SOLUTION OF THE THERMOELASTICITY PROBLEM IN THE FORM OF A TRAVELING WAVE AND ITS APPLICATION TO ANALYSIS OF POSSIBLE REGIMES OF SOLID-PHASE TRANSFORMATIONS

A. G. Knyazeva

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Using the known self-similar solutions of the theory of temperature stresses and thermal theory of combustion on the basis of coupled models of solid-phase combustion proposed for the description of various physicochemical transformations, it is shown that the regime of fast (supersonic) solid-phase transformation (solid-phase detonation) is typical of a reacting medium, as well as the regime of slow combustion. Partial (exact) integration and transformation of variables allow one to reduce the systems of equations that describe various solid-phase processes to shock-wave equations having continuous solutions of the traveling-wave type.

Key words: solid-phase transformations, coupled thermomechanical models, self-similar solution, combustion, detonation.

Introduction. The self-similar solution of the nonlinear problem of the theory of temperature stresses, which describes propagation of a wave with a constant profile (shock wave) moving in a nondeformed quiescent medium, causing deformation of the latter, has been known for a long time [1]. This solution is similar to the solution of the Burgers equation known in the theory of nonlinear waves. The author of the present work became interested in solutions of this type in constructing models of solid-phase transformations, which can propagate over the substance both in the slow and fast regimes.

The regime of solid-phase transformations is known to depend on the hydrodynamic flow pattern. There exist the thermal and hydrodynamic theories of combustion, which describe these transformations. According to the thermal theory of combustion, emergence of different transformation regimes can be caused by the presence of parallel and consecutive stages of chemical transformation, phase transitions, and heat transfer to the ambient medium, i.e., additional sources and drains of heat.

The studies showed that transformations, which can propagate with different velocities, can be described in a unified manner on the basis of coupled thermomechanical models. In particular, the regime of fast transformation in the solid phase for exothermal reactions is typical of the system, as well as the regime of slow combustion (layerby-layer self-sustaining transformation). Additional sources and drains of heat lead to the appearance of both fast and slow regimes.

The properties of self-similar solutions in coupled problems of solid-phase combustion are considered in the present paper.

1. Basic Equations of the Theory of Temperature Stresses. We write some known relations that will be required below. The system of equations of the theory of temperature stresses [2] includes the nonlinear heat-conduction equation

$$\rho c_{\varepsilon} \frac{\partial T}{\partial t} = -\nabla \cdot \boldsymbol{J}_T - 3K \alpha_T T \frac{\partial \varepsilon_{kk}}{\partial t}$$
(1)

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and the equations of motion

$$\rho \,\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \nabla \cdot \hat{\sigma} + \rho \boldsymbol{F},\tag{2}$$

where T is the temperature, J_T is the heat-flux density vector, \boldsymbol{u} is the displacement vector, t is the time, ρ is the density of the substance, c_{ε} is the heat capacity at constant strain, α_T is the linear coefficient of thermal expansion, $\hat{\sigma}$ is the stress tensor, \boldsymbol{F} is the vector of mass forces, $K = \lambda + 2\mu/3$ is the isothermal modulus of triaxial compression, λ and μ are the Lamé coefficients, and $\varepsilon_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ are the components of the tensor of small Cauchy strains. Additional expressions relating the components of stress and strain tensors are the Duhamel–Neumann relations

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \delta_{ij} [\lambda\varepsilon_{kk} - 3K\alpha_T (T - T_0)]. \tag{3}$$

The heat flux is related to the temperature gradient via the Fourier law

$$\boldsymbol{J}_T = -\lambda_T \nabla T,\tag{4}$$

where λ_T is the thermal conductivity.

The real process of thermoelastic deformation of a body is irreversible [2], which is caused by the temperature gradient. There exist various generalizations of the theory of thermoelasticity, including those taking into account the finite velocity of heat propagation and other irreversible processes. If the heat flux obeys the generalized Fourier law

$$\boldsymbol{J}_T = -\lambda_T \nabla T - t_r \dot{\boldsymbol{J}}_T, \tag{5}$$

where t_r is the time of heat-flux relaxation, then Eqs. (1)–(3) and (5) are equations of the so-called generalized thermomechanics [3], which considers the hyperbolic equation of heat conduction. As a generalization of Eq. (1), Nikitenko [4] obtained an equation of the form

$$\rho c_{\varepsilon} \frac{\partial T}{\partial t} = -\nabla \cdot \boldsymbol{J}_T - T \frac{\partial}{\partial t} \left(\varepsilon_{kk} \frac{\partial (Kw)}{\partial T} \right) + Q_T, \tag{6}$$

where Q_T is the density of internal heat sources and w is a function depending on temperature and other thermodynamic variables. This function also enters into the generalization of Eqs. (3):

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \delta_{ij}(\lambda\varepsilon_{kk} - Kw). \tag{7}$$

Other generalizations based on methods of nonequilibrium thermodynamics are also possible [5].

