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EXISTENCE OF SOLUTIONS FOR STEADY DETONATION OF GAS SUSPENSIONS

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The existence of solutions of the traveling-wave type is studied for a system of equations that describes a one-dimensional motion of a suspension of evaporating particles in a viscous and heat-conducting chemically reacting gas. Using topological methods, it is shown that solutions corresponding to weak, strong, and Chapman–Jouguet detonation exist under certain restrictions on energy release and mass transfer.

The problem of constructing profiles corresponding to traveling waves in two-phase media is important. This is primarily related to the study of shock or detonation waves in gas–droplet and bubbly media, gas–solid particles and gas–liquid film systems, etc. The problem of the structure of shock waves or detonation waves in a one-dimensional flow includes two main topics: the existence of solutions of equations of motion for a viscous liquid (which is the carrier phase for heterogeneous media) with a region of rapid variation of its parameters and the description of the wave profile. The solution of the first problem requires the use of analytical methods. The second problem can be effectively solved by numerical methods.

The initial state of the medium ahead of the wave and the final state corresponding to the equilibrium state behind the wave are usually singular points of the dynamic system of ordinary differential equations that describe the motion of the phases. Therefore, prior to integrating this system numerically, one has to prove the existence of a trajectory whose asymptotic ends are singular points.

The wave study should be performed within the framework of the model of hydrodynamics of real liquids, which takes into account the viscosity, thermal conductivity, and diffusion of the substance. The first qualitative solution of the problem was obtained for shock waves in [1, 2] and for gas detonation in [3–6], and strong restrictions were imposed on the flow parameters. For example, the analysis [3–6] is valid only for the Lewis number Le = 1 and Prandtl number Pr = 3/4. The numerical and approximate analytical profiles of detonation waves in two-phase media were constructed in [7]. These studies and also problems of existence of deflagration (combustion) waves are described in detail in [8, 9]. The theorem of existence and uniqueness of homogeneous detonation in a viscous and heat-conducting gas was proved by Majda [10] and that for the case of diffusion of the substance by Gardner [11].

In the present paper, we prove a theorem on existence of solutions corresponding to steady detonation waves in a reacting suspension of particles in a viscous and heat-conducting gas. The problem is formulated in [12], where the conditions of existence of solutions are also given. The rigorous proof of the theorem described below is based on the use of the Conley index — a topological invariant, which is a generalization of the Morse index [11, 13].

Formulation of the Problem. We study the motion of particles (the condensed or the c-phase) suspended in a viscous and heat-conducting gas, which satisfies the equation of state of an ideal gas. We assume that the motion of the medium is one-dimensional, and the interaction of particles proceeds only in the gas phase, which is valid if the volume concentration of particles is rather low. The system of initial

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equations that describe the motion of the two-dimensional medium is divided into two subsystems (for the gas and for the c-phase) related to each other only via their right parts [14]. We assume that the interphase mass transfer is determined by evaporation of the c-phase, where the gas temperature is higher than the particle temperature, and also by gasification of particles due to interphase friction for different phase velocities; the phase temperatures and velocities in the initial quiescent state are identical; the chemical reactions proceed only in the gas; the evaporated substance reacts instantaneously, and the magnitude of the thermal effect is determined by the mass concentration of the substance; the internal energy of the particles and the mean molecular weight of the gas are constant. Without loss of generality, we assume that the viscosity η, the thermal conductivity λ, and the ratio of specific heats γ of the gas are also constant quantities.

Let D be the velocity of the traveling wave, x be the spatial coordinate in the laboratory coordinate system, and t be the time. We introduce a self-similar variable $\xi = Dt - x$. In a coordinate system moving with velocity D, the initial system of partial equations reduces to a system of ordinary differential equations with respect to the variable ξ, which is similar to that given in [12]:

$$\eta \frac{du}{d\xi} = \rho_{\text{in}} D\Big(\frac{RT}{u} + u\Big) - (p_0 + \Omega + \rho_{\text{in}} D^2) \equiv F_1(u, T, k, w),$$

$$\lambda \frac{dT}{d\xi} = \rho_{\text{in}} D\Big(\frac{RT}{\gamma - 1} - \frac{u^2}{2} + Q + \frac{\Omega(u - w/2 - D/2)}{\rho_{\text{in}} D} - I_0(k) - \frac{D^2}{2} + u\Big(D + \frac{p_0}{\rho_{\text{in}} D}\Big)\Big) \equiv F_2(u, T, k, w),$$

$$\frac{dk}{d\xi} = (1 - k)\,\frac{C_1(w - u)^n + C_2(T - T_0)}{w} \equiv F_3(u, T, k, w), \tag{1}$$

$$\frac{dw}{d\xi} = \frac{C_3(u - w)}{w} \equiv F_4(u, T, k, w), \qquad p = \rho RT, \qquad \rho u = \rho_{\text{in}} D.$$

