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The formation of shock waves in a dense gas using a molecular-dynamics type technique

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The formation of shock waves in dense argon is studied using a numerical technique related to the molecular-dynamics approach. The kinetic and total pressures, density, temperature and mass velocity are calculated when a simulated tungsten piston is driven into the stationary gas. It is found that the pressure generated is similar to that found using binary collision assumptions, however the temperature is lower and the density much higher than under more rarefied conditions. Results are also given for the same experiments when the generating piston is composed of dense argon atoms. It is shown that the results are almost independent of the type of piston material and that the shock structure is a function of the gas interparticle force law only. The reflexion of a spherically imploding shock wave in dense argon is also examined and it is found that the shock wave reflects before reaching the centre due to high tangential stresses. Some data is also given upon the velocity distribution and wall pressure fluctuations.

Introduction

The stimulus for the present research was the study of the implosion of a hemispherical shock wave in the driving chamber of the UTIAS implosion driven hyper-velocity launcher (Glass 1967). A binary collision study was undertaken (Macpherson 1970) using the Monte-Carlo technique described in Macpherson (1969). Briefly mentioned in Macpherson (1970) were some preliminary results using an early version of the present technique, and the cautionary note was placed upon these results that "the method was still under development and the results only presented tentatively". It transpires that the results presented were actually calculated at 3 atmospheres rather than 100 atmospheres as stated and that generally the temperature was overestimated in these earlier results. The reason for the overestimate of temperature will be described below but was generally due to molecules sometimes being allowed to come too close to each other before being repelled. The present discussion generally augments the earlier treatment and presents more accurate results.

The usual shock wave relations using perfect gas approximations can be used safely for dilute gases in the number density range 10^{16} to 10^{18} particles/ml and the pressure range 10^{-2} to 1 atm. As pointed out by Devanathan & Bhatnagar (1969) the following assumptions are made in the classical theories: (i) the statistics

of the assembly is adequately represented by the single particle distribution function so that the particles can move freely except for occasional encounters with other particles; (ii) the interaction between the particles is purely binary and takes place in a period of time much less than the duration of the mean flight time. It is also suggested that above 10 atmospheres marked discrepancies between theory and experiment occur. Some extension of the classical theory can be made using various equations of state, but during the reflexion of an imploding spherical shock wave the equation of state must be continually altered as the centre is approached and the derivation of the appropriate state equation becomes more difficult.

In the present treatment a numerical study is made of the generation of a planar shock wave in argon of initial number densities $0{\cdot}73 \times 10^{21}$ and $0{\cdot}25 \times 10^{22}$, by a tungsten piston. As will be shown below, the piston material does not influence the results as the boundary conditions are chosen so that there is no heat transfer out of the gas. Thus the shock properties are a function of the gas only. Even changes of potential forces between the wall atoms and gas atoms do not influence the results. The piston is driven into the gas at such a speed that a shock wave of Mach number 10 would be developed in a rarefied gas. This was performed for both initial number densities and the results presented. Similarly a piston velocity was chosen to develop a Mach number 20 shock and the experiment performed in the medium with the higher initial number density. The reflexion of an imploding spherical shock wave is simulated by a spherical piston imploding into a gas of initial number density $0{\cdot}25 \times 10^{22}$. Initially it was hoped to present a comprehensive treatment of many aspects of the dense gas shock problem but the computer run times are so great that only a few cases could be studied. Generally the present study has shown that the technique described here, which is related to molecular dynamics† (Rahman 1964), can be used to study shock wave generation when the above classical assumptions no longer apply. A few results are presented and it is suggested that if other techniques will not solve a shock generation problem in a dense gas then the present method will. However, the user must be prepared for the exercise to be extremely costly in terms of computer run time.

Method of calculation

The usual molecular-dynamics technique (Rahman 1964) is to assign random positions and velocities to a small number of particles and to store these values in the computer. The molecules are then allowed to move in time steps of 10^{-14} sec by solving the set of Newtonian equations for the whole system of interacting particles. Interaction between particles is assumed to cease after some given radius from the given molecule typically $2{\cdot}25\sigma$, where σ is the zero potential radius in a Lennard-Jones potential. A predictor-corrector formula is used to increase the accuracy of the calculations.

† I am indebted to Dr R. E. Duff who pointed out to me the similarity to molecular dynamics at the 7th Shock Tube Symposium. The method, however, was developed without knowing of the molecular-dynamics technique.

As mentioned above, the present technique is similar to the molecular-dynamic approach, but as it was developed independently it has a number of differences. The main aim of the differences is to decrease the computation time at the expense of accuracy. This is necessary to handle the large number of particles involved in generating a shock and even with the approximations used the computer time is very high. Further, it is not obvious that the standard molecular-dynamic technique could calculate the high energy impacts occurring in the generation of a Mach 20 shock wave for example. It may happen that similar physically incorrect results may result as in Macpherson (1970).

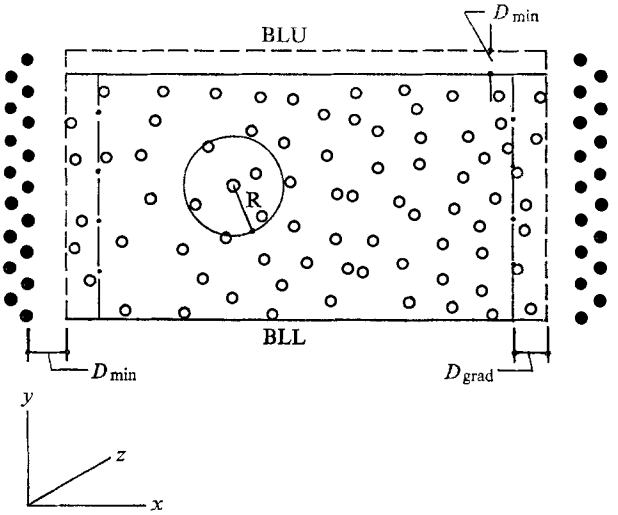


FIGURE 1. Two-dimensional view of argon gas molecules [○] and tungsten wall molecules [●] used in studying planar shock waves. Actual simulation was in three dimensions.

Consider a small prism of argon, typically a few hundred angstroms (Å) long and 100 Å square, contained between two walls of tungsten. The walls are simulated by assuming the metal atoms are in two layers as shown in the two-dimensional sketch in figure 1. Tungsten atoms were chosen as considerable data is available upon argon–tungsten interactions at UTIAS where this work was commenced. For the pressures expected behind a Mach number 10 shock wave (12,000 atmospheres), a wall was chosen rather than reflexion by image molecules because as the density of the gas increased the density of the 'image molecule piston' would increase. Initially, probably only the image of the molecule would be important, but later the surrounding images would have to be considered. Thus a variable density boundary would be produced. By choosing two rows of fixed atoms, either tungsten or argon, constant boundary conditions were obtained throughout the experiment. A two-dimensional figure has been shown for clarity although the actual simulation was in three dimensions. They are taken to be in a body centred cubic lattice with interparticle distance 3·16 Å. However, these atoms are assumed not to move relative to each other during the experiment. This was necessary as not only would the calculation of the vibration of each atom have required considerable extra computer time, but storage of the velocity

and position co-ordinates would have been impossible with the core storage available in the computer used by the author. With fixed positions it was not necessary to store atom positions, assuming that a tungsten atom was situated at the point (0, 0, 0). As the wall atoms are not displaced by the gas atoms collisions, energy is conserved and the gas atoms move in a potential field. Further, as the wall atoms have no internal structure and are not allowed to vibrate there is no mechanism for heat transfer between the wall and gas atoms. Thus the fixed wall atoms provide an adiabatic wall. The argon atoms were simulated by choosing random positions and a Maxwellian velocity distribution. The number of particles was chosen to give the desired initial pressure assuming that the gas was a perfect gas. When inserting each new atom two restrictions were placed upon the position: (i) the distance between the centre of the new particle and any existing particle must be less than $0{\cdot}9\sigma_A$; (ii) no gas molecule must be closer to the wall than $D_{\min} = \sigma_T$, figure 1; where σ_A and σ_T are the zero potential radii for argon–argon interaction and argon–tungsten interaction respectively. This was necessary as two molecules could be placed unrealistically close together so that even in time 10^{-14} sec the velocities would increase to unrealistic values. The periodic boundary condition was invoked on the lateral boundaries. That is, molecules which move out across BLU, figure 1, enter through BLL at the same x co-ordinate. Thus it was necessary to keep all particles a distance—$D_{\min}$ from BLU during the initial set up. In most parts of the region the velocities were taken from a Maxwellian distribution appropriate to 300 °K; however, near the wall, the Maxwellian velocity was increased slightly due to particles coming within the attractive field of the wall. This distance D_{grad}, figure 1, was taken to be 7·5 Å. The increase in velocity was such as to conserve energy of the particle. It was realized that this was incorrect physically for, as has been pointed out to the author by Dr F. Goodman, the density, assuming perfect gas properties, should obey a relationship like that proposed by Steele & Halsey (1955). This was not followed as it was thought that the shock would be developed sufficiently rapidly that the adsorption by the stationary wall would not be significant. This was thought reasonable from the binary studies of shock generation by Bird (1969). However, the shock wave generation is slower and it appears that it would have been better to allow some density variation. It does not seem however that the shock properties would be altered if an initial density variation were allowed.

