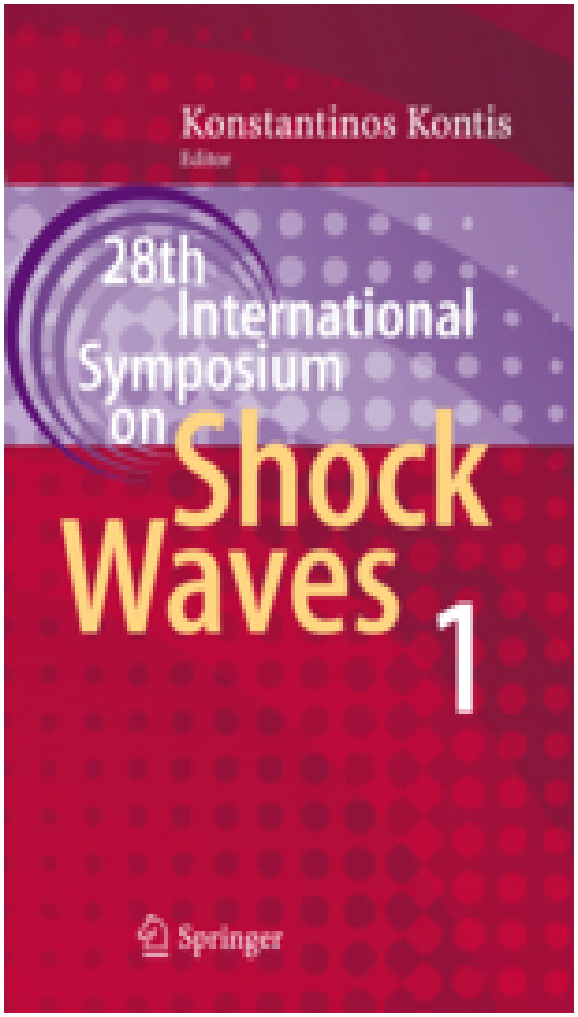
Konstantinos Kontis
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Structure of shock waves in dense media

Z.A. Walenta and A. Slowicka

1 Introduction

The behaviour of shock waves propagating in a gas has been studied for more than a century, experimentally, theoretically and numerically. It was established, in particular, that the thickness of a shock wave (the layer, in which parameters of the medium vary rapidly in space) is of the order of several mean free paths of the gas molecules, provided that the shock is of moderate intensity. Distributions of the parameters of the medium inside the shock resemble the hyperbolic tangent function. The necessary condition for the above to be fulfilled is that the gas is dilute, which means that its molecules interact (collide) with only one neighbour at a time, and between collisions they move with constant speed along straight lines (concept of a mean free path – the average distance travelled this way). Duration of a single collision is negligibly short as compared to the time of free flight (mean free time). In dilute gas the mean free path of the molecules is much larger than the diameter of the molecule and larger than their average separation distance (Figure1 – left).

Shock waves may also be generated in dense media: dense gases, liquids and solids. Under ”dense medium” we understand medium consisting of molecules so closely packed, that the average distance between the closest neighbours is of the same order of magnitude as the distance characteristic for the intermolecular forces. A simplified model of a dense medium consists of hard sphere molecules of finite size, interacting with each other during collisions only. The gaps between neighbouring molecules in such medium are smaller, or at most equal to the diameter of a molecule (Figure1 – right).

In such simplified, dense medium the mean free path can be defined too, however the molecules may collide with the closest neighbours only. The speed of transfer of momentum and energy in such a medium is, in average, approximately equal to the ratio of the sum of the mean free path and the diameter of the molecule to the

Institute of Fundamental Technological Research
Pawinskiego 5b 02-106 Warszawa, Poland

