Journal of Applied Mechanics and Technical Physics, Vol. 36, No. 3, 1995

GAS-DYNAMIC SHOCK WAVES IN A RELAXING GAS

M. A. Rydalevskaya

UDC 533.6

Shock waves in the rarefied gas of anharmonic oscillators are considered. This paper studies the nonequilibrium stationary distributions of molecules in vibrational levels which are realized behind the direct shock wave under various physical conditions.

It is known that the different degrees of freedom of molecules relax at different rates. In many cases, this makes it possible to partition a shock wave into relaxation zones of various thickness [1]. One may assume that some of the degrees of freedom have already relaxed at the boundaries of these zones whereas others remain frozen.

Within this approach, the generalized gas-dynamic consistency conditions take the form [2]

$$\left[\left(\rho\frac{v^2}{2}+e\right)\theta\right]=[p\mathbf{v}\cdot\boldsymbol{\nu}],\quad [\psi_\lambda\theta]=0,\ \lambda=1,\ldots,\Lambda,\quad [\rho\mathbf{v}\theta]=[p]\boldsymbol{\nu}, \tag{1}$$

where $[\alpha]=\alpha^{(+)}-\alpha^{(-)}$; $\alpha^{(-)}$ and $\alpha^{(+)}$ are used to denote the parameter α before the shock wave and at the boundary of the relaxation zone in question behind the shock wave, ρ, $\mathbf{v}$, and e are the density, velocity, and energy of a unit volume of the gas respectively, p is pressure, $\boldsymbol{\nu}$ is a unit normal vector to the strong discontinuity surface, θ is the speed of its propagation, and ψ_λ is the density of macroparameters that is conserved within a selected zone. To describe the gas-dynamic flows, we use the system of determining macroparameters which correspond to the additive invariants of molecular collisions. These invariants have to be taken into account for a distance of the same order as the relaxation zone thickness [3–5].

In the present paper, relations (1) are used to study nonequilibrium regimes of vibrational relaxation of a chemically homogeneous diatomic gas. These regimes may be realized behind the shock waves. For the sake of simplicity, only straight shock waves are considered.

As known, the rotational degrees of freedom of molecules are the first ones among the internal degrees which become excited and then the vibrational ones follow. In addition, the exchange between translational and rotational energy (i.e., *TT*-, *RR*-, and *RT*-exchanges) occur considerably more often than collisions which result in changing the vibrational energy of molecules. This allows us to single out a zone of translational-vibrational relaxation in the shock wave, wherein the vibrational degrees of freedom may be considered frozen [1].

In the case of frozen vibrational degrees of freedom, the state of a gas behind the shock wave has been studied in many works. Figure 1 shows the dependence of the temperature $T^{(+)}$ of the gas behind the shock wave on its temperature $T^{(-)}$ before the shock wave at various velocities $v^{(-)}$ of the gas. The calculations were conducted for oxygen over the range of temperatures $T^{(-)}$ from 500 to 1500 K and velocities $v^{(-)}$ from 500 to 1000 m/sec. The nonrigid oscillating-rotator model has been used for that purpose.

If the temperature of the gas both ahead and behind the shock wave is such that it is possible to take into account only the lowest vibrational levels of molecules, then a harmonic-oscillator model fits very well. In this case, the so-called resonant *VV*-transitions are singled out among those collisions of molecules which lead to the change of vibrational states of molecules. These transitions occur more frequently than *VT*-transitions. This makes it possible to single out a zone of the shock wave wherein *VV*-relaxation takes place parallel with the translational-rotational relaxation, while *VT*-transitions are neglected. In this case, the two-temperature

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St. Petersburg State University, St. Petersburg 199004. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 36, No. 3, pp. 92–97, May–June, 1995. Original article submitted December 10, 1993.

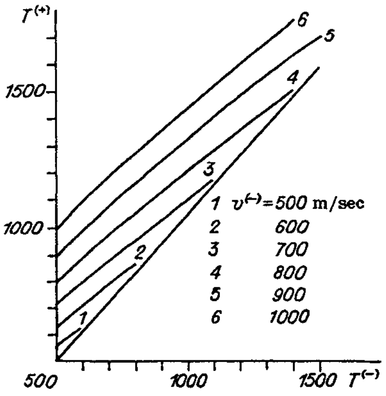

Fig. 1

Boltzmann distribution is reached behind the shock wave. The temperature $T^{(+)}$ of the gas is practically the same as $T^{(+)}$ provided that the vibrational degrees of freedom are frozen. Also, the vibrational temperature $T_V^{(+)}$ coincides with the temperature $T^{(-)}$ of the gas.

