Asymptotically exact value of the distribution function of molecular pairs in a shock-compressed highly dispersed gas mixture

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Abstract. The aim of this work is to obtain asymptotically strong expressions for the distribution functions of pairs of molecules inside the shock wave front. An asymptotically exact expression is obtained for the distribution function of the pairs of molecules of the heavy component of a binary shock-compressed gas mixture at the beginning of its translational relaxation. This result is extremely important for experimental modeling of the effect of high-speed overshoot in shock tubes.

1. Introduction

The previous works of the authors [1-4] on the analytical study of the overshoot effect in shock waves were based on the commonly used a priori approximations of single-particle distribution functions over the velocities of molecules. These include, for example, the well-known bimodal Tamm-Mott-Smith approximation. Recall that the essence of the overshoot effect is the excess of the values of a macroscopic parameter or the values of the distribution function of pairs of molecules inside the shock wave front over the corresponding values behind it. In the latter case, the overshoot effect for the distribution function of pairs of molecules is also called high-speed translational nonequilibrium [5]. The authors of [1-4] were able to identify the main four physical factors that control the mechanism of high-speed translational nonequilibrium. The corresponding analytical representations were obtained for each of the factors:

Factor 1. Effective reduction of the threshold of chemical reactions inside the shock wave front due to the "beam" nature of the bimodal Tamm-Mott-Smith distribution function.

\[
\tilde{G} = \frac{G}{G_1} = 2\pi \left( \frac{T_1}{T_0+T_1} \right)^{\frac{3}{2}} \frac{kT_1}{gu} \exp \left[ \frac{mg^2}{4kT_1} - \frac{m(g-u)^2}{2k(T_0+T_1)} \right],
\]

\[\tilde{G}_{\text{max}} \approx \frac{e}{\sqrt{2}} e^{\frac{1}{2}z}.\]

Here \(G, G_1\) are the distribution functions of pairs of molecules, respectively, inside the front and behind the shock wave front, and \(\tilde{G}\) is their ratio; \(T_0, T_1\) are the gas temperatures, respectively, before and
behind the shock wave front; \( g \) is the relative velocity of pairs of molecules; \( u \) is the shift of the macrospeeds of supersonic and sound flows, respectively, before and behind the shock wave front; \( m \) is the mass of the molecule; \( k \) is the Boltzmann constant; \( \epsilon^{-1} \) is the compression ratio in the wave.

Functions (1) and (2) are relative functions of the distribution of pairs of molecules inside the shock wave front, with function (2) being the maximum value of function (1) achieved inside the wave. The value (2) is obtained as a result of the limiting asymptotic hypersonic transition:

\[
M_0 \to \infty, \epsilon \to 0, \epsilon \cdot M_0^2 > 1,
\]

where \( M_0 \) is the Mach number in front of the shock wave front [1-4].

The effect of high-speed overshoot in accordance with the notation (1) and (2) is achieved when the inequality is fulfilled \( \mathcal{G} > 1 \).

It can be seen from formula (2) that the effect of high-speed overshoot always occurs in the hypersonic approximation.

The factor 1 was actually established earlier in numerical and analytical studies of the translationally nonequilibrium constants of threshold inelastic binary collisions inside the shock wave front in [6]. The distribution function of pairs of \( \mathcal{G} \) molecules was not considered in [6]. The limit transition (3) was also not considered. However, these two aspects together allow us to strictly asymptotically understand the action of the main mechanism of high-speed overshoot.

**Factor 2.** By the excitation of the internal degrees of freedom of the gas particles.

The effect of this factor is actually to increase the overshoot effect in accordance with the formula (2) at \( \epsilon \to 0 \). It should be remembered that the limit transition \( \epsilon \to 0 \) corresponds to the transition \( I \to \infty \), since \( \epsilon \) is inversely proportional to the total number of excited internal degrees of freedom of molecules \( I \). The excitation of a large number of internal degrees of freedom of light carriers, such as \( NH_3, C_2H_6, \) etc., is quite real. The fact is that the translational relaxation of small amounts of the heavy component carried by the lung is proportional to the ratio of their masses. In binary mixtures of interest for nanotechnology and controlled fusion, this ratio varies from \( 10^3 \) to \( 10^4 \). During this long time of translational relaxation of the heavy component to equilibrium with the light component, the latter will have time to excite the corresponding number of internal degrees of freedom \( I \).