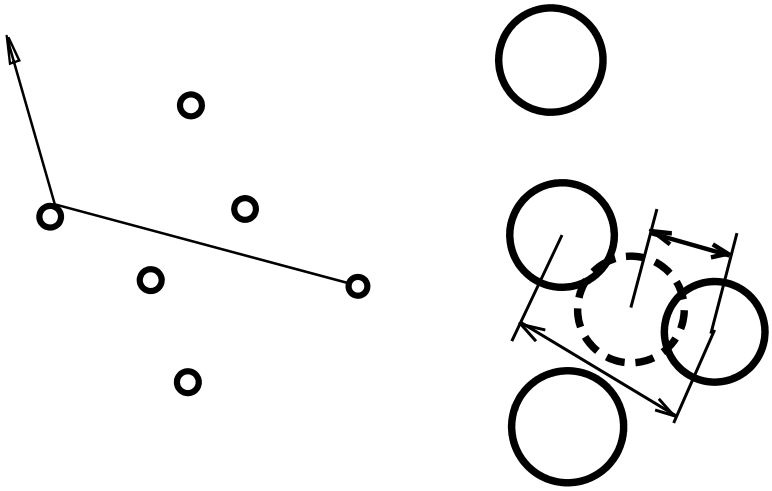

Fig. 1 Left: dilute gas – mean free path larger than average distance between molecules. Right: dense medium – gaps between neighbouring molecules (hard spheres) smaller than diameter of a molecule – collisions occur between closest neighbours only.

mean time between collisions. In fact, the same applies also to dilute gases, however the diameter of the molecule is there negligibly small as compared to the mean free path. The sum of the mean free path and the molecular diameter may therefore be considered as the length scale characteristic for the momentum and energy transfer. As can be seen from Figure1 – right, this sum is very close to the average distance between the centres of the neighbouring molecules (the ”mean molecular distance”). This, in turn, is close to the inverse of the cubic root of the number density of the molecules of the medium. The parameter defined in this way was introduced for the first time by Bridgman in 1923 [1] The last definition is particularly useful if more realistic molecular models are employed (e.g. molecules interacting with Lennard-Jones potential). The molecules of a dense medium are then in permanent contact through the long-range forces and no mean free path can be defined. It will be demonstrated, that the thickness of the shock wave in dense gas (Argon), related to the cubic root of the number density is of the same order of magnitude as that in dilute gas related to mean free path and that this thickness gradually decreases with increasing density. This is contrary to the results of the earlier investigators (Montanero et al. 1999 [2], Schlamp et al. 2007 [3]), who related the shock thickness to the mean free path in the whole range of densities.

2 Flow arrangement – details of simulation and experiment

2.1 Molecular Dynamics – general description of the procedure

All Molecular Dynamics computations reported here were performed with the program MOLDY [4]. This program has originally been designed for stationary configurations of the molecules, however it is easy to supplement with additional procedures for calculating the behaviour of the flowing medium. To produce the flow we place the molecules regularly in space give them random velocities according to the Maxwellian distribution for the required temperature and wait until the system equilibrates. During the equilibration period we perform velocity scaling in order to suppress the unwanted temperature rise (which would occur because the molecules had initially higher potential energy than in equilibrium). When the system is in equilibrium we make the medium move adding the macroscopic velocity V to the x – component of the thermal velocity of each molecule. At the same time we insert the impermeable, reflecting planes into the flow, which generate the shock and rarefaction waves. The number of Argon atoms taken for each simulation run was equal to 125000. The time step was assumed equal to 0.001 of a picosecond, the equilibration period was 10000 time steps long (10 picoseconds). The subsequent actual simulation of the flow was stopped when the produced shock and rarefaction waves met disturbing each other.

2.2 Physical conditions for the simulated flow

In the present research we simulate the flow of Argon at initial temperature T = 300 K and initial velocities: V = 404.8 m/s, 607.2 m/s and 809.6 m/s For the case of dense medium we take three values of the initial density ρ, as specified below. The corresponding values of the mean molecular distance λ are also given: 1) $\rho = 1000kg/m^3$, $\lambda = 4.048A$; 2) $\rho = 307.09kg/m^3$, $\lambda = 6.0A$;
3) $\rho = 125.55kg/m^3$, $\lambda = 8.0A$. Argon atoms have no electric charge and interact with each other only with the Lennard-Jones interaction potential.

2.3 Direct Simulation Monte-Carlo

The flow configuration used for DSMC calculations was identical with that of Molecular Dynamics. Here it was not necessary to go through equilibration process before the actual simulation. The program used was a modification of that by Bird [5] and the sampling procedure for collisions was due to Yanitskiy [6]. The computation domain was split into cells of linear dimension equal to 0.25 of the

mean free path in the region in front of the shock. The total number of molecules in the computation domain was 24 million.

