Analytical theory of high-speed nonequilibrium in a binary mixture of gases with a predominant light component

I V Demidov, M M Kuznetsov, Y D Kuleshova, A V Tikhonovets
Moscow Region State University, ul. Vera Voloshina, 24, Mytishchi, Moscow Region, 141014, Russia
Moscow Aviation Institute (National Research University), Volokolamskoye sh., 4, Moscow, 125993, Russia
E-mail: kuznets-omn@yandex.ru, juliaybogdanova@mail.ru, tikhonovets.a.v@gmail.com

Abstract. Analytical estimates are obtained that allow, first of all, to determine the fundamental conditions for the existence of a high-speed effect. In addition, an analytical assessment of the greatest value of this effect is given.

1. Introduction

The effect of high-speed nonequilibrium, discovered earlier in numerical studies, was directly related to the values of the distribution function of pairs of colliding molecules. The effect is that the value of this function inside the wave significantly exceeds its value behind the wave when the gas is in thermodynamic equilibrium [1].

In the works of the authors [2-5] this effect was studied purely analytically.

The main efforts of the authors in the implementation of this work were aimed at identifying the main dimensionless parameters of the problem, which determine both the condition for the existence of the effect and its largest value.

The predominance of the light component in the binary mixture is a necessary condition for such a study due to two factors:
1) as numerical studies have shown, the effect of high-speed disequilibrium becomes significant only if the concentration of the light component \( n_l \) prevails over the concentration of the heavy \( n_h \). In most calculations, the concentration of the heavy component \( n_h \) was several percent of the concentration of the light component and less;
2) the constancy of temperatures and macrospeeds included in the bimodal Tamm – Mott-Smith distribution, namely, in the second "hot" Maxwell function associated with the values of these parameters in thermodynamic equilibrium behind the shock wave, is always valid only in a one-component gas. In mixtures of gases, however, it will not always be true, but only in the case of \( n_l \gg n_h \) [6, 7].

The possibility of using a bimodal distribution at \( n_l \gg n_h \) for each of the components of a binary mixture in its classical form allows us to fully use its analytical capabilities.

As it is shown in this paper this leads to the allocation of a bilinear symmetric form in the desired distribution function of pairs of molecules analytical representation. By applying the subsequent transformations associated with the bilinear form, it is possible to obtain the final result in a simple analytical form.
2. Distribution function of pairs of light and heavy components

As noted above, the distribution function of pairs of molecules $G^{(Lh)}$ is constructed based on molecules single-particle bimodal distributions for each component of the mixture

$$F^{(i)}(y) = \chi^{(i)}(y)F_0^{(i)} + (1 - \chi^{(i)})F_1^{(i)},$$

$$\chi^{(i)}(y) = \frac{n_0^{(i)}}{n_0^{(i)} + n_1^{(i)}},$$

$$F_1^{(i)}(c) = \frac{m_y}{2\pi k T_i}^3 \exp\left[ -\frac{m_y(c-u_i)^2}{2k T_i} \right]$$

Here, the superscript $i$ corresponds to one of the components of the mixture: light $y = l$, or heavy $y = h$, with $m_l < m_h$; the total volume concentrations of the mixture of components $n_l$ and $n_h$ are composed of their partial $n_0^{(y)}$ and $n_1^{(y)}$, where: $n_y = n_0^{(y)} + n_1^{(y)}$; $y = l, h$; single-particle functions $F_i^{(y)} (i = 0, 1)$ are Maxwellian distributions; $m_y$ is the mass of the $y$ - component molecule; $u_i$ and $T_i$ are the velocity and temperature of the flow in front of ($i = 0$) and behind ($i = 1$) the wave; $k$ is the Boltzmann constant; ($c - u_i$) is the actual velocity of the molecule.

As in a simple one-component gas, the partial concentrations included in the numerator and denominator of formula (2) are functions of the $x$ coordinate that varies in the wavelength. The partial parameters of the flow: the temperature $T_i$ and the macrospeed $u_i$ remain unchanged and coincide, respectively, with the thermodynamic temperature and the macrospeed of the flow at the entrance to the wave ($i = 0$) and at the exit from it ($i = 1$).

The pairs of molecules distribution function obtained on the basis of relations (1-3), as shown in [8], has the following form:

$$G^{(Lh)} = \chi^{(l)} \chi^{(h)} G_0^{(Lh)} + \chi^{(l)}(1 - \chi^{(h)}) G_{01}^{(Lh)} + (1 - \chi^{(l)}) \chi^{(h)} G_1^{(Lh)} + (1 - \chi^{(l)})(1 - \chi^{(h)}) G_1^{(Lh)}.$$  

(4)

For the purposes of further discussion, we will focus a little more on the structure of the relation (4).

