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AN ANALYSIS OF THE POSSIBILITY OF THE ISENTROPIC COMPRESSION OF HYDROGEN WITH A REAL EQUATION OF STATE†

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The possibility of the isentropic compression of hydrogen with a real equation of state up to high values of the density at which an anomaly, associated with the transition of hydrogen from the molecular phase to the atomic phase, is observed in the behaviour of the isentrope, is investigated. The possibility of penetrating the above-mentioned part of the change in the density during the compression of the gas in a shock-free manner is analysed. The problem is not about obtaining very high degrees of compression, which greatly exceed the value of the density in the anomalous range; when necessary, it is also assumed that density values which are less than, but close, to the anomalous range have already been obtained by a preliminary shock-free compression. It is shown that, in the case of the shock-free compression of plane, cylindrical and spherical layers of a uniform gas, which is initially at rest, an infinite density gradient of the gas arises in the flow before the final instant of compression if the density has reached values in the anomalous range. Self-similar solutions which describe the shock-free compression of initially uniform cylindrical and spherical volumes of hydrogen at rest are investigated. It is shown, using a numerical solution of the corresponding systems of ordinary differential equations, that isentropic compression up to density values both in the anomalous range and even higher is possible in this case. A unified approach to the mathematical investigation of the shock-free, strong compression of a gas was proposed in [1]. In particular, an analogue of a centred Riemann wave, which is continuously adjacent to the quiescent, uniform gas, is constructed for a gas with an arbitrary equation of state. The possibility of the shock-free compression of a gas with an arbitrary equation of state up to a certain density, which is greater than the initial density, is thereby proved. The form of the equation of state of the gas has to be specified for a more detailed description of the process of isentropic compression. The strong compression of hydrogen with a real equation of state, which is determined in appropriate physical experiments, is of the greatest interest in solving the problem of controlled thermonuclear synthesis [2].

It has been established experimentally [3] that, during the isentropic compression of hydrogen up to very high densities in the range $0.9\ \mathrm{g/cm^3} < \rho < 1.25\ \mathrm{g/cm^3}$, the rate of increase of the pressure from 260 to 380 GPa changes substantially (Fig. 1) and that this is associated [3] with the transition of hydrogen from the molecular state to the atomic state.

The aim of this paper is to investigate mathematically the possibility of the shock-free compression of hydrogen with an indicated isentrope up to density values in the anomalous range and higher.

In order to obtain the relation $c^2 = c^2(\rho)$ (here c is the speed of sound and $c^2 = p'(\rho)$), numerical and graphical differentiation of the relation $p = p(\rho)$ being considered was carried out and a certain averaged curve was taken as $c^2(\rho)$. After this, a change was made to dimensionless variables, with a choice of the density scale of 0.5 g/cm^3 and of the speed of sound scale of 16 km/s. The pressure scale is not specified and the previous notation is retained for the dimensionless variables.

A graph of $c^2 = c^2(\rho)$ in dimensionless variables is shown in Fig. 2. In this case, the establishment of the relation $p(\rho)$ by integrating the function $c^2(\rho)$ gives a good result both on the whole as well as in the most interesting range of variation of the dimensionless density $1.8 < \rho < 2.5$. The relative error does not exceed 0.5%. It is subsequently assumed that $c(\rho)$ is an analytic function when $\rho > 0$.

When $1.80 < \rho < 2.16$, the second derivative $p''(\rho)$ is negative and, therefore, the medium being considered when $1.80 < \rho < 2.16$, according to Ovsyannikov's terminology (the O terminology), is not a normal gas.

