Problems with a direct simulation Monte Carlo method applied to the shock structure in a binary gas mixture

B. SCHMIDT and M. WÖRNER (KARLSRUHE)

IT HAS BEEN found that the direct simulation Monte Carlo method as developed by G. A. Bird gives results independent of the number of molecules per cell for the shock structure in binary gas mixtures if the number of molecules per cell is sufficiently large. Up to a certain number, separation of the components, shock thickness and the temperature relaxation downstream of the shock are dependent on the number of molecules per cell. Two facts are responsible for the observed distortions of the computed results: the calculation procedure for the molecule collisions and the small perturbation propagation speed across a simulation cell.

Stwierdzono, że zastosowanie bezpośredniej metody symulacyjnej Monte Carlo opracowanej przez G. A. Birda prowadzi w dwuskładnikowych mieszaninach gazowych do wyników niezależnych od liczby cząsteczek w komórce, jeśli tylko liczba ta jest dostatecznie wielka. Do pewnej granicy rozdział składników, grubość fali uderzeniowej i relaksacja temperatury wzdłuż strumienia zależą od liczby cząsteczek w komórce. Zaobserwowane zniekształcenia wyników obliczeń wynikają z dwóch przyczyn: z procedury obliczeniowej dotyczącej zderzeń cząsteczek i z małej prędkości propagacji zaburzeń wewnątrz komórki symulacyjnej.

Констатировано, что применение непосредственного имитационного метода Монте-Карло, разработанного Г. А. Бирдом, приводит в двухкомпонентных газовых смесях к результатам независящим от числа молекул в ячейке, если только это число достаточно велико. До некоторого предела разделение компонентов, толщина ударной волны и релаксация температуры вдоль потока зависят от числа молекул в ячейке. Наблюдаемые искажения результатов расчетов вытекают из двух причин: из расчетной процедуры, касающейся столкновений молекул и пз малой скорости распространения возмущений внутри имитационной ячейки.

1. Introduction

SEVERAL forms of direct simulation Monte Carlo methods are in use ([1] to [4]). The differences among the methods are mainly in the calculation procedure for the collisions between the model molecules. It is of crucial importance that the simulation of the collision process be done in a proper way. The result is very much influenced by the collision procedure.

In applying BIRD's method [1, 5] to the shock structure in a binary mixture of inert noble gases, it was found that under certain conditions the temperatures of the components do not relax to the common equilibrium value (Rankine Hugoniot value) downstream of the shock wave. This has been observed especially when the number of molecules per cell of the simulation procedure was small. The reason seems to be a distorted statistical balance in connection with the collision calculation procedure. An attempt has been made to explain this phenomenon by describing the simulation method used.

2. The numerical simulation method

For the calculation of the one-dimensional shock structure the field in front of the shock generating piston (see Fig. 1) is divided into a sufficient number of cells. The size of each cell, in this case its length in the x-direction, should be about one mean free path $\overline{\lambda}_1$ at the beginning of the calculation. State "1" is the undisturbed condition ahead of the shock wave. The calculation starts by putting an equal number of molecules of each component in each cell. It is impractical to fill the cells according to the mixture ratio with such a number of molecules that the component in minority 'is well represented. In general the number of molecules per cell would become too large and computer problems would follow. The storage capacity would be exhausted soon and the demand in computing time would be excessive. Bird [1, 5] circumvented this problem by putting at the beginning of the simulation an equal number of molecules of each component into each
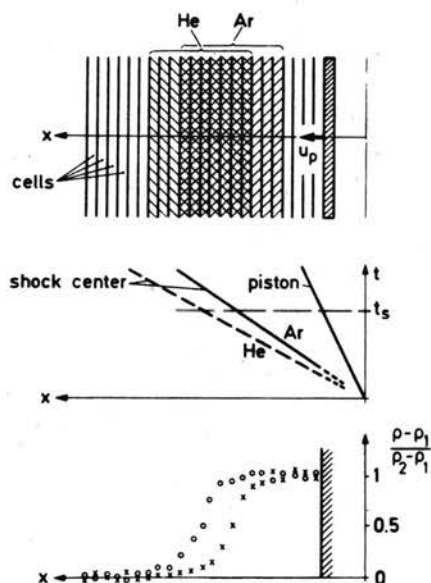