Here u is the gas velocity in the coordinate system moving with velocity D, T and ρ are the gas temperature and density, and k and w are the degree of outburning and the velocity of the c-phase, respectively ($k = 1 - v/v_0$, where v is the volume of one particle). The subscript 0 corresponds to the initial state of the phase parameters of the medium; p is the pressure, R is the gas constant, $Q = -kq$ is the thermal effect of chemical reactions, C_1, C_2, C_3, q, and n ($n > 1$) are constants, and

$$I_0 = (\gamma p_0/(\gamma - 1) + k\sigma_0 e_0)/\rho_{\text{in}}, \quad \Omega = (1 - k)\sigma_0 D^2(1 - w/D), \quad \rho_{\text{in}} = \rho_0 + k\sigma_0, \tag{2}$$

where σ_0 and e_0 are the initial density and thermodynamic component of the internal energy of particles, respectively, and ρ_{in} is the mean initial density of the medium.

The initial autonomous dynamic system (1), (2) yields an adequate description of the processes of interphase interaction for $k \in [0, 1]$ and $T \geqslant T_0$. Below we study the solutions of the system for all values of T and k; the solution whose existence is proved below satisfies the restrictions $k \in [0, 1]$ and $T \geqslant T_0$.

To refine the heat-release model, we introduce the ignition temperature $T_i > T_0$ and assume that the evaporated substance of the c-phase does not react if $T < T_i$. By analogy with [11], we introduce a narrow transitional region in the neighborhood of the hyperplane $T = T_i$, where the evaporated substance burns out rapidly. In passing through this region, the phase trajectories retain continuity and smoothness, and afterwards the magnitude of the thermal effect is determined only by the gasification rate. The procedures of constructing isolating neighborhoods are similar for the refined and simpler models.

We normalize system (1), (2) using constants corresponding to the initial values of the gas parameters: p_0, ρ_0, T_0, and u_0 ($u_0^2 \equiv p_0/\rho_0$). In the dimensionless variables, the system acquires the form

$$\eta \frac{du}{d\xi} = F_1(u, T, k, w), \qquad \lambda \frac{dT}{d\xi} = F_2(u, T, k, w),$$

$$\frac{dk}{d\xi} = F_3(u, T, k, w), \qquad \frac{dw}{d\xi} = F_4(u, T, k, w), \tag{3}$$

where the functions F_i $(i = 1, \dots, 4)$ of the dimensionless variables u, T, k, and w (for convenience, we retain the notation for all basic variables) are obtained from the initial variables by substituting T for RT and 1 for p_0, ρ_0, and T_0.

We note that the energy release in this case is determined only by the degree of gasification k. The kinetic equation is the third equation of system (3). In the theory of combustion, the chemical-reaction rate should be assumed to be zero at temperatures slightly higher than the initial one, since the nonzero rate leads to an infinite growth of parameters at infinity. In this case, for $k = 1$, the right part of the third equation is equal to zero, which is similar to a certain extent to the requirement of vanishing of the reaction rate. None of the trajectories of the system passing through points with $k < 1$ intersects the hyperplane of the phase space $k = 1$ except for the curves approaching asymptotically the points corresponding to the equilibrium states.

The subsequent study is performed in the phase space (u, T, k, w). This approach is widely used in the theory of combustion and detonation [9]. Below we show the existence of trajectories in the phase space, whose limits are isolated singular points — the states of equilibrium (rest points) of system (3). We will call these points the initial and final states of the medium, though, strictly speaking, for finite values of ξ, the medium cannot go out of or come to these states from other points of the phase space. We note that along these trajectories, due to the monotonicity of k ($F_3 > 0$), there is a unique correspondence between the values of the parameter ξ eliminated during the transition to the phase plane and the degree of gasification k: $dk = F_3\, d\xi$.

Singular Points of the Dynamic System. We study the behavior of the trajectories of system (3) in the phase space (u, T, k, w). We assume that the values of the parameter D (velocity of the traveling wave) are greater than some critical value D_* ($D_*^2 > \gamma$), which corresponds to shock and detonation waves. If $k \neq 1$, then the only singular point in which all the right parts of system (3) vanish simultaneously is the point $A_0(D, 1, 0, D)$, which corresponds to the initial state of the medium ahead of the wave.