According to Rozhdestvenskii's and Yanenko's terminology [5] (the R–Ya terminology), a gas is normal if $p_{VV} > 0$ and is not normal if $p_{VV} < 0$ ($V = 1/\rho > 0$ is the specific volume). Since [4]

$$V^3/p_{VV} = 2p_\rho + \rho p_{\rho\rho}$$

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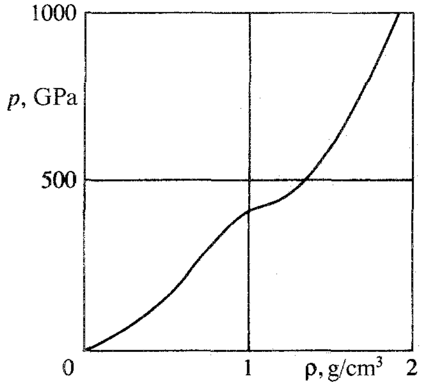

Fig. 1

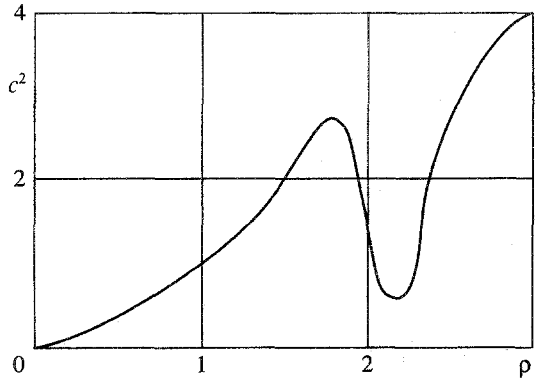

Fig. 2

a gas which is normal according to the O terminology is also normal according to the R–Ya terminology. However, equations of state are possible when a gas which is normal according to the R–Ya terminology is not normal according to the O terminology.

It follows from the last equality that the sign of the derivative p_{VV} is identical to the sign of the expression

$$2p_\rho + \rho p_{\rho\rho} = 2\rho c(\rho)\alpha(\rho), \quad \alpha(\rho) = c(\rho) = c(\rho)/\rho + c'(\rho)$$

Consequently, when $\rho > 0$, $c(\rho) > 0$, the signs of p_{VV} and $\alpha(\rho)$ are identical. It is well known that, in a centred Riemann wave, the gas flow is recovered using the following formulae (t is the time)

$$\frac{x}{t} = u(\rho) \pm c(\rho); \quad u(\rho) = \pm\int\frac{c(\rho)}{\rho}d\rho \tag{1}$$

Hence, apart from the sign, the expression $\alpha(\rho)$ is a derivative of the function

$$x_1(\rho) = u(\rho) \pm c(\rho) \tag{2}$$

and a change of sign of the derivative p_{VV} is equivalent to the non-monotonicity of the function (2), which specifies the flow in the centred wave. Note that it is necessary to differentiate the function $c(\rho)$ to determine the function $\alpha(\rho)$, and to integrate the fraction $c(\rho)/\rho$ to determine $x_1(\rho)$. Since the initial function $p(\rho)$ is only approximately specified, the second of the above-mentioned operations is carried out more accurately.

A graph of the function $x_1(\rho)$ for the equation of state being considered is shown in Fig. 3 and, to be specific, the upper sign is taken in the formula for the centred wave, that is, the centred compression wave moves from left to right. When recovering the function $u(\rho)$, we put $u(0.44) = 0$.

Hence, according to the R–Ya terminology also, the medium is not a normal gas when $\rho_1 < \rho < \rho_2$, where $\rho_1 \approx 1.84$, $\rho_2 \approx 2.16$.

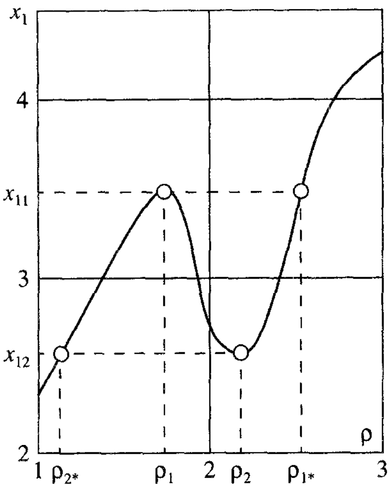

Fig. 3

When $0 \leqslant \rho \leqslant \rho_1$, the centred Riemann wave is uniquely defined using formula (1). Hence, a plane layer of gas which is initially at rest with a density less than ρ_1 can be compressed in a shock-free manner up to a density $\rho = \rho_1$. However, at the instant when the density of the gas on the compressing piston becomes equal to ρ_1, an infinite gradient occurs in the gas flow (actually, on the piston) and the derivative of the density with respect to the spatial variable becomes unbounded.