The simplest classical problem of the theory of temperature stresses is formulated as the problem of a thermal shock on the surface of a half-space free from the action of mass and external mechanical forces. At the time t = 0, the temperature of the ambient medium (or solid body surface) changes instantaneously from the value T_0 to the value T_s . Hence, body deformation in this case can be caused only by time-dependent heating or cooling of the body surface. The solution of the problem reduces to solving the equations

$$\rho c_{\varepsilon} \frac{\partial T}{\partial t} = \lambda_T \frac{\partial^2 T}{\partial x^2} - 3K \alpha_T T \frac{\partial \varepsilon_{kk}}{\partial t}, \tag{8}$$

$$\rho \,\frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} \tag{9}$$

with the boundary conditions

$$x = 0; T = T_s, u = 0 (or \sigma_{11} = 0), (10)$$
$$x \to \infty; \lambda_T \frac{\partial T}{\partial x} = 0$$

and the initial condition

$$t = 0;$$
 $T = T_0, \quad u = 0.$ (11)

In (1)–(11), u is the component of the displacement vector in the direction of the Ox axis and $\varepsilon_{kk} = \varepsilon_{11} = \varepsilon = \partial u/\partial x$; the remaining components of the displacement vector and strain tensor equal zero. The following relations are valid for stress tensor components: $\sigma_{11} \neq 0$, $\sigma_{22} = \sigma_{33} \neq 0$, and $\sigma_{12} = \sigma_{23} = \sigma_{31} = 0$.

Using relations (3), the problem can be reformulated in stresses or displacements:

$$\rho c_{\varepsilon} \frac{\partial T}{\partial t} = \lambda_T \frac{\partial^2 T}{\partial x^2} - 3K\alpha_T T \frac{\partial^2 u}{\partial t \partial x}, \qquad \rho \frac{\partial^2 u}{\partial t^2} = (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} - 3K\alpha_T \frac{\partial T}{\partial x}$$

Sometimes, it is convenient to write Eq. (9) in the form

$$\rho \frac{\partial^2 \varepsilon}{\partial t^2} = (\lambda + 2\mu) \frac{\partial^2 \varepsilon}{\partial x^2} - 3K\alpha_T \frac{\partial^2 T}{\partial x^2}.$$
(12)

In the classical theory of thermoelasticity [2], with allowance for smallness of the coupling coefficient

$$\omega_0 = \frac{(3K\alpha_T)^2}{\lambda + 2\mu} \, \frac{T_0}{c_\varepsilon \rho},$$

the heat-conduction equation is linearized at the temperature of the nondeformed state. Therefore, in most papers that require temperature stresses to be evaluated, the effect of coupling is neglected. Solutions of the problems of linear theory are well studied. These solutions are waves rapidly decaying with distance from the heated surface. There are no solutions of the traveling wave type in the linear theory of thermoelasticity. Such solutions appear in the coupled nonlinear theory [1].

2. Solution of the Traveling-Wave Type. For certainty, we assume that $T_s > T_0$. Then, in the variables

$$\theta = \frac{T - T_0}{T_s - T_0}, \qquad \xi = \frac{x}{x_*}, \qquad \tau = \frac{t}{t_*}, \qquad e = \frac{\varepsilon}{\varepsilon_*}, \tag{13}$$

where

$$x_* = \sqrt{\varpi_T t_*}, \qquad \varepsilon_* = \frac{3K\alpha_T}{\lambda + 2\mu} \, (T_s - T_0), \qquad \varpi_T = \frac{\lambda_T}{\rho c_\varepsilon}$$

and the scale t_* is of no principal importance, Eqs. (8) and (12) take the form

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} - \omega(\theta + \sigma) \frac{\partial e}{\partial \tau}, \qquad \frac{\partial^2 e}{\partial \xi^2} - \frac{\partial^2 \theta}{\partial \xi^2} = \alpha^2 \frac{\partial^2 e}{\partial \tau^2},$$

where

$$\omega = \frac{(3K\alpha_T)^2}{\lambda + 2\mu} \frac{T_s - T_0}{c_\varepsilon \rho}, \qquad \sigma = \frac{T_0}{T_s - T_0}, \qquad \alpha^2 = \frac{\rho}{\lambda + 2\mu} \frac{\varpi_T}{t_*}.$$