If $k = 1$, system (3) decomposes into two subsystems, since the functions F_1 and F_2 are independent of w. In this phase hyperplane, the curve $F_1(u, T, 1) = 0$ is a parabola whose branches are turned downward (with respect to the axes u and T). The curve $F_2(u, T, 1) = 0$ is a parabola whose branches are turned upward (Fig. 1). For each fixed value of the thermal effect of chemical reactions q for $D > D_*$, these parabolas have two intersection points: A_1, where $u^2 > \gamma p/\rho$, and B_1, where $u^2 < \gamma p/\rho$ (the points correspond to weak and strong detonation). For $D = D_*$, the parabolas touch each other and the two points merge into one ($u^2 = \gamma p/\rho$), which corresponds to the Chapman–Jouguet detonation. If $D < D_*$, then the only remaining singular point of system (3) is A_0.

We note that the Chapman–Jouguet state can be reached for a finite value of ξ in the case of nonideal (in particular, heterogeneous) detonation. This is observed if the whole system is divided into two subsystems related to each other only through their right parts. If the perturbations are transferred only by the carrier phase (gas), the right parts of only the gas-dynamic subsystem vanish at the Jouguet point. The mapping point goes out of the state of equilibrium in the case of a finite value of ξ (for example, due to the velocity nonequilibrium of the phases). In our problem, the situation is different. The singular points are equilibrium for all equations of the system and can be reached only for $\xi \to \infty$ or $\xi \to -\infty$.

To determine the type of singular points, we write the characteristic equation $\det A = 0$, where the matrix A has the following form:

$$A = \begin{pmatrix} R_1(-T/u^2 + 1)/\eta - m & R_1/(\eta u) & \sigma_0 DT/(\eta u) & 0 \\ R_1(D - u + 1/R_1)/\lambda & R_1/(\lambda(\gamma - 1)) - m & (F_2)'_k/\lambda & 0 \\ 0 & 0 & -C_2(T - 1) - m & 0 \\ C_3/u & 0 & 0 & -C_3/u - m \end{pmatrix}.$$

Here $R_1 = (1 + \sigma_0)D$.

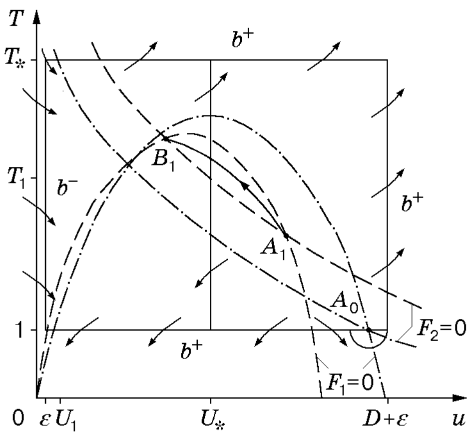

Fig. 1. Projection of isolating neighborhoods on the plane (u, T): the dashed and dot-and-dashed curves refer to $k = 1$ and $k = 0$, respectively.

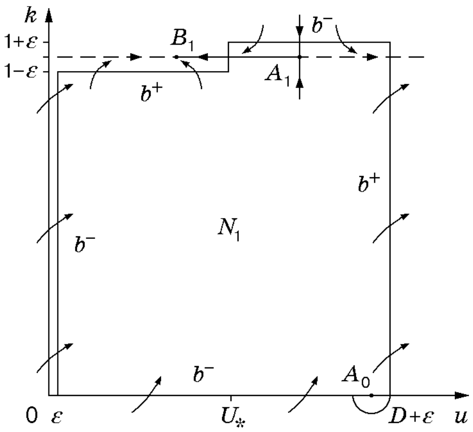

Fig. 2

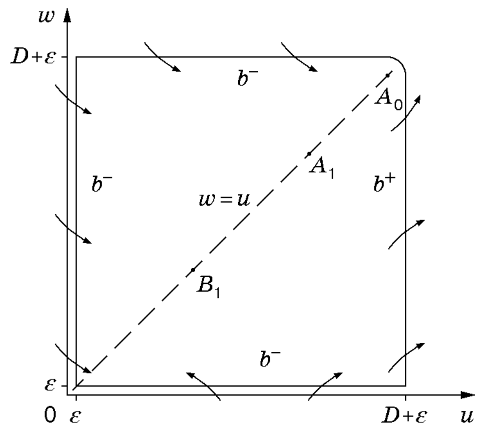

Fig. 3

Fig. 2. Projection of the isolating neighborhood N_1 onto the plane (u, k).

