and suggested that it would be balanced by a concentration of argon near a piston producing the wave. Although no attempt was made to look in detail at the unsteady process, a local depletion of helium was evident near the piston during the formation of the wave.

3.3. *Weak shock waves*

The Monte Carlo simulation method is not suited to very weak waves since the disturbance eventually becomes of the same order as the statistical scatter in computer runs of feasible length. However, the argon–helium mixture was studied at a shock Mach number of 1·4 and it was found that the results were qualitatively similar to those at a shock Mach number of 2·05. It was not considered worthwhile to attempt to investigate weaker waves because of the inordinate amount of computing required.

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REFERENCES

Bird, G. A. 1967 The velocity distribution function within a shock wave. *J. Fluid Mech.* (to be published).

Center, R. E. 1967 Measurement of shock wave structure in helium–argon mixtures. *Phys. Fluids* (to be published).

Chapman, S. & Cowling, T. G. 1939 *Mathematical Theory of Non-uniform Gases.* Cambridge University Press.

Liu, C. Y. 1965 *Phys. Fluids*, **8**, 1190.

Oberai, M. M. 1965 *Phys. Fluids*, **8**, 826.

Oberai, M. M. 1966 *Phys. Fluids*, **9**, 1634.

Sherman, F. S. 1960 *J. Fluid Mech.* **8**, 465.