The molecules are assumed to move for a short length of time Δt in a force field which remains constant during this period. A similar assumption was made by Lennard-Jones & Devonshire (1937) and it was from this idea that the present work developed. Further, the force field is generated only by other molecules within a sphere of given radius R, typically 7·5 Å. In the case of molecules near BLU or BLL the sphere is assumed to extend to the other side of the prism of gas. Thus the ith particle, shown encircled in figure 1, will be assumed to move while all the surrounding molecules remain stationary. Having found the new velocity and position for the ith particle it is returned to its original position and the new values stored. The $(i+1)$th particle is then examined and so on until the whole field is covered. The particles then take up their new positions and velocities and the cycle is repeated. In practice the method was to order the particles in

increasing x and to calculate the interaction between the ith and $(i+1)$th particle. The required force values for the $(i+1)$th particle were then stored as the negative of that for the ith particle. This saved double calculation. Wall effects were allowed for by considering the interaction of the gas atom with the closest sixteen tungsten atoms. Originally the technique by Jackson & French (1969) of assuming that outside a given distance from the wall the wall effects should be integrated to infinity, was tried. It was found that very large fluctuations in wall pressure occurred. This may be due to the nature of the wall model used here.

The motion of the ith molecule, with mass M and position vector $\hat{r}_i$ and velocity vector $\hat{v}_i$ at time t_1, was calculated by the Taylor series expansions

$$\hat{r}_i(t) = \hat{r}_i(t_1) + \hat{\dot{r}}_i(t_1)\,(t-t_1) + \hat{\ddot{r}}_i(t_1)\,(t-t_1)^2/2! + \hat{\dddot{r}}_i(t_1)\,(t-t_1)^3/3! \tag{1}$$

$$\hat{v}_i(t) = \hat{v}_i(t_1) + \hat{\ddot{r}}_i(t-t_1) + \hat{\dddot{r}}_i(t-t_1)^2/2!, \tag{2}$$

where $\hat{\ddot{r}}_i = (1/M)\,\partial\phi/\partial r_i$ and $\hat{\dddot{r}}_i = (1/M)\,(\partial^2\phi/\partial r_i^2).V_i$ where ϕ is the potential function at r_i.

In the present case ϕ is generated by the surrounding atoms at r_j distance r_{ij} from r_i.

$$\hat{\ddot{r}}_i = \sum_{\substack{j \\ j \neq i}} \frac{1}{M} \frac{\partial \phi_{ij}}{\partial r_{ij}} \cdot \frac{\hat{r}_i - \hat{r}_j}{r_{ij}}, \tag{3}$$

$$\hat{\dddot{r}}_i = \sum_{\substack{j \\ j \neq i}} \frac{1}{M} \cdot \frac{\partial^2 \phi_{ij}}{\partial r_{ij}^2} \frac{\hat{r}_i - \hat{r}_j}{r_{ij}} . V_r, \tag{4}$$

where V_r is the relative velocity of the two particles. Thus by letting $(t-t_1)$ be small, i.e. $\Delta t = 10^{-14}$ sec for a Mach 10 shock wave, the positions and velocities could be found. Checks were not made upon energy and momentum conservation as, if sufficient terms were taken in the expansion, due to the potential character of the fields, energy and momentum would be automatically conserved. As will be seen in the results, the shock properties agree with the Rankin-Hugoniot pressure relations, thus the conservation laws were in fact obeyed. Even using the third derivative it was found that in time Δt particles could move unrealistically close together. In the next time step they would then be driven apart with such high velocities that the whole system would eventually become unstable. Thus when two particles would, in a given time step, become less than 2·15 Å apart it was assumed in a side calculation that these two particles collided on their own. The time step was reduced by a factor of 10 and ten small steps were taken. When the new positions and velocities were found the equivalent value of $\hat{\dddot{r}}_i$ was calculated which would take the particles from their initial velocities to the final velocities. This value of $\hat{\dddot{r}}_i$ was then used in the normal calculation assuming all relevant particles were interacting. This device was only needed during the early stages of establishing the Mach 10 shock although it was needed throughout the whole of the Mach 20 wave generation. The time step Δt was reduced to $0{\cdot}4 \times 10^{-14}$ sec in the latter case.

In the earlier treatment (Macpherson 1970) similar assumptions were made except that instead of using a Taylor series expansion it was assumed that the

change in potential energy in time Δt was converted into a change in kinetic energy, i.e.

$$\Delta\phi = \Sigma(\partial\phi_{ij}/\partial r_i)(t-t_1)V_{ij}(t_1), \tag{5}$$

$$V_i(t) = (V_i(t_1)^2 - 2\Delta\phi . V_i(t_1)(t-t_1)/M)^{\frac{1}{2}}. \tag{6}$$

However, further study of individual collisions showed that it was possible under some conditions for unrealistically close approach between molecules to occur before repulsion. An example of this occurs when two molecules are chasing each other with the rearmost molecule having the higher velocity and overtaking the front one. This gave high velocities and hence high temperature peaks. In the present technique the $\hat{\ddot{r}}_i$ term provided early warning of the approach of the second molecule. Although it was thought that the present technique would allow larger time steps than 10^{-14} sec this did not occur. Rather, the time steps in Macpherson (1970) should have been smaller.

An experiment consisted of setting the molecules up, as described above, to simulate a temperature of 273 °K (T_0) and a kinetic pressure as required (P_0), then allowing them to collide for $0{\cdot}55 \times 10^{-13}$ sec or fifty-five cycles. From initial studies it appeared that this would be sufficient time to allow the largest fluctuations due to the expanding gas to be damped. It was realized that the gas was not in a steady state by this time but it appeared that sufficient computer time to achieve an equilibrium state could not be reasonably obtained. This would amount to several hours before the experiment commenced. However, these fluctuations do not appear to seriously affect the general results. After the initial settling time the piston was moved at the velocity necessary to generate the desired Mach number assuming binary collisions (Macpherson 1969). In order to prevent excessively violent collisions between wall atoms and gas atoms, the potential was calculated, assuming that the wall had moved through half the distance it would during the time interval Δt. In all cases the Lennard-Jones potential

$$\phi = t((\sigma/r)^{12} - (\sigma/r)^6) \tag{7}$$

was used.

For argon–argon interaction $t = 1{\cdot}71 \times 10^{-14}$ ergs,

$$\sigma = 3{\cdot}42\,\text{Å};$$

for argon-tungsten interaction $t = 1{\cdot}78 \times 10^{-13}$ ergs,

$$\sigma = 3{\cdot}07\,\text{Å},$$

where r = interparticle distance.

In the imploding shock wave study the piston was assumed to be constructed of argon atoms closely spaced in two rows. As the piston imploded the spacing was reduced as with fixed spacing it would appear to the gas atoms that the piston was rotating circumferentially.