It is quite difficult not only to describe the flow of the gas being considered after the above-mentioned infinite gradient has occurred but even to predict the flow configuration which occurs after this instant of time. The possible difficulties in this case are illustrated most simply by the example of the compression of a plane layer when the flow is defined by formula (1) and the relation $\rho = \rho(t, x)$ is established using the graph shown in Fig. 3.

Due to the fact that the function $x_1(\rho)$ is non-monotonic for all values of x in the range $x_{12} \leqslant x \leqslant x_{11}$ (see Fig. 3), we can postulate the existence of a non-zero jump in the density ($[\rho] \neq 0$). For example (see Fig. 3)

$$[\rho]_{x = x_{12}} = \rho_2 - \rho_{2*} < 0, \quad [\rho]_{x = x_{11}} = \rho_{1*} - \rho_1 > 0$$

A problem regarding the decay of a discontinuity [4, 5] is then obtained, which holds at any point in the range $[x_{12}, x_{11}]$. It is possible that it is necessary to locate the discontinuity at the point $x = x_{12}$, where the first two-valued property of the relation $\rho = \rho(t, x)|_{t=\text{const}}$ occurs. In order to solve the resulting problem on the decay of a discontinuity, it is not only necessary to know the isentrope $p = p(\rho)$ (Fig. 1) but, also, the general equations of state in the form $p = p(\rho, S)$, $e = e(\rho, S)$ (S is the entropy and e is the internal energy) [4, 5]. If these relations are known for the range of variation of the density and pressure of hydrogen being considered, it is possible that, using previously developed approaches [5–7], the configuration of the flow, which arises after such a discontinuity decays, can be successfully predicted. Both values specifying the density jump (both the pair (ρ_{2*}, ρ_2) and the pair (ρ_1, ρ_{1*}), as well as any pair of values of ρ which corresponds to points x in the range $[x_{12}, x_{11}]$), fall on the part of the curve $c^2(\rho)$ where $[c^2(\rho)]' \geqslant 0$, although they are separated by a region in which $[c^2(\rho)]' < 0$. It can therefore be assumed that the decay of such a discontinuity occurs as in the case of a normal gas, that is, with the formation of a compression shock wave.

Hence, it can be concluded from what has been said above that it is impossible to compress a plane layer of gas in a shock-free manner from a density of less than $\rho = \rho_1$ up to a density greater than $\rho = \rho_1$.

Remarks. 1. The generalized solution of the problem of a centred Riemann wave when the point $(t = 0, r = r_*)$, $r_* > 0$ in the flow is singular has been presented in [1] for the cylindrical and spherically symmetric cases. Here, the leading terms, which described the singularity in the flow in these cases, are identical with the expressions using formulae (1). The shock-free compression from $\rho < \rho_1$ to $\rho > \rho_1$ of cylindrical and spherical layers of the gas being considered, which, at the instant of time $t = 0$, have non-zero internal radii, is therefore also impossible.

2. The function $C^2(\rho)$ can be changed so that the difference in the values of its local extrema is smaller: $\rho_{max} = 2.75$, $\rho_{min} = 2.59$. Then, the function $x_1(\rho)$ becomes monotonic. Consequently, the new gas which has been

obtained is normal according to the R–Ya terminology but will not be normal according to the O terminology. In this case, the shock-free compression of plane, cylindrical and spherical layers of the gas up to anomalous density values is possible.

