

The last of these formulae is particularly important because it defines all the possible P_1^* , V_1^* points which can be reached in a single shock compression from the initial conditions P^* , V^* . This follows from the fact that $E_1^* - E^*$ is related to P_1^* , V_1^* by the LJD equation of state as well as by the Rankine-Hugoniot relation. It is therefore possible to eliminate $E_1^* - E^*$ and obtain a specific relationship between P_1^* and V_1^* provided that P^* and V^* are specified. The locus of points obtained in this way will be referred to as a "Hugoniot" compression curve, and P^* , V^* will be called the "starting point".

(b) *Single Shock Compression of a Classical Liquid from $P^* \approx 0$*

We shall consider first a set of starting points corresponding to an LJD liquid which is either at atmospheric pressure or under its own vapour pressure. In these circumstances P^* is very small and can be considered to be zero. The LJD theory then gives a unique relationship, which we have already derived (David and Hamann 1961), between V^* and the reduced temperature T^* .

We can trace the Hugoniot curve from any particular starting point in the following way. We first suppose the fluid to be compressed isothermally from V^* to a smaller volume V_1^* . This generally raises its internal energy, although not sufficiently to satisfy equation (6). We then imagine the fluid to be heated at constant volume until it reaches a temperature T_1^* at which the LJD energy *does* equal the Hugoniot energy. This point (P_1^* , V_1^* , T_1^*) must lie on the Hugoniot curve starting at ($P^*=0$, V^* , T^*). By repeating the operation for a range of final volumes we can find the general form of the Hugoniot curve.

In principle the calculations can be performed automatically on a computer, but in our work we have used the existing LJD compilations of Wentorf *et al.* (1950), together with suitable interpolation formulae.† We have calculated Hugoniot curves from seven starting temperatures in the range $T^*=0.7$ to 1.0 , and, for comparison, worked out the corresponding isothermal and adiabatic compression curves from the same starting points. We have also estimated some of the thermodynamic properties of the fluid along the Hugoniot curve, again by interpolation in the tables of Wentorf *et al.* (1950).

(c) *Shock Compression of a Quantal Liquid from $P^* \approx 0$*

Lennard-Jones and Devonshire's theory is based on classical statistical mechanics, which are known to be inadequate for light liquids such as helium, hydrogen, and neon. For these it is necessary to use a more general equation of state involving de Boer's (1948) quantal parameter Λ^* . In earlier papers (Hamann 1952, 1957; David and Hamann 1953) we have derived an equation of this kind by applying a quantum correction to the classical theory. We have now used this equation to compute a single Hugoniot curve for a quantal liquid ($\Lambda^*=1$) starting from $P^*=0$, $T^*=0.75$.

† Dr. W. Fickett and Dr. W. W. Wood of the Los Alamos Scientific Laboratory have recently confirmed our results for liquid argon (Fig. 2) by automatic calculations on the IBM 704 computer (personal communication).

(d) Conditions after Adiabatic Expansion from a Shocked State

After the passage of a shock wave through a material the substance expands into its surroundings. This expansion occurs adiabatically because shock waves of rarefaction are forbidden by thermodynamics (Hirschfelder, Curtiss, and Bird 1954, p. 789). We can therefore follow the course of the expansion of a shocked LJD fluid by tracing points of constant entropy starting from a Hugoniot point $(P_1^*, V_1^*, T_1^*, S_1^*)$ and moving to a series of points of lower pressure and larger volume $(P_2^*, V_2^*, T_2^*, S_2^*=S_1^*)$. In this way we have traced adiabats from several points on the Hugoniot based on the starting point $P^*=0, T^*=0.75$.

For reasons to be discussed in the next paragraph, it is sometimes important to know the contribution which the expansion makes to the forward flow velocity of the material. This is given by the Riemann integral

$$w_2^* = \int_{P_1^*}^{P_2^*} \left(-\frac{\partial V^*}{\partial P^*} \right)_{S^*} dP^*, \quad (7)$$

where the integration is carried out along the expansion adiabat (see, for instance, Rice, McQueen, and Walsh 1958). The total flow velocity in the direction of the original shock is then $w_1^* + w_2^*$. In evaluating (7) we have found it convenient to fit the adiabat to an empirical equation of the form used by Tait (1900), and then perform the integration numerically by means of Simpson's rule.

If the material expands into a vacuum, then the final pressure is zero and the corresponding value of $w_1^* + w_2^*$ is the velocity, in molecular units, of the free surface of the material after shock acceleration. If on the other hand the material expands into another substance, say air, it generates a shock wave in the second substance and the boundary conditions require that the absolute pressure P_2 and velocity $w_1 + w_2$ at the interface must lie on the pressure/flow-velocity curve for the second material. If this Hugoniot relation is known, as it is for ideal gases, then the interfacial conditions can be worked out. These conditions are important because they determine whether or not the original material will vaporize after the passage of a shock wave. In the present calculations we have considered the expansion of a shocked LJD fluid into air, which we have assumed to obey the ideal gas relationship

$$w_1 = (P_1 - P) \left(\frac{5\hat{V}}{P + 6P_1} \right)^{\frac{1}{2}}. \quad (8)$$

(e) Conditions at the Head-on Collision of Two Plane Shocks

It is worthwhile to consider the conditions which exist after the head-on collision of two plane shock waves in an LJD fluid. We shall designate these conditions by the subscript 2, and the conditions in one of the initial shocks by the subscript 1. The Rankine-Hugoniot relations (4)–(6) can then be rewritten

$$U_2^* = -V_1^* [(P_2^* - P_1^*) / (V_1^* - V_2^*)]^{\frac{1}{2}}, \quad (9)$$

$$w_2^* = -[(P_2^* - P_1^*)(V_1^* - V_2^*)]^{\frac{1}{2}}, \quad (10)$$

$$E_2^* - E_1^* = \frac{1}{2}(P_2^* + P_1^*)(V_1^* - V_2^*), \quad (11)$$