This relation is obtained by multiplying the single-particle distributions (1) with subsequent integration over the entire space of the velocities of both colliding molecules, except for the modulus of their relative velocity $g$ (where $g = |c_l - c_h|$).

We show that formula (4) can be algebraically transformed to the form containing as one of the terms a bilinear symmetric form by the product of dimensionless coordinates $\chi^{(l)}, \chi^{(h)}$, and as the other—a linear form by these coordinates

$$G^{(Lh)} - G_1^{(Lh)} = -\left(G_{01}^{(Lh)} + G_{10}^{(Lh)} - G_1^{(Lh)} - G_0^{(Lh)}\right)\chi^{(l)} \chi^{(h)} + \left(G_0^{(Lh)} - G_1^{(Lh)}\right)\chi^{(l)} + \left(G_1^{(Lh)} - G_0^{(Lh)}\right)\chi^{(h)}.$$  

(5)

It is easy to see that in the right part of the formula (5), the negative term containing the product of dimensionless coordinates $\chi^{(l)} \chi^{(h)}$ is a symmetric bilinear form by permutation of these coordinates. The parameters: $G_0^{(Lh)}, G_{01}^{(Lh)}, G_{10}^{(Lh)}, G_1^{(Lh)}$ do not depend on the coordinates and are functions of the molecules relative velocity modulus $g$. The representation of single-particle functions in accordance with expression (1) can be understood as the decomposition of these functions into basis vectors consisting of a "cold" Maxwell distribution at the entrance to the shock wave $F_0^{(i)}(y)$ and a "hot" - $F_1^{(i)}(y)$ at the exit from it. In the bilinear term in the formula (5), each of the dimensionless parameters $G_0^{(Lh)}, G_{01}^{(Lh)}, G_{10}^{(Lh)}, G_1^{(Lh)}$ is the result of the action of the bilinear functional $A(e_1^{(i)}, e_1^{(j)})$ on the corresponding pair of basis vectors: $e_1^{(i)} = F_1^{(i)}(y), e_1^{(j)} = F_1^{(j)}(y)$. The bilinear functional in this problem, as already mentioned, is the integration of the mixture components single-particle functions over the velocity space of the different mixture components colliding molecules (with the exception of integration over the molecules relative velocity).

Thus, the pairs of molecules distribution function (5) depends parametrically on the molecules relative velocity modulus $g$ and the coordinate in the shock wave "$x$". This coordinate is included in the partial dimensionless densities $\chi^{(l)}$ and $\chi^{(h)}$. The right part of the formula (5) depends on the variable arguments of the problem: the relative velocity $g$ and the coordinates in the wave "$x$". In this case, the variable $g$ is included only in the dimensionless parameters $G_0^{(Lh)}, G_{01}^{(Lh)}, G_{10}^{(Lh)}, G_1^{(Lh)}$; the coordinate "$x$" is only in the dimensionless densities $\chi^{(l)}$ and $\chi^{(h)}$. This is one of the advantages of the original analytical a priori representation of the single - particle distribution function (1) by Tamm-Mott-Smith.
We see that the transition to the distribution function of pairs of molecules also preserves this fundamental simplicity.

3. The centrality of the curve geometrically corresponding to the distribution function of pairs of molecules

To fulfill the goals set in the work, it is necessary to perform a number of transformations that are traditional for bilinear forms. First of all, we note that geometrically, relations (4) and (5) can be considered as equations of second-order curves in the coordinates $\chi^{(l)}$ and $\chi^{(h)}$. We show that by a linear transformation that translates the old coordinates $\chi^{(l)}$ and $\chi^{(h)}$ into the new $\chi_l$ and $\chi_h$:

$$\chi^{(l)} = \chi_l + d_l, \quad \chi^{(h)} = \chi_h + d_h, \quad (6)$$

the curves of dependencies (4) and (5) will become symmetric in the new coordinates. This will be expressed in the fact that the left parts of the equations (4) and (5) will remain unchanged when the coordinates $\chi_l$ are replaced by $-\chi_l$, $\chi_h$ by $-\chi_h$. In this case, the center of symmetry position will be shifted by the distances $d_l$ and $d_h$ (in the old coordinates) relative to the origin of the old coordinates $\chi^{(l)} = \chi^{(h)} = 0$. The coordinates of the center ($d_l$, $d_h$) are determined from the condition of the absence of linear terms in equations (4) and (5) after switching to new coordinates in them.