**Factor 3.** Dilution of the mixture with a light carrier in a highly dispersed mixture of gases.

In this mixture, the concentrations of \( n_l \), \( n_h \) and the molecular weights of \( m_l, m_h \), respectively, of the light (index \( l \)) and heavy (index \( h \)) components are related by the following inequalities:

\[
n_l \gg n_h, m_h \gg m_l, n_l m_l \geq n_h m_h.
\]

The analysis of the action of this factor, similar to the analysis of the action of factors 1 and 2, leads to the following final asymptotic formula [1-4]:

\[
\mathcal{G}_{\text{max}}^{(h,h)} \approx \epsilon \epsilon^*_e \exp\left(\frac{1}{2 \epsilon \epsilon^*_e}\right),
\]

\[
\mathcal{G}_{\text{max}}^{(l,l)} \approx \mathcal{G}_{\text{max}}^{(l,h)} \approx \epsilon^*_e \exp\left(\frac{1}{2 \epsilon \epsilon^*_e}\right).
\]

Here \( \epsilon_* = \frac{m_l}{m_h} \).

In the case of a collision of pairs of heavy component molecules, the maximum value of the high-speed overshoot is \( \mathcal{G}_{\text{max}}^{(h,h)} \) it will also depend, as follows from (5), on the small parameter \( \epsilon_* \ll 1 \). This leads to a significant increase in the maximum of this effect in comparison with the cases of pairs of molecules of only a light component or the case of a mixed composition of pairs. A similar conclusion was previously obtained in numerical studies [5].

**Factor 4.** Anisotropy of the kinetic temperature field.

In experimental [7] and numerical [5] studies of the overshoot effect, this effect was also established for the values of the longitudinal kinetic temperature \( T^\parallel \). The kinetic temperature \( T^\parallel \) is measured along the flow in the shock wave, and the similar temperature \( T^\perp \) is measured perpendicular to it. Earlier, both experimentally and strictly theoretically, it was shown that inside the wave front...
there is an overshoot of the value $T^\parallel$ over the equilibrium value of the temperature $T_1$ behind the wave front. The temperature $T^\perp$ never exceeds $T_1$.

It is known that both temperatures $T^\parallel$ and $T^\perp$ are equally included in the ellipsoidal single-particle distribution of gas molecules in their velocities. As shown in numerical calculations, this distribution, applied for the heavy component, agrees well with them. In contrast to the ellipsoidal one-particle distribution, the distribution of pairs of molecules obtained analytically from it contains only $T^\parallel$ in the exponential dependence indicator. The asymptotic representation of the high-speed overshoot, due to the anisotropy of the kinetic temperatures, has the following form:

$$
\tilde{G}_{max}(h, \varepsilon) \approx \varepsilon \cdot \exp \left( \frac{\Delta T^\parallel}{\varepsilon \varepsilon_*} \right),
$$

(7)

$$
\Delta T^\parallel = \frac{T^\parallel - T_1}{\tau_h},
$$

(8)

It follows from these formulas that the value of the high-speed overshoot (7) strongly depends on the values of $\Delta T^\parallel, \varepsilon, \varepsilon_*$. The analysis of all the above factors was based on a priori analytical approximation of single-particle distribution functions. These approximations are generally accepted in the analytical study of the structure of shock wave fronts. On the basis of these approximations and an analytical study of the collision integral in the Boltzmann equation, the authors of [1-4] were also able to find the distribution function of pairs of molecules. It is this function that determines whether or not the effect of high-speed overshoot exists, as well as the non-Arrhenius form of the coefficients of the rates of threshold chemical reactions.