Results

The results are presented in the form of temperature, pressure and density calculated in narrow zones. A fixed number of twenty-one divisions was used at all piston positions, so that at times when the total distance was small the results

were obtained on a finer grid. The kinetic temperature was calculated as the sum of the squares of the peculiar velocities (Chapman & Cowling 1968) and is referred to as T_k the kinetic temperature. This combines with the density to give the kinetic pressure P_k. The virial of Clausius (Jeans 1952) is used to calculate the total pressure P_T. This gives

$$3P/\rho = \Sigma mc^2 + \Sigma(xX + yY + zZ), \tag{8}$$

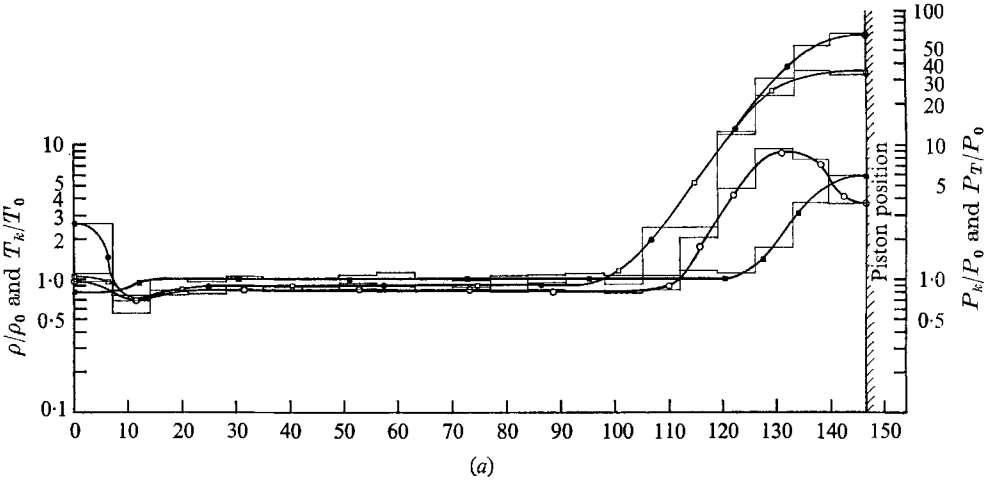
where x, y, z are the position co-ordinates of the molecule and X, Y, Z are the forces acting upon the molecule. In the case of a potential which is dependent upon the distance between the molecules this reduces to

$$3P/\rho = \Sigma mc^2 + \Sigma rF(r), \tag{9}$$

where $F(r)$ is the force between the particles distant r apart. Provided the sign of $F(r)$ is taken as positive or negative according to whether it is a repulsive or attractive force the relation (9) may be used for mixed signed forces as in the present case. The forces between the wall molecules and the gas molecules must be included in X, Y, Z for the zones near to the wall. It was decided to follow Jeans and to show the energy stored in intermolecular forms as pressure equivalent. An alternative derivation providing a potential temperature could have been found. Due to difficulties in displaying results on one figure, only kinetic pressure is shown; the potential pressure may be found as the difference between the total pressure and the kinetic pressure. As it was convenient to perform the summations before the zones were established, it was assumed that no contribution to the summation was made by particles on the left side of a given zone and that the total of the interacting forces on the right side were added to the given zone. The pressures were non-dimensionalized with respect to the kinetic pressure initially established. Similarly density and temperature were non-dimensionalized with respect to the initial conditions. The results are shown as block diagrams with a line sketched through the results for identification. No attempt has been made to use a curve fitting technique as generally the accuracy obtainable from one 'experimental' run is not sufficient to make such an exercise worthwhile. Thus the block diagrams should be studied although in some regions of the undisturbed flow this is not possible. However, even in these regions the fluctuations obtained are of interest.

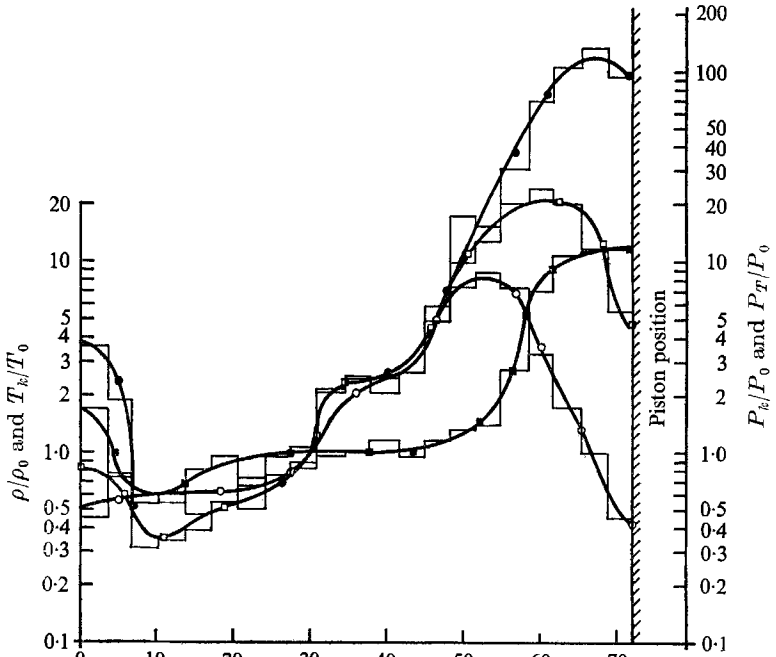
Using a piston velocity of $0{\cdot}29 \times 10^5$ cm/sec, a tungsten surface, initial number density of $0{\cdot}245 \times 10^{22}$ and initial distance between walls of 204 Å, the density ratio, kinetic temperature ratio, kinetic and total pressure ratios are shown for three times in figure 2. Assuming binary collision theory the start of test conditions would be 100 atmospheres, 21 mean free paths between walls, Mach number 10 shock wave and resultant test times of approximately 4, 9, 10 mean time between collisions (τ). The shock equilibrium values of density, temperature and pressure ratios using binary collision theory for a Mach number 10, $\gamma = 1{\cdot}67$ ideal gas would be 3·93, 31·7, 124·6 respectively. The time to develop these values after the piston commences moving has been shown (Bird 1969) to be about one mean collision time in the undisturbed gas. In figure 2(*a*) after 4τ the binary collision results have not been achieved although the equilibrium

temperature profile with a peak value of about 10 at approximately two mean free paths from the piston has been established. It appears that the equilibrium values are obtained between 4 and 5τ and the established profile is shown in figure 2(*b*) at time 9τ. The total pressure is approximately the same as the binary collision theory, the density ratio is about 2½ times greater and the temperature ratio less than 10. The slow rise to equilibrium values is due to the large proportion of



(*a*)

Distance from l.h.s. wall, Å



(*b*)

Distance from l.h.s. wall, Å

FIGURE 2. For legend see facing page.

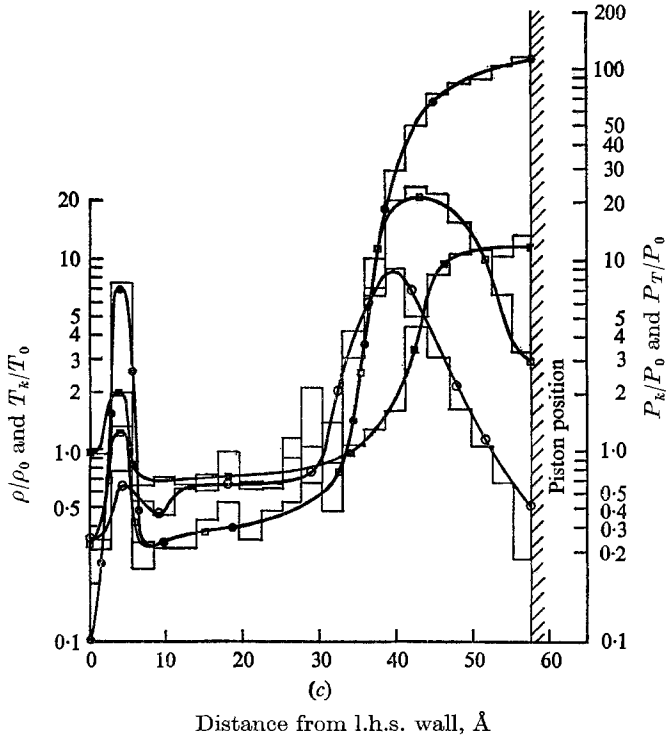


FIGURE 2. Shock wave generation by a tungsten piston moving into argon with initial number density $0{\cdot}245 \times 10^{22}$. Piston velocity $0{\cdot}293 \times 10^6$ cm/sec. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total pressure ratio. (*a*) Time $0{\cdot}199 \times 10^{-11}$ sec after piston started moving. (*b*) Time $0{\cdot}449 \times 10^{-11}$ sec after piston started moving. (*c*) Time $0{\cdot}4986 \times 10^{-11}$ sec after piston started moving.

pressure due to inter-molecular forces, the kinetic equilibrium being established much quicker. A maximum temperature ratio of 18 was found at a time $0{\cdot}5\tau$, but this damped fairly rapidly as the density increased. The final result of physical significance is shown in figure 2 (*c*) at time 10τ. The results at the stationary wall suggest that there is an oscillation set up at the wall as the peak increases apparently with time. This is due to there being 21 zones between the walls at all times. Thus as the piston approaches the wall the width of the zones decreases, in this case by a factor of almost 4 between the start and end of the experiment. Hence density gradients, such as at the bottom of the potential well will be shown more clearly as the zone width decreases. In figure 2 (*c*) the physical adsorption at the stationary wall has altered the initial conditions so that further results could not be obtained. A very large positive pressure peak is found at a distance from the wall corresponding to the distance of the bottom of the potential well of the Lennard-Jones potential between tungsten and argon. The pressure closer to the wall then becomes negative. Due to the large gradients in properties probably the last results which can be confidently used are those in figure 2 (*b*). As indicated by the long development times the Mach number of the wave is much less than 10,

although the mass velocity of the fluid behind the shock is the same as the binary collision results. Approximate contours of constant mass velocity are shown in figure 3. It should be emphasized that this figure is generally produced from only one set of results and thus the position of the curves are probably only accurate to 4 Å. The results in figures 2 and 3 were repeated for varying run times with different initial random particle positions and velocities. Figure 2 (*a*) is the average of 6 results although 2 (*b*) and 2 (*c*) are produced from only one test. Generally the scatter between runs was small and less than would be suggested by theories such as those by Smoluchowski (Lee, Sears & Turcotte 1963, p. 298).