When the excitation of higher vibrational levels of the molecules needs to be taken into account, an anharmonic-oscillator model must be used for them. In this case, the vibrational energy of a molecule reckoned from the zeroth level may be written as

$$\varepsilon_v = v\varepsilon_1 - \Delta\varepsilon v(v-1), \qquad \Delta\varepsilon = xh\nu,$$

$$\varepsilon_1 = h\nu(1-2x), \qquad x \ll 1.$$

The anharmonic oscillator model is not equidistant. Thus, it is impossible to state for any vibrational transition that the vibrational energy of the colliding molecules is equal to that of the resulting molecules. The quantity $\Delta\tilde{\varepsilon}_{\mathrm{vibr}} = \varepsilon_{v'} + \varepsilon_{v_1'} - \varepsilon_v - \varepsilon_{v_1}$ is called the defect of vibrational exchange resonance:

$$(v) + (v_1) \rightleftarrows (v') + (v_1').$$

However, even under the above conditions, the processes of vibrational energy relaxation can be separated according to their rates. This makes it possible to single out a zone of partial (rapid) vibrational relaxation at the boundary of which there is a nonequilibrium distribution of molecules among the vibrational levels.

The task of determining the corresponding vibrational populations and choosing a system of determining macroparameters at the boundary of such a zone is an important stage in describing nonequilibrium flows behind the shock waves.

In the case where one may confine oneself to considering the lower vibrational levels, it is possible to single out an area of the shock wave where the translation-rotation TT-, RR-, and RT-exchanges go parallel with quasiresonant single-quantum VV-exchanges in which the total number of quanta of colliding molecules is conserved. It is the total number density of molecules n and the number of quanta accumulated in the system that enter conditions (1) as macroparameters ψ_λ . In this case, the Treanor distribution is reached behind the shock wave [6]. Calculations show that in this case the temperature $T^{(+)}$, when the vibrational degrees of freedom are frozen, coincides with the temperature $T^{(+)}$ behind the shock wave, and the so-called temperature $T_1^{(+)}$ of the first vibrational level coincides with the temperature $T^{(-)}$ of the gas before the shock wave to an accuracy 10^{-3} K.

As known, the Treanor distribution may be employed only at the lower levels, because starting with a certain level v_0, it grows monotonously as the number v increases. This growth contradicts all experimental data known so far. For that reason, populations of higher vibrational levels in the relaxation zones behind the shock wave are usually studied by means of numerical or approximate analytical integration of the system of differential relaxation equations.

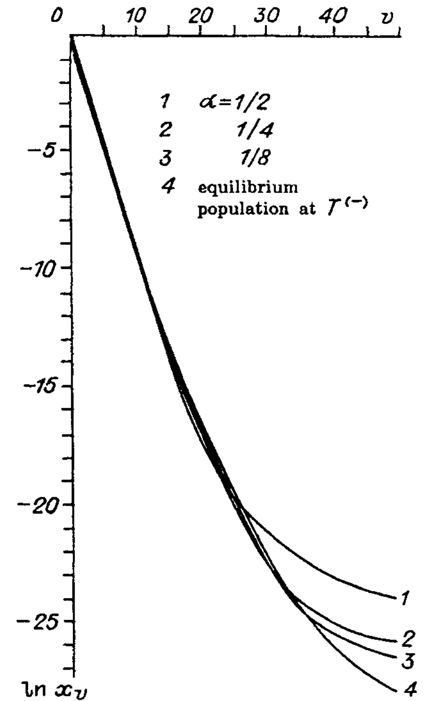

Fig. 2

In the present paper, the populations of the whole vibrational spectrum within the relaxation zones behind the shock waves is studied by singling out the rapid and slow processes in the same way as was done in considering the populations of the lower vibrational levels. Such singling out is based upon the data in [7, 8] according to which it is possible to conclude that the frequency of vibrational transitions of each specific type is first of all determined by the ratio of the corresponding defect of the resonance and vibrational energy of colliding particles.

This makes it reasonable to assume that under certain conditions it is possible to single out a zone of the shock wave in which it is necessary to take into account not only *TT*-, *RR*-, and *RT*-transitions but also such vibrational transitions under which the defect of the resonance $\Delta\tilde{\varepsilon}_{\mathrm{vibr}}$ is not greater than the fraction α $(0 < \alpha < 1)$ of the vibrational energy of colliding particles. In this case, one may assume that the thickness of the zone is of the same order as the product of the reciprocal of the probability of the slowest vibrational exchange during which the defect of the resonance is not greater than the fraction α of the vibrational energy of colliding particles and the mean free path of the molecules. Obviously, the greater α, the thicker the relaxation zone.