We consider solutions of the nonlinear system of equations, which are waves with a constant profile [6] moving with a velocity V. We pass to the coordinate $X = \xi - V\tau$, assuming the wave to move to the right. Then, the shock-wave solution should satisfy the system

$$-V\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \omega(\theta + \sigma)V\frac{de}{dX};$$
(14)

$$\frac{d^2e}{dX^2} - \frac{d^2\theta}{dX^2} = \alpha^2 \frac{d^2e}{dX^2} \tag{15}$$

and the conditions

$$\begin{aligned} X \to -\infty; \qquad \theta = \theta_1 = 1, \\ X \to +\infty; \qquad \theta = \theta_2 = 0. \end{aligned}$$
(16)

Equation (15) is readily integrated. Taking into account the absence of disturbances at infinity $(X \to +\infty)$, we have

$$\frac{de}{dX} = \frac{1}{1 - (\alpha V)^2} \frac{d\theta}{dX}, \qquad e = \frac{1}{1 - (\alpha V)^2} \theta.$$
(17)

Hence, the heat-conduction equation takes the form

$$-V\left(1+\frac{\omega}{1-(\alpha V)^2}\left(\theta+\sigma\right)\right)\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2}.$$
(18)

Under the condition $(\alpha V)^2 > 1$ or $V^2 > 1/\alpha^2$, Eq. (18) coincides in form with the Burgers equation (see, e.g., [6]) written in self-similar variables. Indeed, using the quantities

$$U = \omega^{-1}((\alpha V)^2 - 1 - \omega \sigma), \qquad \nu = ((\alpha V)^2 - 1)/(V\omega),$$

we obtain the equation

$$-U\frac{d\theta}{dX} + \theta\frac{d\theta}{dX} = \nu\frac{d^2\theta}{dX^2},\tag{19}$$

whose normal (non-self-similar) form is

$$\frac{\partial\theta}{\partial\tau} + \theta \,\frac{\partial\theta}{\partial\xi} = \nu \,\frac{\partial^2\theta}{\partial\xi^2}.\tag{20}$$

Solutions of Eq. (19) in the form of a wave with a constant profile exist for $V^2 > (1 + \omega \sigma)/\alpha^2$ or $v_n^2 > c^2(1 + \omega_0)$, where $v_n = V\sqrt{\frac{\omega_T}{t_*}}$ is the wave velocity, $c = [(\lambda + 2\mu)/\rho]^{1/2}$ is the velocity of sound, and $\omega_0 \equiv \omega \sigma$. The exact solution of the nonlinear equation (19) satisfying conditions (16) can be presented as

 $\theta = 1 - (1 + \exp(-X/(2\nu)))^{-1}, \qquad U = 1/2,$

which readily yields the velocity V for prescribed temperatures ahead of the wave front and behind it. This solution is a weak shock wave. Since strains and stresses are linearly related to temperature, the strains and stresses in the wave front satisfy the equation of the form (18) or (19). The Burgers equation has also an exact solution, which is reduced to the ordinary linear heat-conduction equation by means of the Cole–Hopf substitution. This allows one to study the evolution of the initial disturbance of a given form to a stationary profile. In particular, it is shown [6] that the temperature remains continuous in passing through the shock wave in a heat-conducting medium. As $\nu \to 0$, the solutions of Eq. (20) converge to shock-wave discontinuous solutions of the equation

$$\frac{\partial\theta}{\partial\tau} + \theta \,\frac{\partial\theta}{\partial\xi} = 0,\tag{21}$$

satisfying the condition

$$U = (\theta_1 + \theta_2)/2, \qquad \theta_1 > U > \theta_2.$$

Similar conclusions were drawn for inelastic media in [7, 8] and other papers.

