Analytical properties of nonequilibrium threshold in shock waves

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Abstract. Are the main results of numerical research of the effect of high speed threshold Nonequilibrium activated kinetic processes in shock-compressed gases. In parallel to it are corresponding analytical results of the authors.

1. Introduction
Analytical properties of threshold of kinetic processes in the shock waves are directly related to the so-called effect of high-speed translational Nonequilibrium [1]. The effect of significant excess number of pairs of molecules that have overcome the threshold energy of a chemical reaction inside the shock wave front, over the appropriate number of pairs of molecules behind it, was previously installed in the paper [2] on the through numerical Monte Carlo simulation.

The numerical research of shock wave Monte Carlo also identified all of the basic physical factors accelerating the flow of kinetic processes in shock waves:

- effectively reduction the threshold of chemical reactions inside the front shock wave due to the nature of the bimodal distribution function Tamm-Mott-Smith;
- speed reduction of equilibrium chemical reactions in a "hot" area behind the front shock wave due to the strong dilution of "Rayleigh gas" by predominant light carrier;
- reducing the speed of the high-speed equilibrium of chemical reactions in a "hot" area behind the front shock wave due to energy dissociation expense (reduction of equilibrium statistical temperature compared to kinetic inside front shock wave);
- velocity acceleration high-speed chemical reactions due to anisotropy field of kinetic temperatures inside the shock wave.

It should also be noted that the relative effect of a high-speed "overshoot" increases with the energy threshold of inelastic collisions between pairs of molecules. For threshold velocity constants of chemical reactions this fact repeatedly emphasized in works of V Yu Velikodnıy (see for example [3]). In the works of the same author, apparently, was first proposed by an analytical approach to the study of threshold progressively nonequilibrium processes on the basis of the bimodal distribution of molecules within the shock wave. His research focused on the impact of the first factor to the effect of "overshoot" speeds of translational nonequilibrium threshold chemical reactions. Influence of anisotropy field of kinetic temperatures on the magnitude of this effect was considered in [1].

An analytical approach to the study of the effect of threshold progressively Nonequilibrium in shock wave has some fundamental advantages (in the sense of final results) compared to numerical.
But this is achieved through a substantial simplification of the mathematical model of the consider effect. So, using the ellipsoidal distribution function of the molecules in the gas mixture components [1], you can show a certain interdependence of four determining physical factors. To take into account the impact of these factors on translational nonequilibrium velocity of threshold chemical reactions can offer a universal formula for some chemical kinetics [4].

2. Binary gas mixtures with constant and variable approximation parameters in Maxwellian “wings” of Bimodal distributions

Previously two theorems on high velocity translational nonequilibrium in shock wave for one-component (or pure) gas were formulated in authors works. Besides was noted that the proof of this theorems in the case of a shock-compressed gas binary mixture involves overcoming some significant difficulties. Chief among that is the fact that in gas mixtures the bimodal molecular velocity distribution cannot be unconditionally applied for the calculation of shock wave structure, as has been done in a simple gas. As a rule, the range of applicability of the classical bimodal Tamm – Mott-Smith distribution with constant approximation of auxiliary macroscopic velocities and kinetic temperatures for groups of molecules in supersonic and subsonic “wings” of this distribution is limited by small concentration values of one of the mixture components. In this case only it is possible to preserve all the advantages of the bimodal approximation of partial distribution functions in binary gas mixture to obtain a simple analytical solution for shock wave structure. Because of that the obtaining of necessary and sufficient high velocity translational nonequilibrium conditions for arbitrary values component concentration of gas mixtures becomes much more complex. In this paper a rigorous formulation and the substantiation of these conditions is given. These conditions apply to the case of variability of the auxiliary approximation macro parameters of “hot” bimodal distribution wing in binary gas mixture. All the same time the values of auxiliary macroscopic velocities and kinetic temperatures for groups of molecules in subsonic “wing” are constant. In binary mixtures of gases with distribution functions for the light and heavy components can be three distribution functions of the module of relative molecular velocity for pairs molecules. These functions are: G(ll) is the distribution function of pairs inside a light-light component, the second – G lh – function pairs light-heavy component, the third – G hh is a function of pair heavy-heavy component. The numerical realization of corresponding overshoot effect of bimodal distributions for pair molecules was examined in particular case of small concentration of heavy component in binary gas mixture (Rayleigh gas). It is known that in Rayleigh gas this effect for function G(hh) is most noticeable. The numerical calculation of this effect took into account the molecular rotational degrees of freedom in polyatomic gas.

3. Analytical estimate of high-speed overshoot value for pair molecules distribution in binary gas mixture

Analytical properties of bimodal distribution of pairs molecules allow to establish the existence of maximum values for the relative effect of ”overshoot" in the number of pairs of molecules inside front shock waves compared to the appropriate number of pairs of molecules behind the shock wave. Furthermore, to estimate the magnitude of the "overshoot" of pairs of molecules can offer universal analytical expression, finding which requires no detailed numerical calculation of shock wave front structure. For a simple gas it was done in [1]. For binary gas mixtures the presence of maximum for the value of the corresponding "overshoot" was found in [5]. In the present work a formula for its estimate is provided:

$$\left[\left(G^{(\rho,\rho)} / G^{(\rho,\rho)}_{0}\right) - 1\right] > g^{(\alpha,\beta)} (1) \cdot g^{(\alpha,\beta)} (2) \cdot \left[\left(g^{(\alpha,\beta)} (1) + g^{(\alpha,\beta)} (2)\right)ight]^{-1} > 0$$

Here's the first set of square brackets is the value of corresponding of "overshoot" effect for distribution functions of pairs molecules inside the wave front $G^{(\rho,\rho)}$ belong to the corresponding translational equilibrium value $G^{(\rho,\rho)}_{0}$. Other designations are given in [5].
4. Conclusion
Note that all values on to the right of the first inequality, enables to estimate the relative effect of "overshoot" magnitude does not require for its computing knowledge structures of front shock wave. The structure of shock wave knowledge allows to replace the first inequality to equality. In this equality compared to inequality appears an additional multiplier order the unit. However, for practical applications, effect of "overshoot", as shows experiment [6], shall be not less than $10^4$-$10^6$. Knowledge factor order 1 is not fundamental.

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References
[1] Kuznetsov M M, Kuleshova Ju D and Smotrova L V, Bulletin of the Moskow State Regional University 2012. (2) P.108
[2] Genich A P, Kulikov S V, Manelis G B, Chereshnev S L, Izv. ANSSSR MZhG 1990. (2) P.144
[3] Velikodniy V Yu, 1990 Molecular dynamics of gas and the mechanics of nonuniform media M.: Nauka 1990 P.41
[4] Kuznetsov M M and Smotrova L V, Bulletin of the Moskow State Regional University 2013. (3) P. 66
[5] Kuznetsov M M, Kuleshova Ju D, Smotrova L V and Reshetnikova Yu G, Bulletin of the Moskow State Regional University 2016. (3) P. 84
[6] Genich A P, Kulikov S V, Soloviova M E, Chereshnev S L, Fundamental Problems of Shock Vaves Physics. Book of Abstracts 1987. 1 (2). P. 240