In this paper, the next step in the analytical study of the high-speed effect in shock waves is made, which consists in an attempt to abandon the traditional a priori approximations of distribution functions in shock waves. The strong difference in the translational relaxation times of the light and heavy components in a highly dispersed gas mixture actually makes an a priori approximation unnecessary. The unambiguous and only possible analytical form of these functions is established at the end of translational relaxation in the light component and the beginning of this relaxation in the heavy one.

2. Asymptotically accurate translationally nonequilibrium state of a highly dispersed shock-compressed gas mixture

The shock wave in a highly dispersed gas mixture corresponding to the inequalities (4) seems to split into two separate waves. The first of them corresponds to the translational relaxation of the light component, and the second to the relaxation of the heavy one. Due to the overwhelming predominance of the concentration of the light component over the concentration of the heavy one, the establishment of the Maxwellian distribution behind the shock wave in the light gas occurs much earlier than the establishment of this equilibrium in the heavy component.

Figure 1 schematically shows the extent of both shock fronts in the light and heavy components. As is known [8], the length of translational relaxation of the heavy component $\delta_h$ exceeds the length for the light component $\delta_l$ in proportion to the mass ratio $\delta_h \approx \frac{m_h}{m_l}$. 

Here $f_l^M(-\infty)$ and $f_l^M(+\infty)$ are Maxwellian distributions in front of the shock wave front in the light component and behind it; $f_h^M(-\infty)$ and $f_h^M(+\infty)$ are Maxwellian distributions in front of the shock wave front of the heavy component and behind it; $\delta_l$, $\delta_h$ are the width of the fronts of the light and heavy components of the dispersed gas mixture; the section marked with the marker ($\ast$) corresponds to the end of the relaxation of the light component and the beginning of this relaxation for the heavy component.

Note that, in contrast to the Tamm-Mott-Smith bimodal distribution, the Maxwell distributions $f_h^M(-\infty)$ and $f_l^M(+\infty)$ are taken in the same cross section, indicated in Figure 1 by the marker ($\ast$). In the Tamm-Mott-Smith method, the functions $f_h^M(-\infty)$ and $f_l^M(+\infty)$ are taken in different sections corresponding to the flow input into the shock wave and output from it.

As previously mentioned, the ratio $\frac{m_h}{m_l}$ can be quite large: $10^3 - 10^4$, which may be quite sufficient to excite rotational and vibrational degrees of freedom in the light component $\tilde{G}_{neq}^{(lh)}$, see Table 1.

**Table 1.** The value of “overshoot” $\tilde{G}_{neq}^{(lh)}$ at the beginning of the relaxation zone of the heavy component.

| Gas | A  | $(A_2)$ linear, none vibration | $(A_2)$ linear, with vibration | $(A_3)$ nonlinear |
|-----|----|-------------------------------|-------------------------------|------------------|
| $\gamma$ | 5/3 | 7/5 | 9/7 | 7/6 |
| $\varepsilon$ | 1/4 | 1/6 | 1/8 | 1/13 |
| $G_{neq}^{(lh)}$ | 1.31 | 2.37 | 4.84 | 3628 |

Here the symbol A denotes a variety of gas molecules with different number of atoms. Thus, symbols (A), (A2), (A3) denote molecules of monatomic, diatomic and triatomic gases respectively, $\tilde{G}_{neq}^{(lh)} = G_{neq}^{(lh)} / G_{eq}^{(lh)}$, $G_{eq}^{(lh)}$ - the translationally-nonequilibrium distribution function of the pairs of molecules inside the shock front, $G_{eq}^{(lh)}$ is the equilibrium distribution function of the pairs of molecules behind the wave front.

### 3. Conclusion

The effect of high-speed overshoot, which is a direct consequence of the bimodal approximation, is obtained without a priori introduction of this approximation, as an asymptotic property of a highly dispersed gas mixture.
The effect of high-speed overshoot in a two-component highly dispersed gas mixture has a maximum value that is completely determined by the degree of compression in the shock wave.

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