3. Combustion and Detonation. Let the medium have an internal source of heat due to an exothermal chemical reaction. If only thermal stresses and strains are significant and the chemical transformation can be described by the summarized scheme "solid reagent-solid product," the equation of motion remains unchanged [see (9)] and the one-dimensional heat-conduction equation acquires the form

$$\rho c_{\varepsilon} \frac{\partial T}{\partial t} = \lambda_T \frac{\partial^2 T}{\partial x^2} - 3K \alpha_T T \frac{\partial \varepsilon_{kk}}{\partial t} + Q_r k_r \varphi_1(y) \varphi_2(T).$$
(22)

The degree of transformation y satisfies the kinetic equation

$$\frac{\partial y}{\partial t} = k_{\rm r}\varphi_1(y)\varphi_2(T). \tag{23}$$

In the dimensionless variables (13) (with the substitution of T_* for T_s) under the condition that the reaction rate satisfies the Arrhenius law

$$\varphi_2(T) = \exp\left(-E_{\rm r}/(RT)\right),$$

Eqs. (22) and (23) take the form

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial\xi^2} - \omega(\theta + \sigma)\frac{\partial e}{\partial\tau} + \theta_0^{-1}\varphi_1(y)\varphi_2(\theta);$$
(24)

$$\frac{\partial y}{\partial \tau} = \varphi_1(y)\varphi_2(\theta),\tag{25}$$

where

$$\varphi_2(\theta) = \exp\left(-\frac{1+\sigma}{\theta+\sigma}\frac{1}{\beta}\right), \qquad \beta = \frac{RT_*}{E_r}, \qquad \theta_0 = \frac{T_* - T_0}{Q_r/(c_\varepsilon\rho)}, \qquad \sigma = \frac{T_0}{T_* - T_0}.$$

Determining the scale temperature as the temperature of reaction products in the thermal theory of combustion [9] $T_* = T_0 + Q_r/(c_{\varepsilon}\rho)$, we reduce the number of parameters. In this case, the time scale is conveniently defined as $t_* = k_r^{-1}$. The solution of the traveling-wave type (wave with a constant profile) satisfies the system

$$-V\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \omega(\theta + \sigma)V\frac{de}{dX} + \varphi_1(y)\varphi_2(\theta);$$
(26)

$$-V\frac{dy}{dX} = \varphi_1(y)\varphi_2(\theta) \tag{27}$$

and (14), which is partly integrated. Using Eq. (17), we find

$$-V\left(1+\frac{\omega}{1-(\alpha V)^2}\left(\theta+\sigma\right)\right)\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \varphi_1(y)\varphi_2(\theta).$$
(28)

Integrating Eq. (28) with allowance for (27) and assuming that y = 0 in the undisturbed substance, we obtain

$$-V\Big(1+\frac{\omega\sigma}{1-(\alpha V)^2}\Big)\theta-\frac{\omega V}{1-(\alpha V)^2}\frac{\theta^2}{2}=\frac{d\theta}{dX}-Vy.$$

Assuming that $X = \xi - V\tau \rightarrow -\infty$ and y = 1 in the region of reaction products, we obtain the quadratic equation for the temperature of the disturbed substance

$$B\theta_b^2 + (2B\sigma - 1)\theta_b + 1 = 0, \qquad B = \omega/(2((\alpha V)^2 - 1)), \tag{29}$$

the number of its solutions depends on the parameters ω , V, α , and σ .

For $B \leq 0$ [which is possible if $V < \alpha^{-1}$ or $v_n^2 < (\lambda + 2\mu)/\rho$], Eq. (29) has the only real solution. Each value of B < 0 corresponds to only one temperature $\theta_b = \theta_1 < 1$. For $B \to 0$ ($\omega \to 0$), we have $\theta_b \to 1$.

For B > 0, the quadratic equation (29) has two real solutions: $\theta_b = \theta_A$ and $\theta_b = \theta_B$. If α , ω , and σ are fixed, each value of temperature θ_B corresponds to its own value of velocity V satisfying the condition $V > \alpha^{-1}$ or $v_n^2 > (\lambda + 2\mu)/\rho$. Two values of temperature (θ_A and θ_B) correspond to two stationary points of the heat-conduction equation (28) as $X \to -\infty$ (in the region of reaction products), which are similar to the stationary points of the Burgers equation [6], and the point A is a stable singular point. The exact solution of this problem cannot be obtained.

An asymptotic analysis of problem (26), (27), (15) with conditions typical of the combustion theory, which was performed in [10], also yields two types of solutions in the form of a traveling wave.

As $\omega \to 0$, the continuous solution of the first type $(V < \alpha^{-1})$ converges to the solution of the simplest classical problem of the theory of solid-phase combustion, including Eqs. (27) and

$$-V\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \varphi_1(y)\varphi_2(\theta)$$
(30)

with the boundary conditions (16). These equations together with Eq. (15) form a system of equations of noncoupled theory of thermoelasticity written in self-similar variables. According to the combustion theory [9], problem (30), (27), (16) has only one solution. For each value of $\omega \ge 0$, the solution is also unique; the wave with a constant profile propagates with a velocity lower than the velocity of sound.