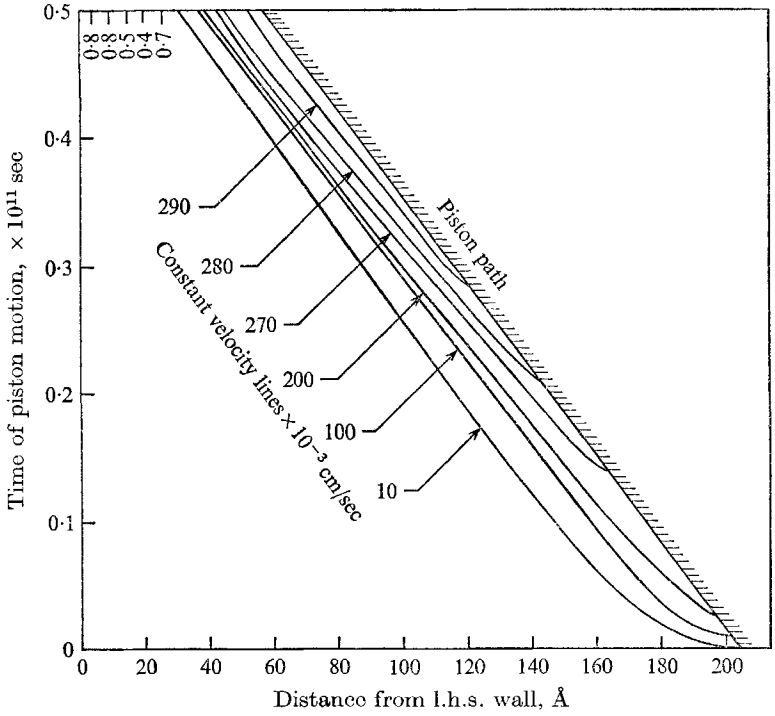


FIGURE 3. Approximate curves of constant mass velocity behind shock wave generated in argon initial density $0{\cdot}245 \times 10^{22}$ number density, piston velocity $0{\cdot}293 \times 10^{6}$ cm/sec.

Longitudinal velocity distribution profiles, integrated with respect to both lateral velocity distributions, were obtained for each zone at the completion of the test. The results are shown in figure 4 plotted with a probability or Poisson ordinate. With this ordinate a Maxwellian distribution will appear as a straight line through the 50 % ordinate and 0·0 abscissa points. These results may be compared with those by Bird (1967) using a binary collision assumption. It is found that a similar result is obtained. The zone near the piston is Maxwellian with a small standard deviation.On moving through the shock the average value becomes negative (in Bird (1967) the average became positive as in the present case the piston moves from the positive x co-ordinate towards the origin) and a second Maxwellian is formed on the positive side. This bump is seen clearly in

the results by Bird (1967). In front of the shock a Maxwellian of larger standard deviation is found. Thus using an entirely different technique from Bird and a dense gas where inter-molecular forces are important, the same velocity distribution profiles have been obtained. This gave added confidence in the present results.

From these results it appeared that the potential of the wall could dominate the shock structure or at least substantially modify it. Thus an experiment was simulated by enclosing the gas between two pistons constructed of argon atoms in a body centred cubic lattice as before, with an intermolecular spacing of 1·5 Å. The argon piston atoms were placed closer together than the tungsten

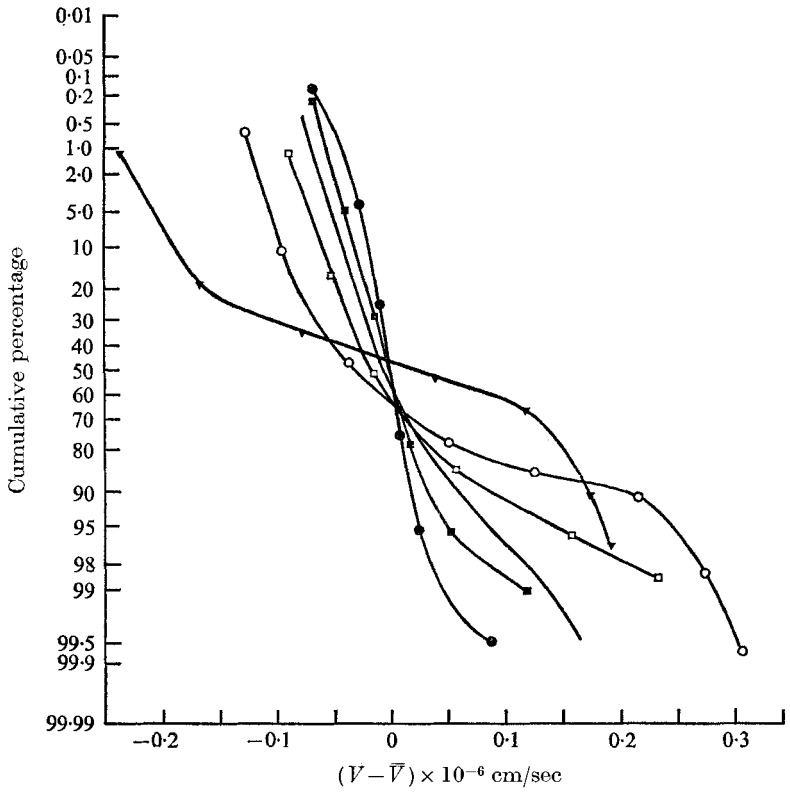


FIGURE 4. Longitudinal velocity distributions integrated across both lateral velocity distributions under conditions specified for figure 2(*c*). Numbering the cells shown in figure 2(*c*) as 1 next to the piston. —●—●—, cell 1; —■—■—, cell 2; ————, cell 4; —□—□—, cell 5; —○—○—, cell 6; —◀—◀—, cell 7.

atoms to prevent the high energy (both kinetic and potential) gas atoms from escaping. Even so the potential force provided by the argon piston was only about one-fifth that provided by the tungsten piston. It would thus be expected that if the wall was influencing the results, a marked difference between the results obtained with a tungsten piston and those with the softer argon piston would be found. Actually the wall effects would only be expected to influence the flow a few mean free paths from the wall. At 10,000 atmospheres the mean free path is about a molecular diameter or less.

The results in figure 5 are shown at time 9τ after the piston commenced moving, and can be compared with figure 2(*b*). The effects of the stationary wall upon the gas at the left-hand side are seen to be much less than before; however the shock properties are within expected statistical scatter. This strongly suggests that the results are a function of the gas inter-molecular potential only. Using a 360/65 IBM computer the computation time to obtain figures 2(*b*) and 5 was 8 h; to continue to obtain figure 2(*c*) required an additional 4 h. The time varies by the cube of the density approximately and as the shock develops the cycle time becomes much greater. Thus only a limited number of cases could be studied due to the high computer time requirements.