As a result, we get

$$\Delta G^{(l,h)} = -\chi_l \chi_h + g_{01}^{(l,h)} g_{10}^{(l,h)}, \quad (7)$$

where

$$\Delta G^{(l,h)} = \frac{G^{(l,h)} - G_1^{(l,h)} - G_0^{(l,h)}}{G_1^{(l,h)} - G_0^{(l,h)}}, \quad (8)$$

$$g_{01}^{(l,h)} = \frac{G_0^{(l,h)} - G_1^{(l,h)}}{G_1^{(l,h)} - G_0^{(l,h)}}, \quad (9)$$

$$g_{10}^{(l,h)} = \frac{G_1^{(l,h)} - G_0^{(l,h)}}{G_1^{(l,h)} - G_0^{(l,h)}}, \quad (10)$$

$$d_h = g_{01}^{(l,h)}; d_l = g_{10}^{(l,h)} \quad (11)$$

Note that, as shown in [8], the equations (8-10) can be represented entirely in terms of the values $g_{01}^{(l,h)}$, $g_{10}^{(l,h)}$, $g_{1}^{(l,h)}$, where

$$g_{01}^{(l,h)} = G_{01}^{(l,h)} - G_{1}^{(l,h)}; g_{10}^{(l,h)} = G_{10}^{(l,h)} - G_{1}^{(l,h)}; g_{1}^{(l,h)} = G_{1}^{(l,h)} - G_{0}^{(l,h)} \quad (12)$$

4. The region of existence of the high-speed overshoot effect

In the previous works of the authors [5, 8] necessary and sufficient conditions for the effect of high-speed overshoot were formulated.

The necessary conditions were reduced to the non-negativity of the expression $\Delta G_{ij}^{(l,h)}$, where $i,j = 0,1,$ and

$$\Delta G_{ij}^{(l,h)} = (G_{01}^{(l,h)} + G_{10}^{(l,h)} - G_{1}^{(l,h)} - G_{0}^{(l,h)}) \geq 0, \quad (13)$$

or

$$\Delta G_{ij}^{(l,h)} = g_{01}^{(l,h)} + g_{10}^{(l,h)} + g_{1}^{(l,h)} \quad (14)$$

Sufficient conditions consisted in the non-negativity of each term in equation (14):

$$g_{01}^{(l,h)} \geq 0; g_{10}^{(l,h)} \geq 0; g_{1}^{(l,h)} \geq 0 \quad (15)$$

Inequalities (15) can also be considered as the domain of an effect existence in a certain range of the molecules relative velocity modulus $g$ values, since all the values standing in the left parts of the non-strict inequalities (15) are functions of $g$.

However, in the coordinate space $\chi^{(l)}$ and $\chi^{(h)}$, where $0 \leq \chi^{(l)} \leq 1$, $0 \leq \chi^{(h)} \leq 1$, such a region was not specified, unlike the one-component gas considered in [3].

To establish the boundaries of the desired area, we will return to the old coordinates $\chi^{(l)}$ and $\chi^{(h)}$ in the expression (7):
where \( \chi \) is the function \( \gamma \). 

It is easy to see that when the product of the "new coordinates" \( \chi \) and \( \chi \) is a negative value, the effect of high-speed overshoot \( \Delta G(\chi)\geq 0 \) always exists. In addition, it is greater than the value \( \Delta G_0 \) in the original "old coordinates" \( \chi(l) \) and \( \chi(h) \).

**Figure 1.** The area of existence of the high-speed overshoot effect

![Figure 1](https://example.com/figure1.png)

We transform the right-hand sides of equations (8-10) using the functions (12-14):

\[
\Delta G(\chi) = \frac{\Delta G(l, \chi)}{\gamma_{01} + \gamma_{01} + \gamma_{10}},
\]

\[
\gamma_{01} = \frac{\gamma_{01}}{\gamma_{01} + \gamma_{10} + \gamma_{10}} < 1,
\]

\[
\gamma_{10} = \frac{\gamma_{10}}{\gamma_{10} + \gamma_{01} + \gamma_{10}} < 1,
\]

where \( \Delta G(l, \chi) = G(l, \chi) - G_1(\chi) \).

At the point "X" with coordinates \( (\gamma_{01}(l), \gamma_{10}(l)) \) the overshoot effect \( \Delta G(l, \chi) \) is exactly equal to the product of \( \gamma_{01} \) \( \gamma_{10} \). It has the same value on each of the lines: \( \chi(l) = \gamma_{01}(l), \chi(l) = \gamma_{10} \).

In the fields: \( \chi(h) > \gamma_{01}(l), \chi(l) < \gamma_{10}(l) \) and \( \chi(h) < \gamma_{01}(l), \chi(l) > \gamma_{10}(l) \) the value \( \Delta G(l, \chi) \) will be greater than \( \gamma_{01} \gamma_{10} \).