Solutions of the second type $(V > \alpha^{-1})$ are also continuous and are shock-wave solutions. These solutions describe shock waves in a heat-conducting medium with an exothermal chemical reaction or solid-phase detonation.

Using the quantities U and ν , we write Eq. (28) as

$$-U\frac{d\theta}{dX} + \theta\frac{d\theta}{dX} = \nu\frac{d^2\theta}{dX^2} + \nu\varphi_1(y)\varphi_1(\theta).$$
(31)

As $\nu \to 0$, which corresponds to $V \to \alpha^{-1}$, continuous solutions of Eq. (31) converge to discontinuous shock-wave solutions of Eq. (21).

The stresses and strains in the self-similar problem are completely determined by the temperature and degree of transformation, which can easily be shown by using integrals of the equation of motion (17) and relations between the stresses and strains in dimensionless variables. For the component of the stress tensor σ_{11} (in the direction of front motion), we have

$$s = e - (\theta + \sigma) = -\sigma + \theta(\alpha V)^2 / (1 - (\alpha V)^2),$$

where $s = \sigma_{11}/\sigma_*$ and $\sigma_* = 3K\alpha_T(T_* - T_0)$. (In the case of uniaxial deformation considered, three components of the stress tensor differ from zero: σ_{11} and $\sigma_{22} = \sigma_{33}$.) In the noncoupled problem, the stress (strain) wave 168 with a constant profile, if it is not amplified by an external mechanical action, always runs with a velocity of the wave of chemical transformation, which is lower than the velocity of sound. In this case, the detonation regime of transformation cannot exist notwithstanding the arguments of [11–13]. In the coupled problem ($\omega \neq 0$), there exist two types of waves with a constant profile. The first (subsonic) wave is the consequence of the nonlinear dependence of the rate of chemical heat release on temperature (nonlinear interaction of heat conduction and chemical transformation). The second wave exists due to energy transfer by the wave of mechanical disturbances ("hydrodynamic" transfer of energy) or due to nonlinear interaction of the heat-transfer processes and propagation of mechanical disturbances. The linearized system of equations has no self-similar solutions of this kind.

The "nonuniqueness" of the solution of the simplest coupled problem of solid-phase combustion is demonstrated in [10] by an example of a stepwise heat-release function (in this case, exact solutions of the problem can be found). The wave velocity V is the eigenvalue of the problem of solid-phase combustion (27), (30); system (15), (26), (27) has eigenvalues of two types: $V_1 < \alpha^{-1}$ and $V_2 > \alpha^{-1}$.

Note, for $\varphi_1(y) = 1$, Eq. (28) is a particular case of the Lienard equation whose solution exists and is unique for fixed parameters, including the prescribed value of V [14]. The type of the solution depends significantly on the function at the first derivative, including the values of parameters.

Similar results are obtained by using the generalized Fourier law (5) with a finite time of heat-flux relaxation [15] and also in analyzing the solution of the coupled problem with the relations of the Maxwellian model of a viscoelastic body are used instead of the Duhamel–Neumann relations (see, e.g., [16, 17]).

4. Changes in Volume During Solid-Phase Transformation. The model of solid-phase transformation considered above does not take into account the changes in properties, which should affect physical parameters. A real detonation wave has a transitional zone where the initial substance transforms into detonation products. Since the transitional zone is small as compared to the specimen size and the residence time of particles in this zone is also small, the transitional zone in solving many problems is replaced by a strong discontinuity [18]. Then, detonation can be defined as a hydrodynamic wave process of propagation of an exothermal reaction zone over the substance with a supersonic velocity. A similar approach is used in modeling slow combustion processes: the velocity of front motion is determined by the velocity of chemical heat release in the narrow reaction region; in the limit, the latter is a surface separating reagents and products whose properties are different in the general case. Heating of the substance ahead of the reaction front and, hence, its propagation are ensured by heat conduction. In the present work, it is of interest to consider the process of propagation of the chemical reaction zone over the substance in which the substance properties are continuously changed in the course of transformation of the initial substances into reaction products both in the case of slow and "explosive" transformation. Various models can be constructed to describe these processes, including those that do not imply low strains. In this case, it is necessary to use continuity equations and, possibly, nonlinear equations of state in reagents, products, and reaction zone.