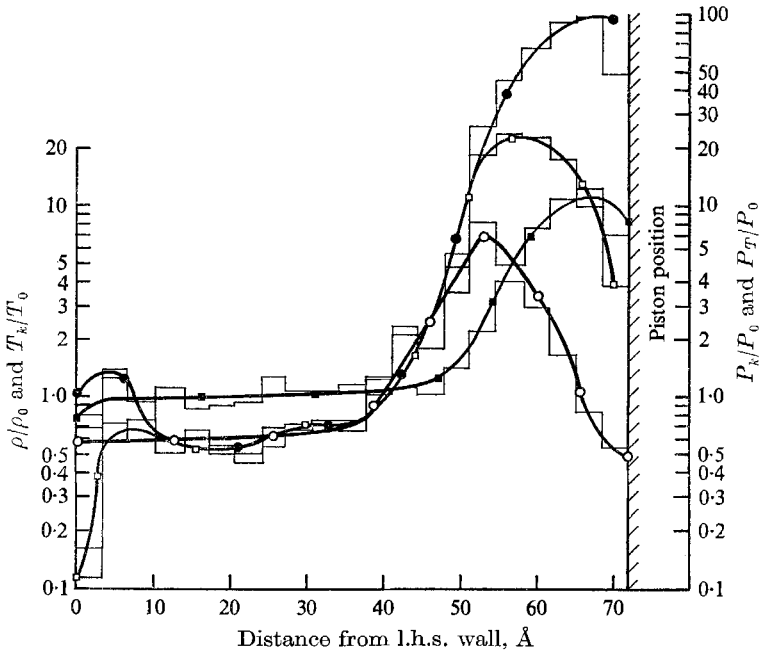


FIGURE 5. Shock wave generation by a dense argon piston moving into argon with initial number density $0{\cdot}245 \times 10^{22}$. Piston velocity $0{\cdot}293 \times 10^6$ cm/sec, result shown at time $0{\cdot}449 \times 10^{-11}$ sec after piston started moving. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total pressure ratio.

A study was performed using a piston velocity of $0{\cdot}586 \times 10^5$ cm/sec, which would generate a Mach number 20 shock wave assuming binary collision theory. The values of density ratio, temperature ratio and pressure ratio would then be 3·98, 126, 501. Figure 6 shows the results with initial number density $0{\cdot}245 \times 10^{22}$. Again the pressure ratio reaches the classical result, the density ratio is approximately $2\frac{1}{2}$ times the classical result and the temperature ratio is just less than 30. The integrated longitudinal velocity distributions are shown in figure 7 and although the standard deviation is greater the same trend is found.

It would be desirable to check the method by generating a shock wave in a gas with initial pressure equal to 1 atmosphere. However, it appears that this would require about 30 h computer time and in addition only about three or four mean

free paths of undisturbed gas could be simulated. One result which goes some way towards such a proof is given at the end of the paper. Using a tungsten piston and an initial number density of $0{\cdot}737 \times 10^{21}$ a simulated experiment was performed. The distance between the walls was 680 Å or 22 mean free paths of the undisturbed gas. After the piston has been in motion for about 10τ a well-developed shock wave is formed as in figure 8. Again the pressure ratio is approximately that obtained from binary collision theory, the temperature ratio is

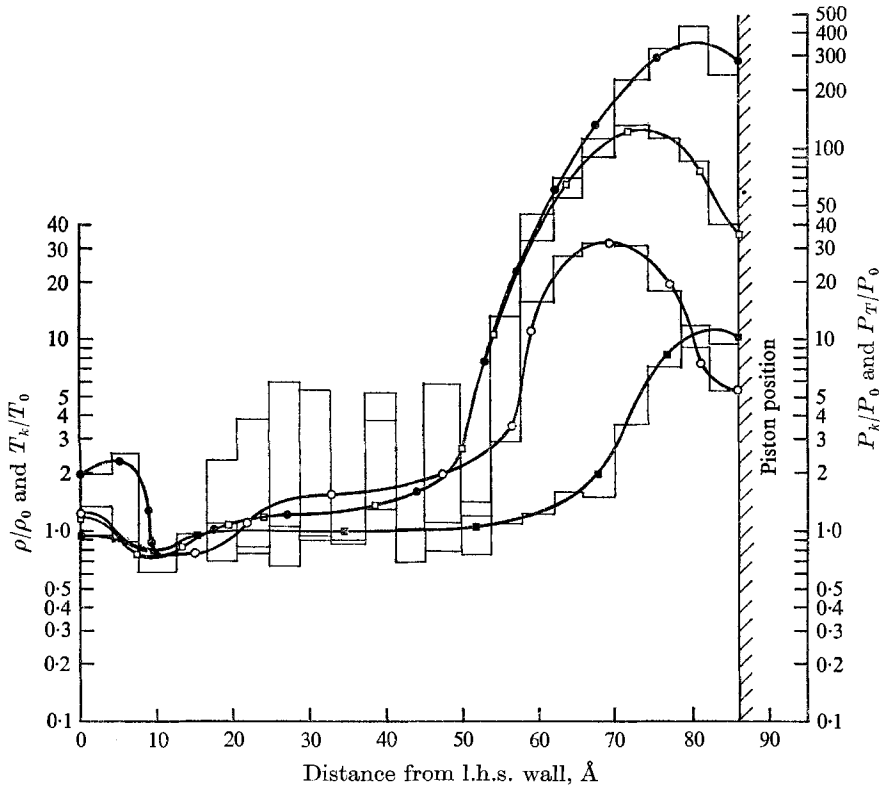


FIGURE 6. Shock wave generation by a tungsten piston moving into argon with initial number density $0{\cdot}245 \times 10^{22}$. Piston velocity $0{\cdot}586 \times 10^6$ cm/sec, result shown at time $0{\cdot}198 \times 10^{-11}$ sec after piston started moving. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total pressure ratio.

again slightly less than 10. However, the density ratio now is over 30 and is about three times that obtained with the higher initial number density. This means that the actual density was the same at the piston face in both cases. This suggests the conclusion that the temperature ratio is limited by a type 'space change' due to the high initial density. Once a certain initial density is exceeded a given piston speed will only generate a limited molecular velocity. Thus if the pressure is determined by the piston forces then the density must accommodate the difference. An examination of the integrated longitudinal velocity distributions gave the results in figure 9. Again the same pattern was reproduced through the shock wave.

The longitudinal force upon the walls for the case of $0{\cdot}245 \times 10^{22}$ initial number density is plotted in figure 10 as a function of time. The fine fluctuating lines indicate the instantaneous variation and the heavy line shows the average force on the stationary wall. Similar fluctuations about the mean were found on the moving piston but only the mean result can be shown. Certainly some of the early time fluctuations are due to the initial expansion process although as can be seen the first $0{\cdot}55 \times 10^{-12}$ sec have not been shown or used in calculating the average. Even large peaks were found on both walls at times $4\text{–}5 \times 10^{-12}$ sec after initial settling period. Some of these effects may be reduced if a non-rigid wall were used.

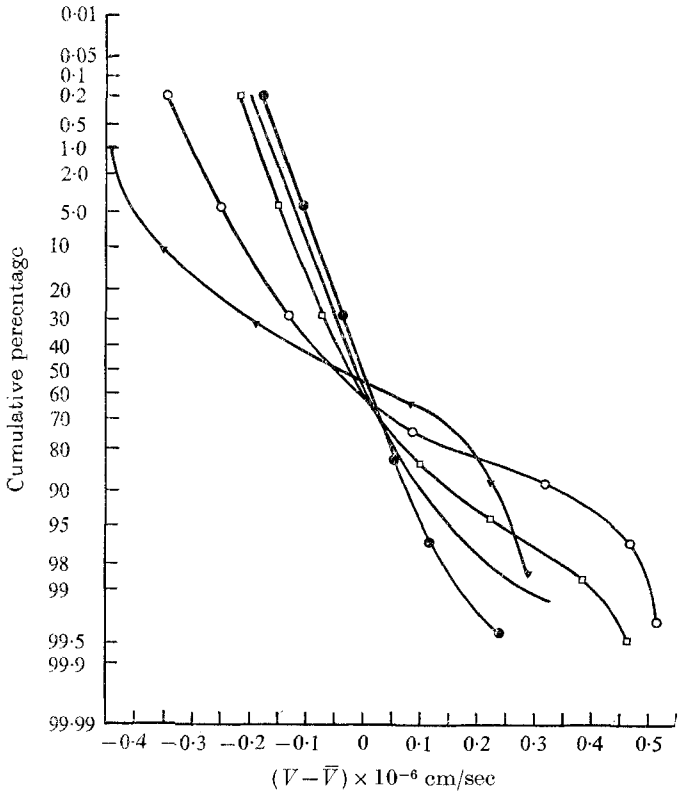


FIGURE 7. Longitudinal velocity distributions integrated across both lateral velocity distributions under conditions specified for figure 6. Numbering the cells shown in figure 6 as 1 next to the piston. —●—●—, cell 1; ————, cell 2; —□—□—, cell 3; —○—○—, cell 4; —◀—◀—, cell 5.