3. It is also impossible to rule out such a hypothetical situation when, in the case of another flow configuration (for example, when the external action is definitely non-monotonic), the shock-free compression of one-dimensional layers of the initial gas, which is not normal according to the R–Ya terminology, becomes possible.

The possibility of the bounded shock-free compression of cylindrical and spherical uniform volumes of gas at rest, with the equation of state being considered (see Figs 1 and 2), is next investigated. The required flows arise at the instant of time $t = 0$, when the compression waves, which, when $t < 0$, are continuously adjoining the homogeneous state of rest through the acoustic C^--characteristic, converge to the axis or to the centre of symmetry. At the instant of time $t = 0$, the compression wave is not focussed at the point $t = r = 0$ and has a continuous distribution from $r = 0$ up to a certain $r = r_* > 0$. In the case of a polytropic equation of state, the unknown self-similar solutions [8] describe [9–11] the isentropic compression of a gas both up to an infinite value of the density as well as up to any previously specified finite value of the density.

A system of equation of gas dynamics [4] in dimensionless variables, introduced in the standard manner

$$\rho_t + u\rho_r + \rho(u_r + \nu u/r) = 0, \quad u_t + uu_t + c^2(\rho)\rho_r/\rho = 0 \tag{3}$$

is used to describe one-dimensional isentropic flows. The value $\nu = 0, 1, 2$ correspond to the cases of plane, cylindrical and spherical symmetry, $r = (x_1^2 + \ldots + x_{\nu+1}^2)^{1/2}$, x_1, x_2, x_3 are the spatial coordinates, u is the gas velocity and $C^2(\rho)$ is specified by a dependence which is determined by the graph shown in Fig. 2.

A standard change of variables $\xi = t/r$, $\tau = t$ is carried out and one puts $\partial/\partial\tau = 0$ in order to construct self-similar solutions of system (3). As a result, instead of system (3), a system of ordinary differential equations in $\rho = \rho(\xi)$, $u = u(\xi)$ is obtained

$$(1 - \xi u)\rho' - \xi\rho u' = -\nu u, \quad -\xi c^2(\rho)\rho'/\rho + (1 - \xi u)u' = 0 \tag{4}$$

In the case when $\nu = 0$, this system is homogeneous. In order that there should not only be a trivial solution, it is necessary to require that its determinant is equal to zero

$$\Delta \equiv (1 - \xi u)^2 - \xi^2 c^2(\rho) = 0$$

which leads to the following relations

$$(1 - \xi u) = \pm\xi c(\rho), \quad du/d\rho = \pm c(\rho)/\rho, \quad \xi = 1/[u(\rho) \pm c(\rho)]$$

As a result, solution (1) written out above is obtained.

When $\nu = 1$ or 2, system (4) is not homogeneous and can be rewritten in the equivalent form

$$\rho' = -\nu\rho u(1 - \xi u)/\Delta, \quad u' = -\nu\xi c^2(\rho)u/\Delta \tag{5}$$

It is impossible to reduce system (5) to a single equation, as we done in the case of a polytropic gas [8] and the singular points of system (5) are therefore unknown in advance.

The solutions of system (5) can be constructed numerically by specifying the initial values

$$\rho(0) = \rho_{00} > 0, \quad u(0) = u_{00} < 0$$

at the singular point $\xi = 0$ and calculating the integral curves in the direction of decreasing ξ, that is, when $\xi \leqslant 0$.

Graphs of the solutions $\rho = \rho(\xi) \geqslant 0$ and $u = u(\xi) \leqslant 0$ of system (5), constructed when $\nu = 2$ in the range $\xi_0 \leqslant \xi \leqslant 0$ from the initial values $\rho_{00} = 3$, $u_{00} = -1$, are labelled in Fig. 4 with the number *1*. In the case of these solutions when $\xi = \xi_0 \approx -2$, the numerators and denominators of both the right-hand sides of system (5) vanish, $u(\xi_0) = 0$, and the value of $\rho^0 = \rho(\xi_0)$ is such that $C^2(\rho^0) = 1/\xi_0^2$. Consequently,