2.4 Experiment

The measurements of the shock wave structure (density) were performed in the low density shock tube at the Institute of Fundamental Technological Research in Warsaw. The tube, was 250 mm in diameter, which made it possible to make experiments at initial densities corresponding to mean free paths up to a couple of millimeters. The initial pressure of the test gas (Argon) in the experiments was about 7.5 Pa, the initial temperature about 300 K, which corresponded to mean free paths about 0.95 mm and the shock thicknesses about 4 mm. Under such conditions it was possible to measure the gas density in the shock with the standard electron beam attenuation technique [7].

3 Results

3.1 Plane, perpendicular shock wave in Argon

In Figure2 – left the diagrams of density distributions inside the shock wave, calculated for the three initial gas densities and the initial velocity V = 404.8 m/s are shown superimposed upon one another.

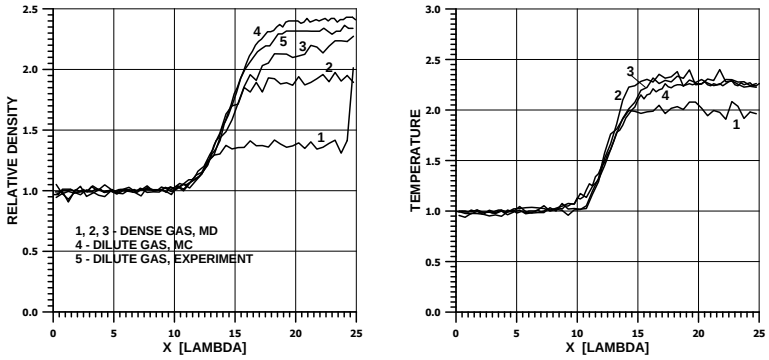

Fig. 2 Left: density distributions, right: temperature distributions inside the shock wave for the initial velocity V = 404.8 m/s

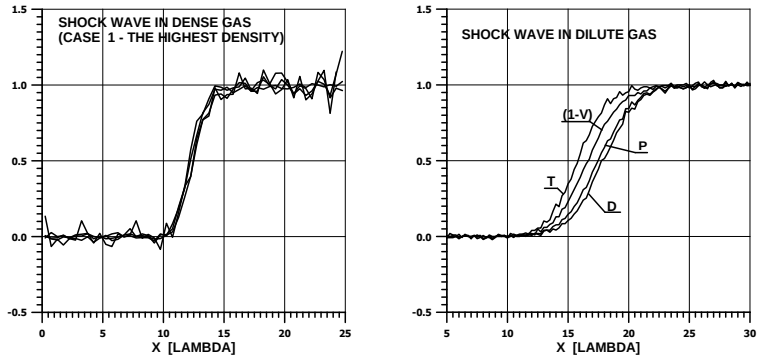

Fig. 3 Left: normalized diagrams of density, pressure, macroscopic velocity and temperature for the highest density. Right: normalized diagrams of density, pressure, macroscopic velocity and temperature for the dilute gas.

The density distributions inside the shock in a dilute gas, taken from DSMC calculations and from experiment, are shown there too. The unit length on the X – axis of this figure is equal to the ”mean molecular distance” (as defined above) for the dense gas and to the mean free path for the dilute gas. From these diagrams it is evident, that the ”mean molecular distance” plays really the same role for dense gases as the mean free path for dilute. It is also worth noting, that the front parts of all presented diagrams are practically identical. The differences can be seen in the rear parts: the higher the initial density, the lower the density ratio across the shock. As a result – in more dense gas the shock wave is relatively thinner. Figure2 – right shows in a similar fashion the temperature distributions. The temperature jumps (temperature ratios) are equally high for all considered cases (including M – C result for a dilute gas) with the exception of the highest gas density. In this case the temperature jump is lower, which is probably due to the fact, that relatively large part of the internal energy is stored in the mutual interactions of the molecules. Figure3 – left presents normalized diagrams of density, pressure, macroscopic velocity and temperature inside the shock wave for the highest density considered. The four curves can hardly be distinguished, which is different from the case of a dilute gas, where the curves are distinctly shifted with respect to each other, as shown in Figure3 – right.

4 Conclusion

The presented results for Argon seem to support the validity of the mean molecular distance” as the proper length scale for the structure of the shock wave in dense

media. The shock thickness under rarefied conditions, related to mean free path and for dense medium, related to the mean molecular distance are close to each other. Moreover – the relative thickness of the shock wave defined above decreeses smoothly when density increases from low to high values.

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