The reflexion of a spherically symmetrical imploding shock wave was studied by considering a sector of gas with included angle approximately 11° in both orthogonal circumferential directions. The radial boundaries consisted of dense argon surfaces as described above with intermolecular spacing 1·5 Å. The centre boundary was a sphere 2 mean free paths in radius, i.e. 19·4 Å. The initial outer piston radius was 620 Å, the initial number density $0{\cdot}245 \times 10^{22}$ and the piston velocity was $0{\cdot}293 \times 10^{6}$ cm/sec. Again the periodic boundary condition was used

along both circumferential directions. The conditions after the piston had moved for about 11τ are shown in figure 11(*a*). The density and temperature ratios are about the same as for the planar case although the temperature profile has a plateau rather than a sharp peak. The kinetic pressure does not dip at the piston surface as the temperature gradient at the piston is less than in the planar case. The total pressure is substantially lower than in the planar case due to the reducing area not producing as high a resistance as in the planar case. The results at a time 22τ are shown in figure 11 (*b*). At this stage all variables except the temperature have risen very substantially. A curious front plateau appears in the density ratio

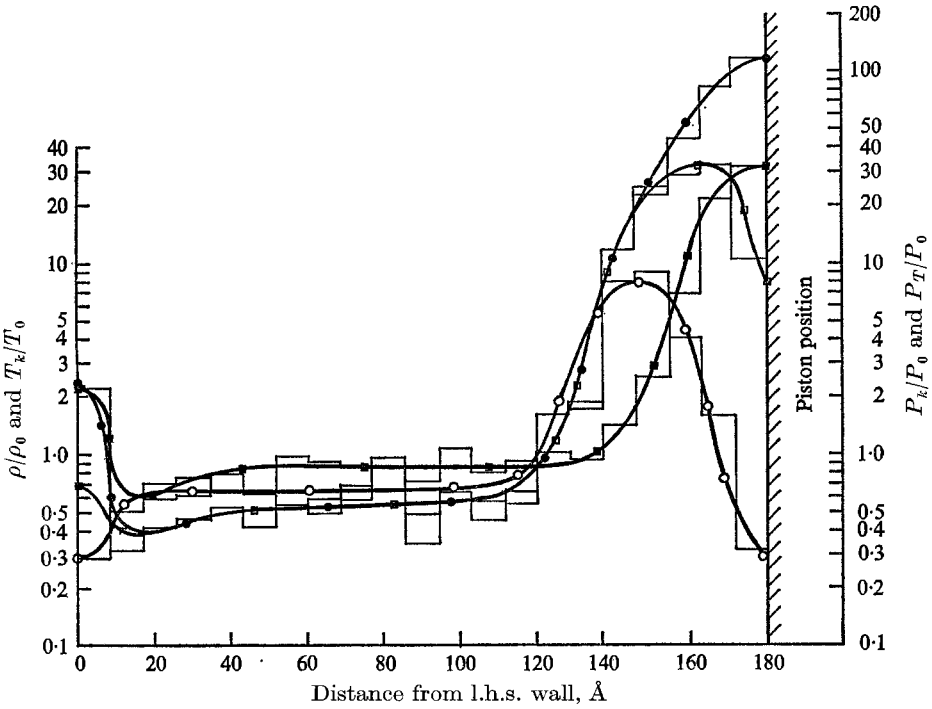


FIGURE 8. Shock wave generation by a tungsten piston moving into argon with initial number density $0{\cdot}736 \times 10^{21}$. Piston velocity $0{\cdot}293 \times 10^6$ cm/sec, result shown at time $0{\cdot}170 \times 10^{-10}$ sec after piston started moving. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total temperature ratio.

although from one set of results it may not be significant. At a time $0{\cdot}6 \times 10^{-12}$ sec later, figure 11 (*c*), a reflected pressure wave can be seen to have developed about 20 Å from the piston. The pressure ratio rises from 600 at the piston to about 1000 at the point where reflexion occurred. Comparing 11 (*b*) and 11(*c*) it can be seen that the pressure pulse also occurs in the density profile. The smoothness of the shock profile development, except near the centre where only a few particles are found, strongly suggests that this refraction is a real effect rather than a numerical instability. The author's practical experience on instability generation is limited to finite difference schemes used in numerical weather forecasting. In these the

instability grows with time from a number of points. In the present case a sudden rise is found as would be expected from a shock wave. However, this refraction effect requires additional study maybe from a continuum viewpoint.

The kinetic temperature profile is not so peaked in 11 (*c*) as in 11 (*b*). The effect of this reflected wave striking the imploding piston was observed in the results at a time $0{\cdot}1162 \times 10^{-10}$ sec. A pressure ratio of $0{\cdot}9 \times 10^{6}$ was formed near the piston in a very narrow region. In an experiment the piston would be sufficiently far from the reflexion point that this event would not arise, thus the results at later times, figure 11 (*d*), probably have no physical significance. The high

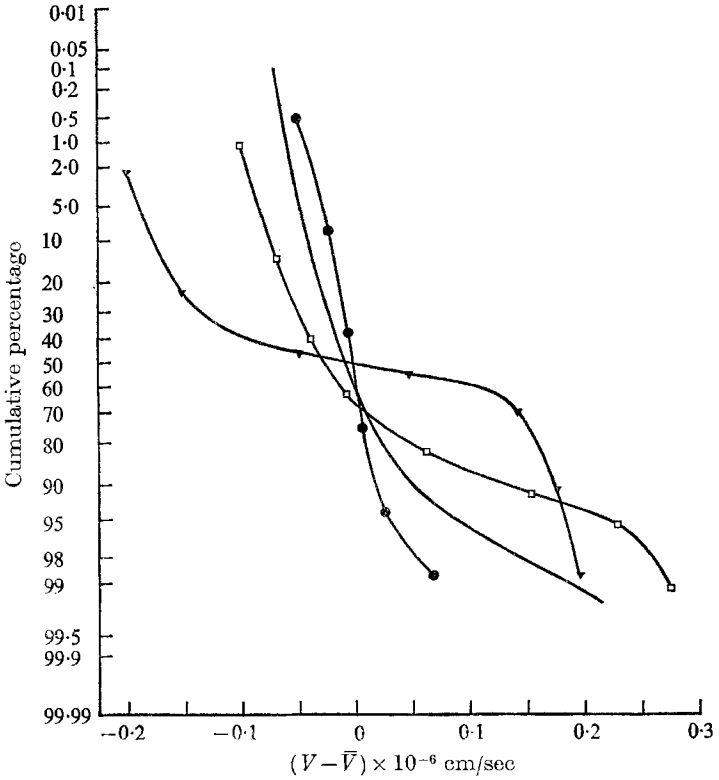


FIGURE 9. Longitudinal velocity distributions integrated across both lateral velocity distributions under conditions specified for figure 8. Numbering cells shown in figure 8 as 1 next to the piston. —●—●—, cell 1; ————, cell 2; —□—□—, cell 3; —◀—◀—, cell 4.

temperature and pressure peaks, figure 11 (*d*), towards the centre are the result of the intense reflected wave moving very rapidly through the dense gas till it reached the relatively rarefied gas near the centre. The molecules at the front of the shock were propelled at high velocities by this wave and gave apparently high temperatures and pressures. The pressures and density profiles show the reinforced wave moving rapidly towards the centre.

One test was performed with an initial density of three atmospheres and the results are shown in figure 12. The piston had been in motion for about $0{\cdot}6\tau$, and it

can be seen that apparently the binary collision temperature, pressure and density ratios have been established as if the shock wave was plane. However as this was for the spherical case and the time to equilibrium found by Bird of $1{\cdot}0\tau$ had not been reached the results are not conclusive. However it can be seen that the temperature limit found previously has not occurred in this case and a ratio of 30 has been achieved. It should be mentioned that these results required about 20 h of computer time before the experiment was terminated.