Fig. 1. Arrangement of piston, cells and generated shock; time-distance plot and raw density data.

cell and represented the mixture by a weighting factor W that is simply the mixture ratio. By a random number guided acceptance-rejection selection procedure, the individual molecule velocity is assumed to obey, in the average, an equilibrium distribution according to the undisturbed conditions ahead of the shock wave. The piston and left border reflect the molecules specularly. Then the piston is suddenly set in motion with a speed corresponding to the shock Mach number of the shock to be generated. The time is advanced in small increments Δt_m, where Δt_m is a fraction of the mean free path $\overline{\lambda}_1$ divided by the shock wave speed u_s. Molecule movement and collision process are uncoupled. When the molecules move in Δt_m according to their individual velocity, no collisions are calculated and vice versa.

Of the four possible types of colliding molecule pairs in a binary mixture, the cross-collisions are selected by a probability procedure influenced by the weighting factor. The post-collision velocities are calculated by using the well-known relations. Each collision calculation executed advances the time counter for this type of collision by the collision time Δt_c. The selection and calculation of collisions is stopped as soon as the sum of all Δt_c reaches Δt_m. The collision time Δt_c is inversely proportional to the square of the number of molecules per cell. Therefore a small N means a relatively large Δt_c and a small number of collisions calculated is the result.

All collisions selected are calculated. But whereas the minority component molecules change their velocity at cross-collisions with every cross-collision calculated, only every W-th cross-collision is effective in the average for the majority component molecules. If N is small, it can happen that over one or more time increments Δt_m no cross-collision is effective for the majority component. The final result may not be balanced statistically and numerically-caused nonequilibrium effects are observed downstream of the shock wave.

A second effect, connected with a small number of molecules per cell, N, is that a disturbance propagates faster if N is small. This can be explained by the probability dependent choice of collision pairs in a cell. If N is large, most randomly selected collisions are between molecules that are much less apart than the cell width. The lower N is chosen, the more collisions are selected between molecules that are close to the opposite boundaries of the cell. Disturbances are propagated by collisions and therefore it is more likely that a signal crosses a cell within few collisions and therefore faster if N is small. This effect explains the broadening of the shock wave if N becomes small.

The procedure of separated calculation of molecule movement and of collisions is repeated until the shock wave has formed and has become separated from the piston. The run ends with the sampling of the different moments to calculate the macroscopic quantities: density, bulk velocity and temperature. Depending on N, 10 to 100 runs are needed for a reasonable low scatter of the data.

3. Results

To find out what number of molecules per cell, N, is needed to generate results independent of N, a number of runs have been started with different numbers of molecules per cell, N, different He-Ar mixtures and for three shock strengths, $M_s = 2$, 3.5 and 6. N has been varied from 4 up to 160 molecules per cell and component. The result is more or less the same for all three shock Mach numbers M_s. Above a certain N the results become less and less dependent on the number of molecules per cell. Figure 2 shows this for the shock thickness Δ taken between 10% and 90% of $(\varrho - \varrho_1)/(\varrho_2 - \varrho_1)$, and the separation s between the two shock profiles of the components at $(\varrho - \varrho_1)/(\varrho_2 - \varrho_1) = 0.5$. "1" is the equilibrium condition upstream, "2" the equilibrium condition downstream of the shock wave. For a 90% Ar–10% He mixture, $M_s = 3.5$, thickness Δ and separation s become almost independent of N for values of N greater than 20 to 40 molecules per cell.
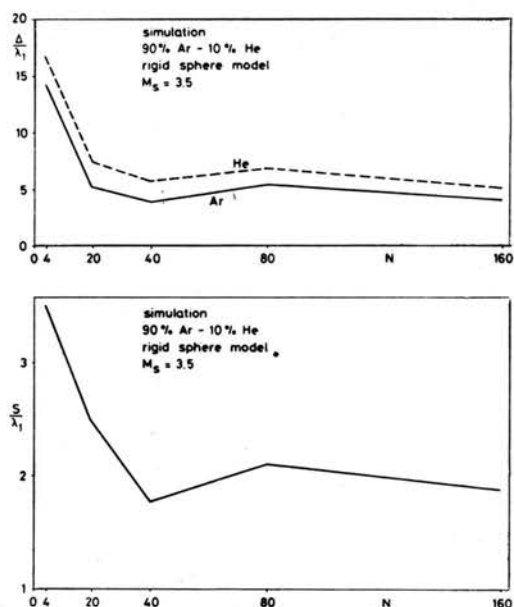
FIG. 2. Shock thickness Δ and separation s as plotted against the number of molecules per cell N for an 90% Ar — 10% He mixture.