A careful study of such vibrational exchanges shows that when $0 < \alpha \leqslant 1/2$, one may associate with them not only the total energy and the unity but also a certain additive invariant $\psi_\alpha(v)\varepsilon_1$ of molecular collisions so that

$$\psi_\alpha(v) = \begin{cases} \psi_\alpha(v_n(\alpha)) + (v - v_n(\alpha))(1 - n\alpha), \\ v \in ([v_n(\alpha),\, v_{n+1}(\alpha)] \cap [0, v^*(\alpha)]), \\ n = 0, 1, \ldots, 1/\alpha, \\ \psi_\alpha(v^*(\alpha)), \quad v \in [v^*(\alpha),\, v_{\max}] \end{cases} \tag{2}$$

when α is small, that is $\alpha \in \left(0, \dfrac{1}{8}\right]$;

$$\psi_\alpha(v) = \begin{cases} v, & v \in [0, \tilde{v}_1(\alpha)], \\ \psi_{\alpha/2}(v) + a(\alpha), & v \in [\tilde{v}_1(\alpha),\, v^*(\alpha)], \\ \psi_{\alpha/2}(v^*(\alpha)) + a(\alpha), & v \in [v^*(\alpha),\, v_{\max}] \end{cases} \tag{3}$$

when $\alpha \in \left(\frac{1}{8}, \frac{1}{4}\right]$, and

$$\psi_\alpha(v) = \begin{cases} v, & v \in [0, \approx{v}_1(\alpha)], \\ \approx{v}_1(\alpha) + (v - \approx{v}_1(\alpha))(1 - \alpha/4), & v \in [\approx{v}_1(\alpha), \approx{v}_2(\alpha)], \\ \psi_{\alpha/4}(v) + a(\alpha) + a(\alpha/2), & v \in [\approx{v}_2(\alpha), v^*(\alpha)], \\ \psi_{\alpha/4}(v^*(\alpha)) + a(\alpha) + a(\alpha/2), & v \in [v^*(\alpha), v_{\max}] \end{cases} \tag{4}$$

when α is relatively large, that is, $\alpha \in \left(\frac{1}{4}, \frac{1}{2}\right]$.
In Eqs. (2)–(4),

$$v_0(\alpha) = 0, \qquad \psi_\alpha(0) = 0, \qquad v_n(\alpha) = \alpha\frac{\varepsilon_1}{2\Delta\varepsilon}\left(n - \frac{1}{2}\right) + 1, \qquad a(\alpha) = \frac{\varepsilon_1}{2\Delta\varepsilon}\frac{\alpha^2}{32},$$

$$\tilde{v}_1(\alpha) = v_1\left(\frac{\alpha}{2}\right) + \frac{2}{\alpha}a(\alpha), \qquad \approx{v}_1(\alpha) = 1 + \frac{11 - 2\sqrt{3}}{32}\frac{\alpha\varepsilon_1}{2\Delta\varepsilon}, \qquad \approx{v}_2(\alpha) = 1 + \frac{10 + 2\sqrt{3}}{32}\frac{\alpha\varepsilon_1}{2\Delta\varepsilon}.$$

The value of $v^*(\alpha)$ is determined from

$$\psi_\alpha(v_{\max}) - \psi_\alpha(v^*) \approx \alpha\psi_\alpha(v^*). \tag{5}$$

When passing through a selected relaxation zone, the following distributions of molecules in the vibrational levels is formed in the gas:

$$n_v = \frac{n}{\tilde{z}_{\text{vibr}}(T, T_1)} z_{\text{rot}}^{(v)}(T) \exp\left\{ -\frac{\psi_\alpha(v)\varepsilon_1}{kT_1} + \frac{\psi_\alpha(v)\varepsilon_1 - \varepsilon_v}{kT} \right\}, \tag{6}$$

where

$$\tilde{z}_{\text{vibr}}(T, T_1) = \sum_v z_{\text{rot}}^{(v)}(T) \exp\left\{ -\frac{\psi_\alpha(v)\varepsilon_1}{kT_1} + \frac{\psi_\alpha(v)\varepsilon_1 - \varepsilon_v}{kT} \right\};$$

T_1 is the temperature of the first vibrational level (as in the Treanor distribution), and $z_{\text{rot}}^{(v)}(T)$ is the rotational statistical sum (the relation between rotations and vibrations of molecules is taken into account here).