Within the framework of the above approximation of low strains, displacements, and velocities and the linear thermal equation of state [Eq. (3)], we try to take into account the basic characteristics of "explosive" transformation: expansion of the substance, which is accompanied by an increase in pressure, and excitation of shock waves.

Not neglecting the coupled character of different processes (in our case, the processes of heat transfer and deformation), i.e., the "small" term in Eq. (1) or (6), we take into account that the components of the stress tensor σ_{ij} in each particle in an elastic body are functions of the components of the strain tensor ε_{ij} , temperature, and other physicochemical parameters [19]. It can easily be shown that, if other parameters are described by scalar functions, such a relation for an isotropic body has the form (7), where the function w depends on temperature and concentrations of reagents and products [4, 20]. Assuming further that the chemical reaction can be described by the simplest global scheme $A \to B$, we find

$$w = 3[\alpha_T(T - T_0) + (\alpha_B - \alpha_A)(y - y_0)].$$
(32)

Here α_B and α_A are the coefficients of "concentrational expansion" of the product and reagent, which are determined in thermodynamics in the same manner as the thermal expansion coefficient and are directly related to partial specific volumes of the substances participating in the reaction [20]. This does not eliminate, however, the dependence of physicochemical properties on temperature and degree of transformation. Using Eq. (7) (or similar equations written in increments), Eq. (32), continuity equation, and usual equations of motion in the form

$$\rho \, \frac{d\boldsymbol{v}}{dt} = \nabla \cdot \hat{\sigma} + \rho \boldsymbol{F},\tag{33}$$

where v is the velocity vector, we obtain the model of an elastic body with a solid-phase reaction proceeding in it. In the case of small strains, accelerations, and displacements, the equations of motion remain in the form (2) and

the continuity equation is not needed. This model of the elastic body is readily generalized to an arbitrary number of components and stages of chemical reactions with the use of additional thermodynamic relations and also to the case of large strains.

The self-similar solution (solution in the form of a traveling wave) for system (22), (23), (9) with additional relations (7) and (32) is constructed in the same manner as in Sec. 3. The one-dimensional equation of motion in terms of strains becomes

$$\rho \frac{\partial^2 \varepsilon}{\partial t^2} = (\lambda + 2\mu) \frac{\partial^2 \varepsilon}{\partial x^2} - 3K \Big(\alpha_T \frac{\partial^2 T}{\partial x^2} + (\alpha_B - \alpha_A) \frac{\partial^2 y}{\partial x^2} \Big).$$

In the dimensionless variables (13), we have Eqs. (24), (25), and

$$\frac{\partial^2 e}{\partial \xi^2} - \left(\frac{\partial^2 \theta}{\partial \xi^2} + g \frac{\partial^2 y}{\partial \xi^2}\right) = \alpha^2 \frac{\partial^2 e}{\partial \tau^2},$$

where $g = (\alpha_B - \alpha_A)/(\alpha_T(T_* - T_0))$ is a dimensionless parameter characterizing the reaction proceeding in the solid substance. For g > 0, the reaction proceeds with an increase in volume; for g < 0, the reaction proceeds with a decrease in volume; for g = 0, the specific volume remains unchanged in the course of the reaction.

In a stationary wave moving to the right with a velocity V, the strains are related to temperature and degree of transformation by the expression

$$e = [\theta + g(y - y_0)] / [1 - (\alpha V)^2].$$

In this case, the heat-conduction equation takes the form

$$-V\Big(1+\frac{\omega(\theta+\sigma)}{1-(\alpha V)^2}\Big)\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \varphi_1(y)\varphi_2(\theta)\Big(1-\frac{\omega(\theta+\sigma)}{1-(\alpha V)^2}g\Big).$$
(34)

Using the quantities U and ν , we can easily show that the solutions of Eq. (34) converge to discontinuous solutions of the shock-wave equation (21) as $\nu \to 0$.

Exact solutions of this problem could not be obtained yet. Using the method of matched asymptotic expansions (for the zero-order reaction), it can be shown [10] that models that take into account the change in volume in the course of transformation admit two types of solutions: subsonic and supersonic (slow combustion regime and solid-phase detonation). These solutions are continuous. The question on the number of these or those regimes remains open.

It should be noted that the coupled model of solid-phase transformation also admits the existence of selfsimilar solutions if the chemical reaction is endothermal (in this case, there is the minus sign at the second term in Eq. (34) and Q_r is replaced by $|Q_r|$ in the definition of scale temperature). The overall exception from the reaction zone is caused either by the fact that the endothermal reaction leads to an increase in volume, and there occurs energy release in the detonation wave due to the work of stresses or by the fact that the endothermal reaction proceeds with a decrease in volume, heat release in the slow wave of solid-phase combustion exceeds the endoeffect of transformation.