Fig. 3. Projection of the isolating neighborhoods onto the plane (u, w).

An analysis of the coefficients of the characteristic equation at the singular point A_0 shows that, in accordance with the Descartes' theorem, for $D \geqslant D_*$ the equation has three roots m with a positive real part and one root with a negative real part; at the point A_1, there are two roots with a positive real part and two roots with a negative real part. At the point B_1, one root has a positive real part and three roots have a negative real part. Thus, all three equilibrium states of the autonomous dynamic system (3) are spatial saddles.

Construction of Isolating Neighborhoods. In what follows, we assume that the parameters D and q acquire values such that system (3) allows the existence of all three singular points. If $D < D_*$, when A_0 is the unique singular point, a traveling wave can exist; after passing through this wave, the medium returns to the initial state A_0. Nevertheless, in our case system (3) does not allow such solutions. Irreversible changes occur along the trajectories, which are related to the processes of energy release and heat and mass transfer. The Chapman–Jouguet detonation ($D = D_*$) is considered below.

In the phase space (u, T, k, w), we construct an isolating neighborhood N_1 that contains two singular points A_0 and A_1 as internal points and does not contain the point B_1, and a neighborhood N_2 that contains the points A_0 and B_1 and does not contain the point A_1. The isolating neighborhood N is a compact and bound subset of the phase space, where each trajectory corresponding to the solutions of system (3) and

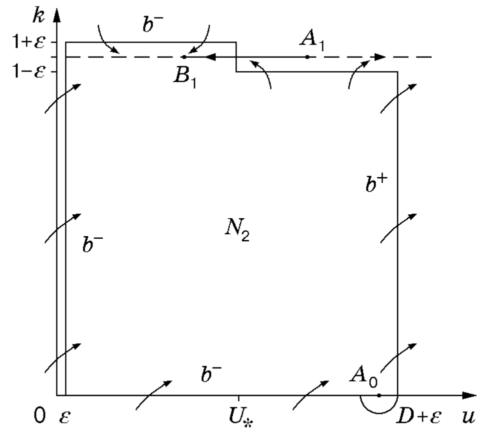

Fig. 4. Projection of the isolating neighborhood N_2 onto the plane (u, k).

passing through its boundary ∂N leaves N in at least one of the directions (as $\xi \to \infty$ or $\xi \to -\infty$). The set $S(N)$ of trajectories of system (3) that remain in N for an arbitrary ξ is called the isolated invariant set. For the isolating neighborhoods that we are constructing, the set $S(N)$ should be maximal, i.e., it should not have common points with the boundary ∂N.

The set N_1 is bounded by the hyperplanes $u = \varepsilon$, $u = D + \varepsilon$, $T = 1$, $T = T_*$, $k = 0$, $k = 1 + \varepsilon$ $(U_* \leqslant u \leqslant D + \varepsilon)$, $k = 1 - \varepsilon$ $(\varepsilon \leqslant u \leqslant U_*)$, and $w = \varepsilon$, $w = D + \varepsilon$. Here ε is a small number, T_* is a rather large number (the values of T on the surface $F_1 = 0$ are smaller than T_*), and $u(A_1) < U_* < u(B_1)$. In addition, we add to the neighborhood a sphere of radius ε with center at the point A_0. The cross sections of the neighborhood N_1 by the planes (u, T), (u, k), and (u, w) are shown in Figs. 1–3, respectively. We denote as b^+ a set of points that belong to the boundary ∂N_1 of the set N_1, and the trajectories passing through b^+ leave N_1; similarly, we denote as b^- a set of input points to N_1 ($b^- \subset \partial N_1$). As is shown in Figs. 1–3, the set of points b^+ consists of the hyperplanes $u = D + \varepsilon$ and $T = 1$, the section $u \in [U_1, D + \varepsilon]$ for $T = T_*$, the set $u \in [\varepsilon, U_*]$ for $k = 1 - \varepsilon$, and also the subset of the hyperplane $u = U_*$, where $k \in [1 - \varepsilon, 1 + \varepsilon]$ and $T \in [1, T_1]$.

For rather small ε, all trajectories passing through the boundary of the ε-neighborhood of the point A_0 leave this neighborhood at least in one direction owing to the saddle type of the point; the intersection of the set of input points of the trajectories to this neighborhood with the boundary ∂N_1 is a bound set with a set of points b^- on the hyperplane $k = 0$, and the output points form a bound set with a set of points b^+ on $u = D + \varepsilon$.