In this case, conditions (1), written in a symmetric form for the direct shock wave, will read

$$n^{(+)}v^{(+)} = n^{(-)}v^{(-)}, \qquad \overline{\psi}_\alpha^{(+)} = \overline{\psi}_\alpha^{(-)},$$

$$\frac{v^{(+)2}}{2} + \frac{5}{2}\frac{kT^{(+)}}{m} + \frac{e_{\text{rot-vibr}}^{(+)}}{m} = \frac{v^{(-)2}}{2} + \frac{5}{2}\frac{kT^{(-)}}{m} + \frac{e_{\text{rot-vibr}}^{(-)}}{m},$$

$$mn^{(+)}v^{(+)2} + n^{(+)}kT^{(+)} = mn^{(-)}v^{(-)2} + n^{(-)}kT^{(-)},$$

where the pressure $p = nkT$; $e_{\text{rot-vibr}}$ and $\overline{\psi}_\alpha$ are mean values of the invariant $\psi_\alpha(v)$ and vibrational-rotational energy per molecule.

Calculations have shown that in the case of frozen vibrational degrees of freedom, the temperature of the gas coincides with the temperature $T^{(+)}$ to an accuracy 10^{-3} K when $\alpha \in (0, 1/8]$ or to within several K when $\alpha \in (1/4, 1/2]$. The temperature $T_1^{(+)}$ coincides with the temperature $T^{(-)}$ of the gas before the shock wave, too.

It can be seen from Eqs. (2)–(6) that distribution (6) coincides with the Treanor distribution at the lower vibrational levels and with the Boltzmann distribution at the higher levels for the temperature of the gas $T^{(+)}$. Behind the shock wave when $T_1^{(+)} < T^{(+)}$ the vibrational populations $n_v^{(+)}(\alpha)$ of the level interval $[0, v^*(\alpha)]$ are positioned lower than the Boltzmann ones (when the temperature $T_1^{(+)} \approx T^-$), although very close to them. According to Eq. (5), as α increases, $v^*(\alpha)$ decreases. This can be easily seen in Figs. 2 and 8, where relative vibrational populations $x_v = n_v/n_0$ are shown. These may be represented as

$$x_v = \exp\left\{ -\frac{\varepsilon_1}{kT_1}\left(\frac{\varepsilon_v}{\varepsilon_1} - \left(\psi_\alpha(v) - \frac{\varepsilon_v}{\varepsilon_1}\right)\left(\frac{T_1}{T} - 1\right)\right)\right\}.$$

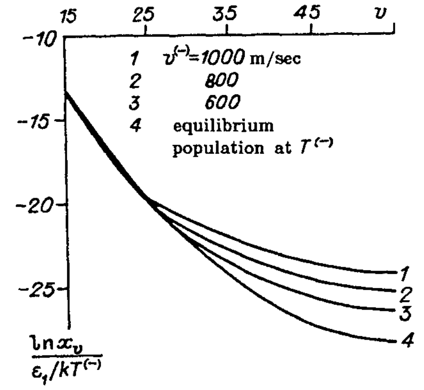

Fig. 3

Figure 2 shows the relative populations of vibrational levels of oxygen molecules behind the shock wave at some fixed temperature $T^{(-)} = 500\,\mathrm{K}$ of gas and velocity $v^{(-)} = 1000$ m/sec of the gas before the shock wave but at different values of α (that is, at different distances from the shock wave front). The graph demonstrates that up to a certain level $v^*(\alpha)$, the relative populations of the vibrational levels coincide, in practice, with the equilibrium populations of the corresponding levels before the shock wave, but after this level they decrease significantly more slowly, similar to the equilibrium populations, which correspond to the temperature $T^{(+)}$ of the gas behind the shock wave. The greater the distance from the shock wave surface (that is, the greater α), the earlier this transition occurs.

Figure 3 shows the relative populations of the vibrational levels of the oxygen molecules behind the singled out relaxation zone of the shock wave that has a definite thickness corresponding to the parameter $\alpha = 1/2$. In this case, the influence of the velocity $v^{(-)}$ before the shock wave on the distribution of molecules in the vibrational levels is studied at the fixed temperature $T^{(-)} = 500$ K of the gas. It is seen from the graph that the higher the velocity $v^{(-)}$ of the flow, the more populated the higher vibrational levels of molecules.

Note, in conclusion, that distributions (6) provide a new way of describing some nonequilibrium regimes of flow behind the shock waves using a reduced quantity of macroparameters and the possibility of studying the transfer phenomena together with the thermal disassociation processes in a nonequilibrium gas of anharmonic oscillators, when the level of the vibrational excitation is arbitrary.

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