5. Generalization of the Simplest Model to the Case of a Compressible Medium. The aboveconsidered coupled models of solid-phase combustion are valid if the medium is assumed to be incompressible, i.e., $\nabla \cdot \boldsymbol{v} = 0$. We assume that strains, accelerations, and displacements are not small. In system (6), (23), (33), partial derivatives with respect to time should be replaced by total derivatives d/dt. We supplement these equations by the continuity equation

$$\frac{d\rho}{dt} + \rho \nabla \cdot \boldsymbol{v} = 0$$

and the linear relation between the components of stress and strain tensors written in increments:

$$d\sigma_{ij} = 2\mu \, d\varepsilon_{ij} + \delta_{ij} (\lambda \, d\varepsilon_{kk} - K \, dw).$$

The one-dimensional system of equations (in the case of one chemical reaction proceeding in the substance) takes the form

$$\rho c_{\varepsilon} \frac{dT}{dt} = \lambda_T \frac{\partial^2 T}{\partial x^2} - 3\rho \alpha_T T \frac{d}{dt} \left(\frac{K}{\rho} \varepsilon\right) + Q_r k_r \varphi_1(y) \varphi_2(T),$$
$$\frac{dy}{dt} = k_r \varphi_1(y) \varphi_2(T), \qquad \rho \frac{dv}{dt} = \frac{\partial \sigma_{11}}{\partial x},$$

$$\frac{d\rho}{dt} + \rho \, \frac{dv}{dx} = 0, \qquad \frac{d\sigma_{11}}{dt} = (\lambda + 2\mu) \, \frac{d\varepsilon}{dt} - K \, \frac{dw}{dt},$$

because $\varepsilon_{kk} \approx \varepsilon_{11}$ in the one-dimensional approximation. The approximation $K/\rho \approx \text{const}$ is valid for most materials. Hence, in the coordinate system fitted to the reaction front moving to the right with a velocity v_n , we have

$$-mc_{\varepsilon} \frac{dT}{dx} = \lambda_T \frac{d^2T}{dx^2} + 3\alpha_T T \frac{K}{\rho} m \frac{d\varepsilon}{dx} - \frac{Q_r}{\rho} m \frac{dy}{dx},$$

$$-m \frac{dy}{dx} = \rho k_r \varphi_1(y) \varphi_2(T), \qquad -m \frac{dv}{dx} = \frac{d\sigma_{11}}{dx},$$

$$m \frac{d\rho}{dx} = -\rho^2 \frac{dv}{dx}, \qquad \frac{d\sigma_{11}}{dx} = (\lambda + 2\mu) \frac{d\varepsilon}{dx} - K \frac{dw}{dx},$$

(35)

where $m = \rho(v_n - v)$ is the mass burning rate and the function w is calculated by Eq. (32).

In the case considered, we can assume that $\varepsilon_{kk} \approx \varepsilon \approx \rho_0/\rho - 1$, which allows us to close and partly integrate system (35) with specified conditions in the reagents $(x \to +\infty)$ and the condition of decay of disturbances in reaction products $(x \to -\infty)$. Indeed, since we have

$$\frac{d\varepsilon}{dx} = -\frac{\rho_0}{\rho^2} \frac{d\rho}{dx}$$

then the third and fifth equations of system (35) yield

$$m \frac{dv}{dx} = \frac{\rho_0}{\rho^2} \left(\lambda + 2\mu\right) \frac{d\rho}{dx} + K \frac{dw}{dx}$$

Using the continuity equation [fourth equation of system (35)], we obtain

$$\frac{dv}{dx} = -\frac{mK}{m^2 - \rho_0(\lambda + 2\mu)} \frac{dw}{dx}.$$
(36)

Similarly, we have

$$\frac{1}{\rho^2}\frac{d\rho}{dx} = \frac{K}{m^2 - \rho_0(\lambda + 2\mu)}\frac{dw}{dx}.$$
(37)

In this case, the heat-conduction equation is replaced by the equation

$$-mc_{\varepsilon}\frac{dT}{dx} = \lambda_T \frac{d^2T}{dx^2} - \frac{3\alpha_T TmK^2 \rho_0}{\rho(m^2 - \rho_0(\lambda + 2\mu))} \frac{dw}{dx} - \frac{Q_r}{\rho} m \frac{dy}{dx}.$$
(38)