The neighborhood N_2 is bounded by the hyperplanes $u = D + \varepsilon$, $u = \varepsilon$, $k = 0$, $k = 1 + \varepsilon$ $(\varepsilon \leqslant u \leqslant U_*)$, $k = 1 - \varepsilon$ $(U_* \leqslant u \leqslant D + \varepsilon)$, $u = U_*$ $(k \in [1 - \varepsilon, 1 + \varepsilon])$, $T = 1$, $T = T_*$, $w = \varepsilon$, and $w = D + \varepsilon$. As for N_1, we supplement N_2 by a sphere of radius ε with center at the point A_0. Here the set b^+ consists of points where $u = D + \varepsilon$, $T = 1$, $T = T_*$ $(U_1 \leqslant u \leqslant D + \varepsilon)$, and $k = 1 - \varepsilon$ $(U_* \leqslant u \leqslant D + \varepsilon)$, and the subset of the hyperplane $u = U_*$, where $k \in [1 - \varepsilon, 1 + \varepsilon]$ and $T \in [T_1, T_*]$. The cross sections of the neighborhood N_2 by the planes (u, T), (u, w), and (u, k) are shown in Figs. 1, 3, and 4, respectively.

We also note that all trajectories of system (3) that have common points with the set $k = 1$ remain on this hyperplane for all values of ξ. In addition, the position of the curves in this set indicates that there exists a unique trajectory that begins at the point A_1 and ends at the point B_1 (along this trajectory, we have $k = 1$). From the physical point of view, this situation corresponds to the shock wave in a gas where the substance of the c-phase has been completely evaporated and reacted. The proof of the existence and uniqueness of this trajectory is similar to that given in [1].

Indices of Isolated Sets. Let S be the maximal invariant set contained in the neighborhood N, i.e., all trajectories of system (3) passing through the boundary ∂N leave N at least in one time direction, and the closure of S is contained in N. The Conley index $h(S)$ of the set N is a homotopical class of equivalence of the factor-space N/b^+ [11, 13]: $h(S) = [N/b^+]$. The Conley index corresponds to the Morse index if the latter is determinate, i.e., for nondegenerate singular points. Thus, for the rest point, which is an isolated invariant set, this index is determined by the number of roots of the characteristic equation that have positive real parts. The Conley index is a topological invariant and is not changed for an arbitrary isolating neighborhood containing this isolated invariant set.

We calculate the index of the singular point A_0. The set of output points for a four-dimensional ε-sphere with center at the point A_0 is a three-dimensional manifold. Factorizing this set, we obtain that the resulting space is homeomorphic to the space of the homotopical type Σ^3. In a similar manner, we can show that $h(A_1) = \Sigma^2$ and $h(B_1) = \Sigma^1$. Here Σ^n is an n-dimensional sphere (pointed). For nondegenerate singular points A_0, A_1, and B_1, the number n coincides with the Morse indices for these points.

We calculate the indices of the isolating neighborhoods. In the four-dimensional phase space $X(u, T, k, w)$, system (3) defines a continuous mapping f: $X \times R \to X$, where $\xi \in R$. If we denote f as $\boldsymbol{x} \cdot \xi$ for $\boldsymbol{x} \in X$, then the relation $(\boldsymbol{x} \cdot \xi) \cdot s = \boldsymbol{x} \cdot (\xi + s)$ is valid. Therefore, f is a flow. This means that the trajectories of system (3) can touch isolating neighborhoods (i.e., passing through the boundary ∂N_i, leave the set N_i in both time directions), and the boundary ∂N_i itself may consist, in particular, of sectors of the trajectories leaving N_i. The index of the isolating neighborhood coincides with the index of the isolating block that does not possess these properties.

For the isolating neighborhood N_1, the set of output points b^+ is doubly connected. If we identify b^+ and collapse it into a point, the resultant space is a space of the homotopical type Σ^2, i.e., $h(S) = \Sigma^2$.

The set of output points b^+ for the isolating neighborhood N_2 is simply connected (as the set of input points b^-). By collapsing b^+ into a point, we obtain that the statement $h(S) = \bar{0}$ is valid for the neighborhood N_2, i.e., the factor-space is a space of the homotopical type of a one-point space.