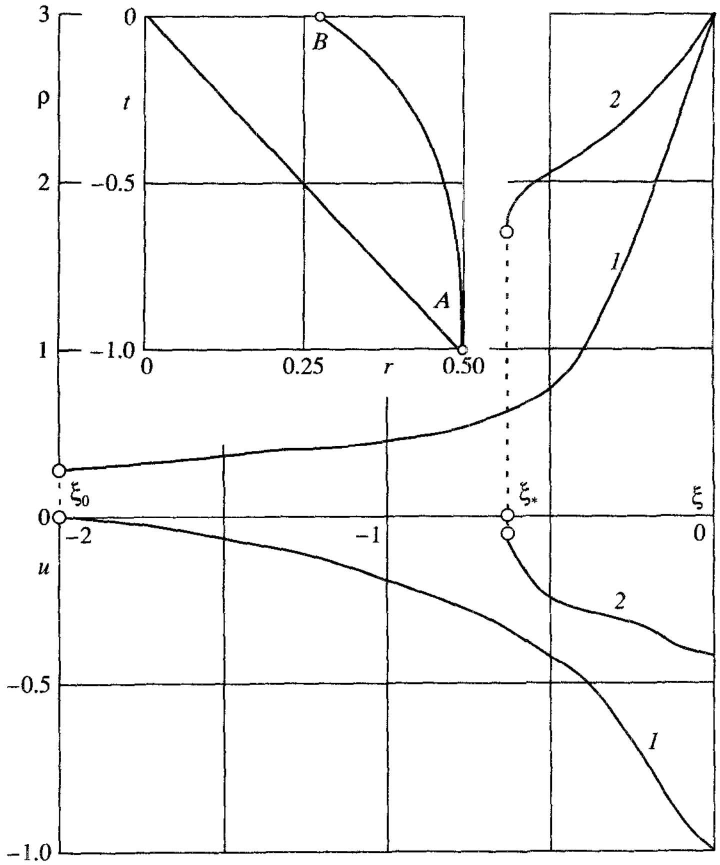

Fig. 4

the line $t/r = \xi_0$ is the acoustic C^--characteristic of the uniform gas at rest with a density $\rho = \rho^0$ and the self-similar compression wave constructed continuously adjoins this uniform state of rest through this characteristic.

The trajectory AB of the motion of the impermeable piston, which creates the self-similar compression wave in the OAB domain, through the characteristic AO, which continuously adjoins the uniform state of rest, is shown in the inset in Fig. 4. In this example, the following values are obtained in the calculations

$$r_A = 0.500751, \quad r_B = 0.261258, \quad \rho_A = 0.4253, \quad \rho_B = 3$$

(r_A, and r_B are the radii of the indicated points and ρ_A, and ρ_B are the values of the densities of the uncompressed and compressed gas, respectively) and the relative difference between the masses of the uncompressed and compressed gas in the example being considered does not exceed 0.2%. This magnitude represents the accuracy of the numerical construction of the self-similar solution of system (3).

The example given above shows that the shock-free compression of a spherical volume of gas with an initial density which is less than the values from the anomalous range of densities up to a density which exceeds the values from the anomalous interval, is possible.

Graphs of the solution of system (5), constructed for $\nu = 2$ with the initial values $\rho_{00} = 3$, $u_{00} = -0.4$, are labelled in Fig. 4 with the number 2. In the case of these solutions when $\xi = \xi_* \approx -0.6$, only the denominators of the two right-hand sides of system (5) vanish and the numerators are non-zero. This fact can be treated as the occurrence of infinite derivatives of ρ_r and u_r with the subsequent formation of shock wave in the gas flow.

Similar phenomena also occur in the case when $\nu = 1$: if the value of u_{00} has a large modulus, shock-free compression is possible. If u_{00} is insufficiently large in modulus, the anomalous density region cannot be successfully traversed isentropically.

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