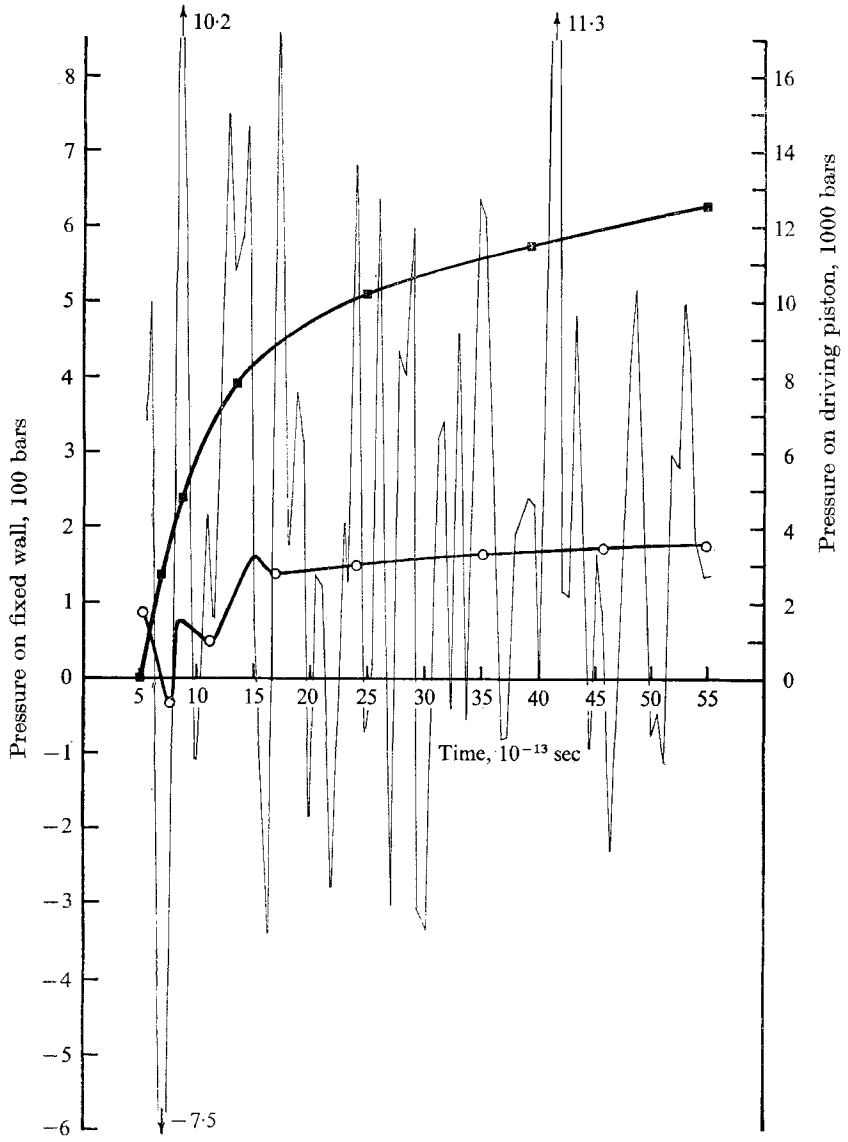


FIGURE 10. Pressure on tungsten walls used to produce results in figure 2. Fine lines are instantaneous values on the fixed wall. Solid heavy lines are mean values back to time $0{\cdot}55 \times 10^{-12}$ sec. —○—○—, fixed wall; —■—■—, moving piston.

Conclusion

It has been shown that the technique presented here can be used to study shock phenomena in dense gases and presumably could be extended to include liquids. Although it has not been shown that the results agree with binary collision theory at low pressures some evidence has been produced to suggest that this probably would occur. Due to the long computer run times involved only a few examples could be studied and thus the conclusions drawn cannot be considered to be all embracing.

At an initial pressure between 3 atmospheres and 30 atmospheres it appears that the temperature ratio developed by a Mach number = 10 shock wave becomes limited to a maximum of 8. This value is maintained for initial pressures up to over 100 atmospheres and is approximately one-quarter of the binary collision result. The nominally Mach number 20 shock wave also gave approximately one-quarter of the binary collision result. The pressure ratio obtained is approximately that calculated by binary collision theory and the density ratio is adjusted to match the temperature and pressure ratios. At higher Mach numbers with initial number densities of $0{\cdot}245 \times 10^{22}$ the pressure again is that calculated by binary collision theory, the density ratio is the same as for Mach number = 10 and the temperature ratio is adjusted to match these. The integrated longitudinal velocity distribution function through all the planar shock waves studied agreed generally with the results found for binary collision theory.

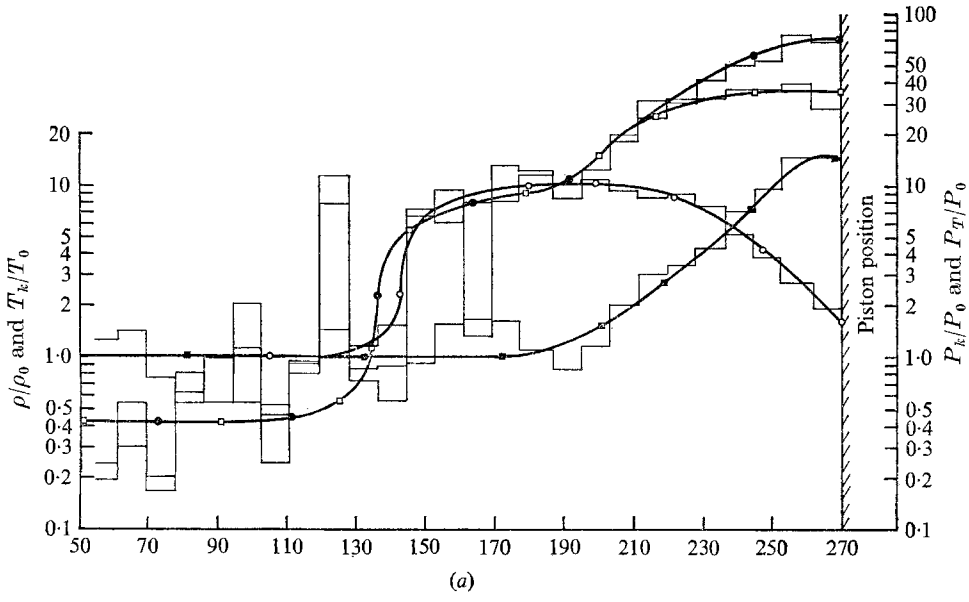
A spherically symmetrical imploding shock wave does not reach the centre before reflexion. With an initial number density of $0{\cdot}245 \times 10^{22}$ the wave reflects about 120 Å from the centre of the sphere. The process is similar to shock wave refraction and a transmitted wave continues to the centre and a reflected wave outward. Possibly as the transmitted wave strengthens refraction may be possible again.

I would like to acknowledge the encouragement and advice I received from Dr G. N. Patterson and Dr I. I. Glass at the Institute for Aerospace Studies at the University of Toronto where this work was started. As acknowledged previously, I am indebted to Dr P. C. Hughes for his advice in setting up the equations, although the author bears full responsibility for any errors.

I would like to express my thanks to the Computer Centre at the University of Manitoba for making available the considerable time necessary to complete this work. Both at the University of Toronto and at the University of Manitoba, this research was supported by the National Research Council of Canada and this support is gratefully acknowledged.

Legend to Figure 11

FIGURE 11. Shock wave generation by an imploding spherical dense argon piston moving into argon with initial number density $0{\cdot}245 \times 10^{22}$. Piston velocity $0{\cdot}293 \times 10^{6}$ cm/sec, results shown at various times after piston commenced moving. Centre is occupied by a sphere of radius 19·4 Å. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total temperature ratio. (*a*) $0{\cdot}672 \times 10^{-11}$ sec after piston started moving. (*b*) $1{\cdot}045 \times 10^{-11}$ sec after piston started moving. (*c*) $1{\cdot}105 \times 10^{-11}$ sec after piston started moving. (*d*) $1{\cdot}165 \times 10^{-11}$ sec after piston started moving.