Existence of Trajectories Connecting Singular Points. We consider the isolating neighborhood N_1. It is known [13] that, if the isolated invariant set S consisted of only two singular points $S = \{A_0, A_1\}$, it would follow that $h(S) = h(A_0) \vee h(A_1)$. Since $\Sigma^3 \vee \Sigma^2 \not\equiv \Sigma^2$, the invariant set $\{A_0, A_1\}$ is not maximum, i.e., there are other trajectories in the neighborhood N_1 that remain in N_1 during the entire time ξ.

It should be noted that the flow prescribed by the mapping f is gradientlike inside the isolating neighborhoods N_i, $i = 1$, 2, if $k \in (0, 1)$. For example, for this flow, there exists the Lyapunov function $G(k) = 1 - k^2$, which is rigorously decreasing along all trajectories in N_i other than those in the equilibrium state. This fact eliminates the possibility of existence of closed trajectories and limiting cycles. Hence, there exist trajectories for which the point A_0 is an α-limiting set and the point A_1 is the ω-limiting set, i.e., trajectories that connect these points.

We consider trajectories in the isolating neighborhood N_2. We note that all the integral curves of system (3) for which the point B_1 is an ω-limiting set compose a three-dimensional manifold S_1 that crosses an infinitesimal neighborhood of the point A_1. If some trajectories that belong to S_1 and enter this small neighborhood do not leave N_2 as $\xi \to -\infty$, then N_2 is not an isolating neighborhood. Nevertheless, owing to the fact that the flow is gradientlike, these curves reach the hyperplane $k = 0$, and the point A_0 should be α-limiting for them, which proves the existence of the sought trajectories.

We assume that all curves of the manifold S_1 that enter a small neighborhood of the point A_1 leave N_2. Then the neighborhood N_2 is isolating. Since in this case we have $h(S) = \bar{0} \neq \Sigma^3 \vee \Sigma^1$, the invariant set S also contains trajectories that differ from the quiescent states A_0 and B_1, which indicates the existence of integral curves connecting these singular points.

We consider the case $D = D_*$. Since there exist trajectories that connect all three singular points for all values of the parameter D greater than the critical value, in the limiting case, where two of them merge into one, the sought trajectory corresponding to the steady-state Chapman–Jouguet detonation continues to exist.

Thus, it is shown in the present paper that, under certain, rather strong limitations on the character of energy release and interphase interaction, there exist solutions of the traveling-wave type, which correspond to weak and strong detonation of gas mixtures, and also to the Chapman–Jouguet detonation in the limiting case.

REFERENCES

1. R. Mises, "On the thickness of a steady shock wave," *J. Aeronaut. Sci.*, **17**, No. 9, 551–554 (1950).
2. D. Gilbarg, "The existence and limit behavior of the one-dimensional shock layer," *Amer. J. Math.*, **73**, No. 2, 256–274 (1951).
3. J. O. Hirschfelder and C. F. Curtiss, "Theory of detonations. 1. Irreversible unimolecular reaction," *J. Chem. Phys.*, **28**, No. 6, 1130–1147 (1958).
4. B. Linder, C. F. Curtiss, and J. O. Hirschfelder, "Theory of detonations. 2. Reversible unimolecular reaction," *ibid.*, pp. 1147–1151.
5. W. W. Wood, "Existence of detonations for small values of the rate parameter," *Phys. Fluids*, **4**, No. 1, 46–60 (1961).
6. W. W. Wood, "Existence of detonations for large values of the rate parameter," *Phys. Fluids*, **6**, No. 8, 1081–1090 (1963).
7. F. A. Williams, "Structure of detonations in dilute sprays," *Phys. Fluids*, **4**, No. 11, 1434–1443 (1961).
8. Ya. B. Zel'dovich and Yu. P. Raizer, *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*, Academic Press, New York (1967).
9. F. A. Williams, *Combustion Theory*, Addison-Wesley, Reading, Massachusetts (1964).
10. A. A. Majda, "Qualitative model for dynamic combustion," *SIAM, J. Appl. Math.*, **41**, No. 1, 70–93 (1981).
11. R. A. Gardner, "On the detonation of a combustible gas," *Trans. Am. Math. Soc.*, **277**, No. 2, 431–468 (1983).
12. D. V. Voronin, "Existence of a steady solution of the problem of detonation-wave propagation in gas mixtures," in: *Mechanics of Fast Processes* (collected scientific papers) [in Russian], No. 73 (1985), pp. 9–25.
13. J. Smoller, *Shock Waves and Reaction-Diffusion Equations*, Springer-Verlag, New York (1994).
14. R. I. Nigmatulin, *Dynamics of Multiphase Media*, Parts 1 and 2, Hemisphere, New York (1991).