The more sensitive quantity is the temperature. Figure 3 shows the temperature profiles of the components He and Ar for a $M_s = 3.5$, shock wave in a 90%Ar–10% He mixture. For $N = 4$ molecules per cell the temperature of helium does not relax to its equilibrium value $(T-T_1)/(T_2-T_1) = 1$. For $N = 160$ molecules per cell it relaxes to equilibrium. Further, the profiles for $N = 160$ are steeper than those for $N = 4$. This is obvious for the density profiles, too (see Fig. 4). Less obvious is that the separation s between the components is smaller for $N = 160$ than for $N = 4$.
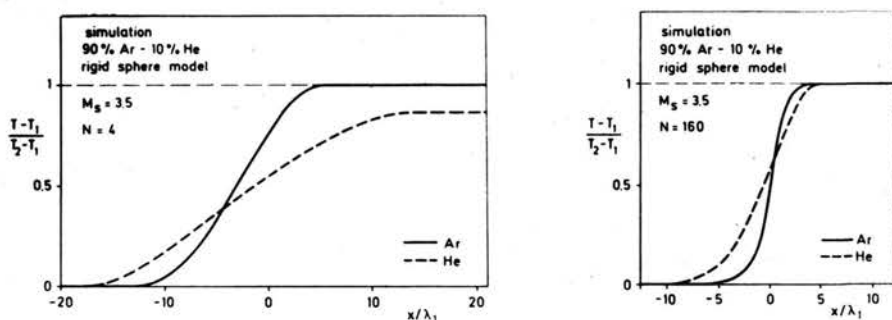

FIG. 3. Shock temperature profiles under variation of the number of molecules per cell N.

Figure 2 shows that 20 to 40 molecules per cell are sufficient to generate molecules per cell independent separations s and thicknessess Δ. The picture is quite different for the more sensitive temperature. As Fig. 5 shows, for the temperatures T_{Ar} and T_{He} downstream of the shock wave, the influence of N is present almost up to $N = 80$ molecules
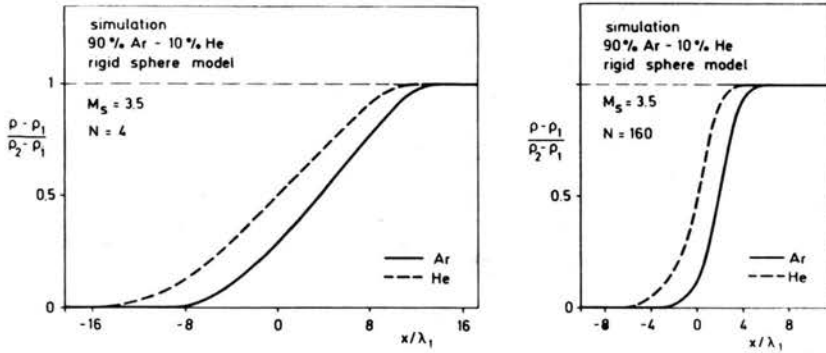
FIG. 4. Shock density profiles under variation of the number of molecules per cell N.
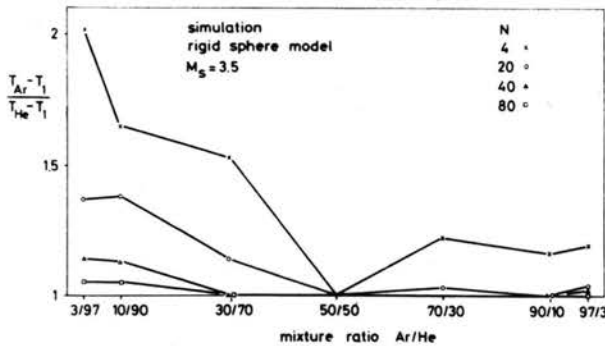