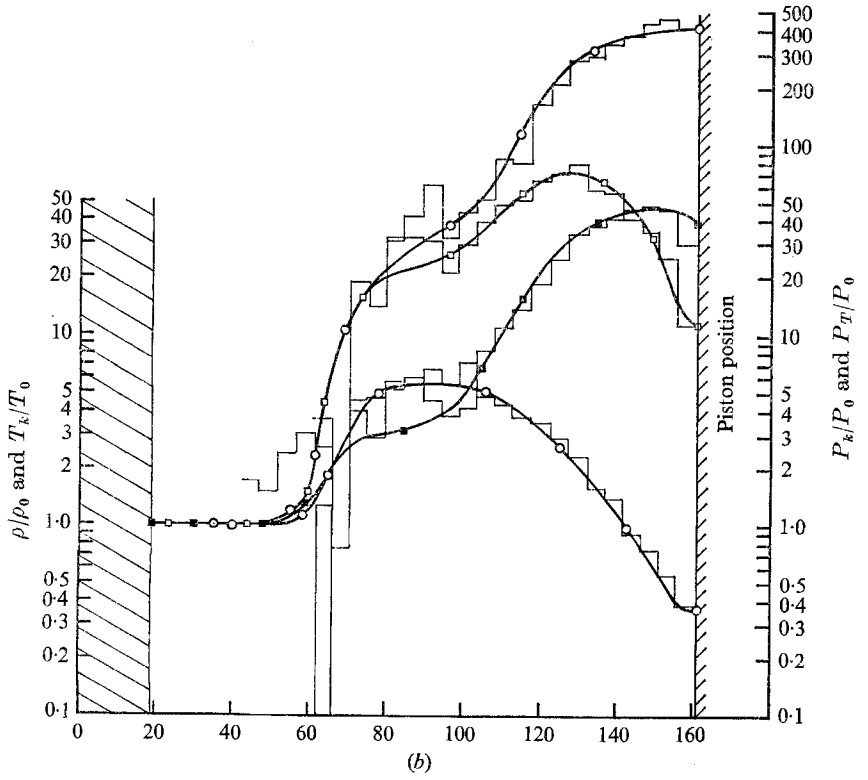
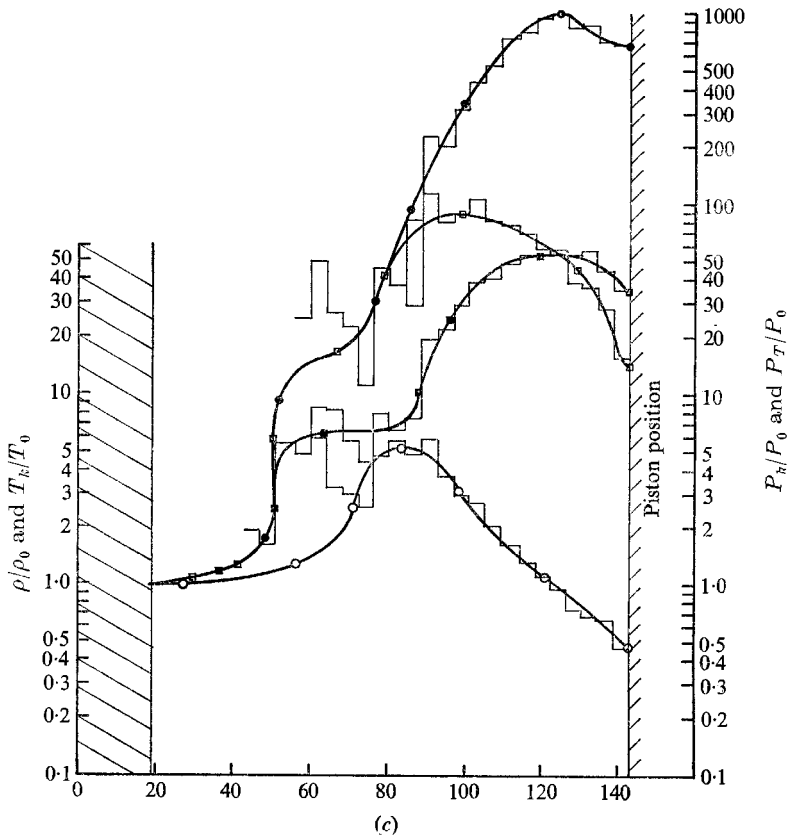


FIGURE 11. For legend see facing page.



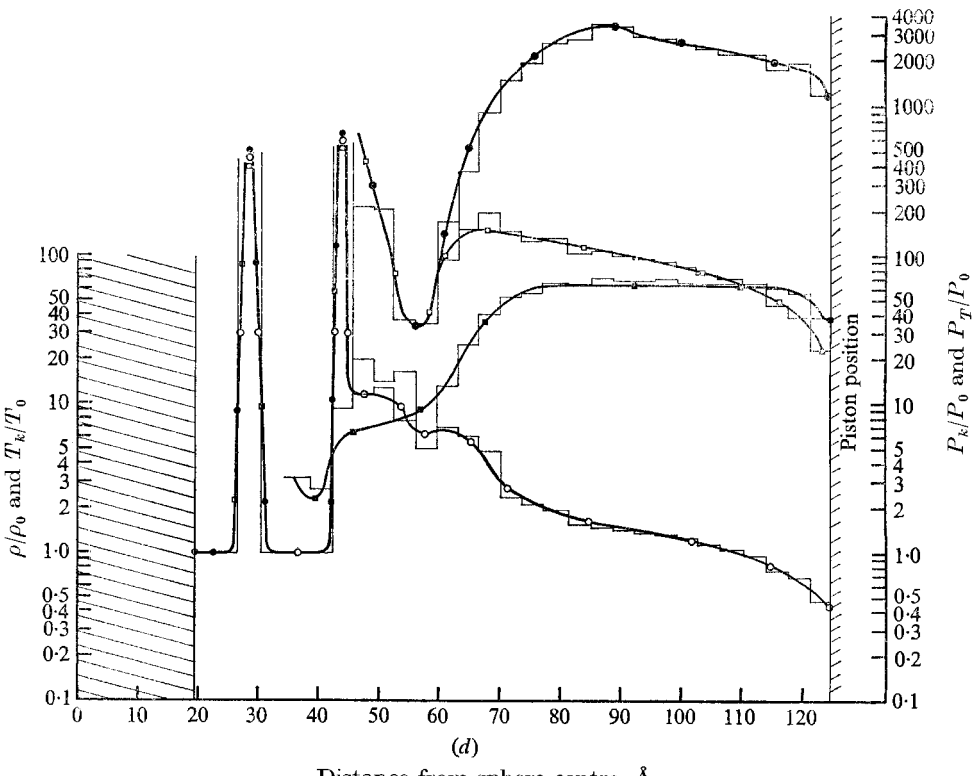


FIGURE 11. For legend see p. 618.

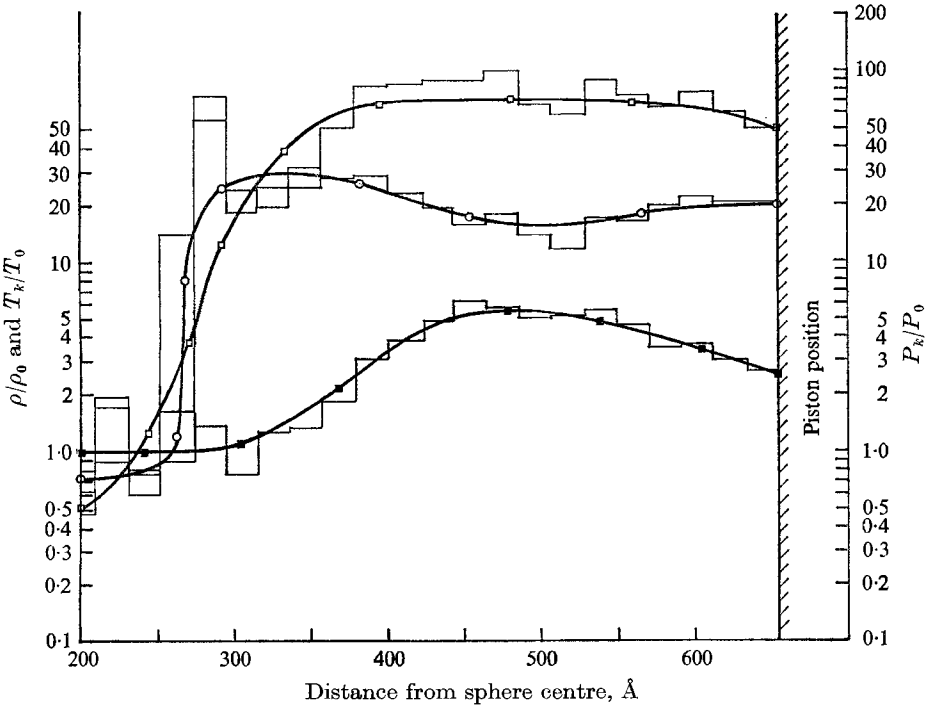


FIGURE 12. Shock wave generation by an imploding spherical dense argon piston moving into argon with initial pressure 3 atmospheres. Piston velocity $0{\cdot}293 \times 10^6$ cm/sec. —■—■—, density ratio; —○—○—, temperature ratio; —□—□—, kinetic pressure ratio; —●—●—, total temperature ratio.

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