In the fields: \( \chi(h) > \gamma_{01}(l), \chi(l) > \gamma_{10}(l) \) and \( \chi(h) < \gamma_{01}(l), \chi(l) < \gamma_{10}(l) \) the value \( \Delta G(l, \chi) \) will be less than \( \gamma_{01} \gamma_{10} \).

At the point \( \chi(l) = 0, \chi(l) = 0 \), i.e. at the origin of the coordinates, the effect is completely absent, \( \Delta G(l, \chi) = 0 \). The effect is also absent on the line with the equation: \( -\chi(l) \chi(l) + \gamma_{01}(l) \chi(l) + \gamma_{10}(l) \chi(l) = 0 \). This curve is drawn in Figure 1 and is located in the upper-right rectangle. Above and to the right of this curve is the function \( \Delta G(l, \chi) < 0 \).

5. Estimation of the highest value of the high-speed overshoot effect

The equation (16) obtained from the expression (5) for the pairs of molecules distribution function \( G(l, \chi) \) also allows us to estimate the largest value of the overshoot effect.

Indeed, as follows from the equation (16), a positive addition to the main value of the effect: \( \Delta G(l, \chi) = \gamma_{01} \gamma_{10} \), can only be written in the following variants:

a) \( \gamma_{01}(l) - \chi(l)(\gamma_{01}(l) + \gamma_{10}(l)) \);

b) \( \chi(l) - \gamma_{01}(l)( \gamma_{10}(l) - \chi(l)) \).
In each of these variants, we will find the largest values of each of the multipliers and multiply them:

\[ \left( \bar{g}_{01}^{(l,h)} - \chi^{(l)} \right) \bar{\Delta} \sup \times \left( \chi^{(h)} - \bar{g}_{10}^{(l,h)} \right) \left| \sup \right. = \left( \bar{g}_{01}^{(l,h)} - \chi^{(l)} \right) \left( 1 - \bar{g}_{10}^{(l,h)} \right) = \bar{g}_{01}^{(l,h)} - \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)}, \] (20)

\[ \left( \chi^{(l)} - \bar{g}_{01}^{(l,h)} \right) \left. \bar{\Delta} \sup \times \left( \chi^{(h)} - \bar{g}_{10}^{(l,h)} \right) \right| \sup = \left( 1 - \bar{g}_{01}^{(l,h)} \right) \left( \bar{g}_{10}^{(l,h)} - 0 \right) = \bar{g}_{10}^{(l,h)} - \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)}. \] (21)

In each of these variants, we will find the largest values of each of the multipliers and multiply them:

\[ \Delta \sup = \bar{g}_{01}^{(l,h)} - \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)} + \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)} = \bar{g}_{01}^{(l,h)}; \] (22)

\[ \Delta \sup = \bar{g}_{10}^{(l,h)} - \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)} + \bar{g}_{01}^{(l,h)} \bar{g}_{10}^{(l,h)} = \bar{g}_{10}^{(l,h)}. \] (23)

Thus, the expressions (22) and (23) give an estimate of the highest value of the high-speed overshoot effect \( \Delta \sup \):

1) if \( \bar{g}_{01}^{(l,h)} \geq \bar{g}_{10}^{(l,h)} \), then \( \bar{g}_{01}^{(l,h)} \leq \Delta \sup \leq \bar{g}_{01}^{(l,h)} \);

2) if \( \bar{g}_{01}^{(l,h)} \leq \bar{g}_{10}^{(l,h)} \), then \( \bar{g}_{01}^{(l,h)} \leq \Delta \sup \leq \bar{g}_{10}^{(l,h)} \).

In Figure 1, each of the values: \( \bar{g}_{01}^{(l,h)} \cdot \bar{g}_{10}^{(l,h)} \) corresponds to its own pair of coordinates at which they are reached. So, the values of \( \bar{g}_{01}^{(l,h)} \) correspond to \( \chi^{(h)} = 1 \) and \( \chi^{(l)} = 0 \), i.e. the point (1;0). The value of \( \bar{g}_{10}^{(l,h)} \) is the point (0;1).

**Conclusion**

The paper shows that in the case of a strong predominance of the concentration of a light component over the concentration of a heavy one, the pairs of molecules distribution function can be represented as the sum of a bilinear symmetric shape and a constant value, which is the "average measure" of the overshoot effect.

Thanks to the selection of a symmetric bilinear form in the analytical representation of the distribution function of pairs of molecules, it was possible to determine both the area of the overshoot effect existence and to estimate the greatest value of this effect. It is important to note that these significant conclusions are obtained analytically. They do not require obtaining a solution to the Boltzmann equation for a mixture of gases in a shock wave.

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