FIG. 5. Ratio of the final temperature of argon and helium down-stream of the shock as function of the mixture ratio and the number of molecule per cell N.

per cell. $N = 20$ is by far not sufficient for relaxation to equilibrium downstream of the shock wave. An exception is the mixture with equal parts of the components, 50% Ar –50% He. Here the weighting factor is equal to one and the number of collisions between the components and within the components is balanced.

The question is now: how accurate are the computed N-independent results of the direct simulation Monte Carlo method as developed by BIRD [1], especially for gas mixtures? A definite answer can be given only by comparison with experimental results. These are difficult to produce and are available in limited number. ROTHE [6] gives some experimental results for very strong shock waves whereas CENTER [7] and HARNETT and MUNTZ [8] give results for weak shock waves ($M_s \approx 2$).

4. Comparison with experimental results

Only a very limited number of experimental data can be compared accurately with calculated simulation results. Most papers lack the necessary basic data of the experiments to calculate the mean free path length ahead of the shock wave or an equivalent to normalize the length scale. The publication of CENTER [7] contains all information

necessary for a comparison. Figure 6 shows the result for a He/Ar mixture with 48% argon. The agreement between simulation and experiment is good except for the end of the shock on the high density side. Center attributes the failure of his data to come up to the theoretical value for this particular Mach number ($M = 2.24$) to shock curvature and radial diffusion in front of the shock holder. The comparison of calculated data with Center's results for 2.2% argon in the He-Ar mixture has not been possible thus far because the data are still being processed in the computer. We are anxious to see how good the agreement is for the other experimental data of Center.
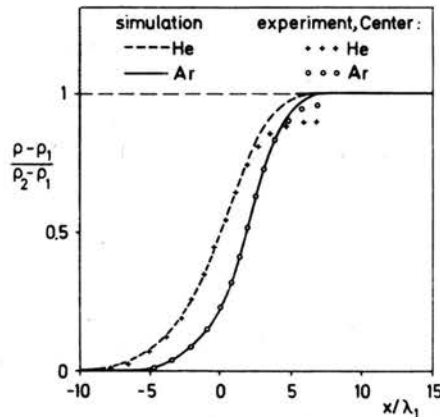

Fig. 6. Comparison of calculated and experimental data for a $M = 2.24$ shock wave in a 48% Ar — 52% He mixture. Simulation: $N = 160$ molecules per cell, mean free path λ_1; [1] page 71; experiment: $\lambda_1 = 0.648$ mm.

5. Conclusions

On the basis of the shock thickness and the component separation in the shock, it is evident that the number of molecules per cell (N) has, up to a certain limit, a certain influence on the calculated shock profiles. This has been found true in the shock Mach number range $2 \leqslant M_s \leqslant 6$ and for binary Ar-He mixtures from 3% up to 97% argon. Sufficient are 80 to 160 molecules per cell.

A comparison of some calculated results with experimental data for a weak shock wave shows very good agreement between the results. It has to be seen if this good agreement holds for other experimental data, too.

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INSTITUT FÜR STRÖMUNGSLEHRE UND STRÖMUNGSMASCHINEN
UNIVERSITÄT KARLSRUHE, BRD.