In the dimensionless variables θ , $\bar{\rho} = \rho/\rho_0$, $\bar{v} = v/\sqrt{\omega_T/t_*}$, and X, Eqs. (36)–(38) yield

$$\frac{d\bar{v}}{dX} = -\frac{V\gamma}{(\alpha V)^2 - 1} \left(\frac{d\theta}{dX} + g\frac{dy}{dX}\right);\tag{39}$$

$$\frac{1}{\bar{\rho}^2} \frac{d\bar{\rho}}{dX} = \frac{\gamma}{(\alpha V)^2 - 1} \left(\frac{d\theta}{dX} + g \frac{dy}{dX}\right);\tag{40}$$

$$-V\left(1-\frac{\omega(\theta+\sigma)}{(\alpha V)^2-1}\,\bar{\rho}^{-1}\right)\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + \left(1-\frac{\omega(\theta+\sigma)}{(\alpha V)^2-1}\,\bar{\rho}^{-1}\right)\varphi_1(y)\varphi_2(\theta),\tag{41}$$

where

$$\omega = \frac{(3\alpha_T K)^2}{\lambda + 2\mu} \frac{T_* - T_0}{c_{\varepsilon} \rho_0}, \quad V = \frac{m}{\rho_0 \sqrt{\omega_T / t_*}}, \quad \alpha^2 = \frac{\rho_0}{\lambda + 2\mu} \frac{\omega_T}{t_*}, \quad \gamma = \frac{3K\alpha_T (T_* - T_0)}{\lambda + 2\mu}.$$

The parameter γ is the product of the thermal strain $\alpha_T(T_* - T_0)$ and the ratio of velocities of the bulk and longitudinal mechanical waves $3K/(\lambda + 2\mu)$.

Assuming that $\gamma \approx \text{const}$ and $\omega \approx \text{const}$, from (39) and (40), with allowance for the condition of the absence of disturbances in the reagents, we find

$$\bar{\rho} = \frac{1}{1 + \gamma(\theta + gy)/(1 - (\alpha V)^2)}, \qquad \bar{v} = -\frac{\gamma V}{(\alpha V)^2 - 1} \left(\theta + gy\right),$$
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i.e., density and velocity are functions of temperature and degree of transformation.

Hence, we have

$$-V\left[1 - \frac{\omega(\theta + \sigma)}{(\alpha V)^2 - 1} \left(1 + \frac{\gamma(\theta + gy)}{(\alpha V)^2 - 1}\right)\right] \frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + F(\theta, y),\tag{42}$$

where

$$F(\theta, y) = \left(1 + \frac{\omega(\theta + \sigma)}{(\alpha V)^2 - 1}g\right)\varphi_1(y)\varphi_2(\theta)$$

is an effective function of chemical heat release, which, as above, can have an arbitrary sign. Further solving of system (40), (27) with previous conditions seems to be possible with the use of asymptotic or numerical methods. Let us analyze these equations under some simplifying assumptions.

For g = 0 and $\varphi_1 0(y) = 1$, we obtain the Lienard equation.

For $V \ll \alpha^{-1}$, we obtain the usual problem of the combustion theory, in which heat capacity depends on temperature but the heat-release function has a more complicated form than in using the Arrhenius dependence. The problem includes Eq. (27) and heat-conduction equation in the form

$$-V[1+\omega(\theta+\sigma)(1-\gamma(\theta+gy))]\frac{d\theta}{dX} = \frac{d^2\theta}{dX^2} + F(\theta,y),$$

where $F(\theta,y) = [1-\omega(\theta+\sigma)g]\varphi_1(y)\varphi_2(\theta)$, with conditions typical of such problems:

$$X \to +\infty: \qquad \theta = 0, \quad y = 0,$$

$$X \to -\infty$$
: $\theta = \theta_b, \quad y = 1.$

In contrast to simpler models, the sought quantity here is the mass burning rate rather than the linear velocity of the front. An approximate analytical solution can be found in the same manner as in [21].

For $V > \alpha^{-1}$, it is convenient to present Eq. (42) in another form. Using the quantities U and ν , we write

$$-U\frac{d\theta}{dX} + (a_0 + a_1\theta + a_2\theta^2)\frac{d\theta}{dX} = \nu \frac{d^2\theta}{dX^2} + \nu F(\theta, y),$$
(43)

where

$$a_0 = \frac{g\sigma\gamma}{(\alpha V)^2 - 1} y, \qquad a_1 = 1 + \frac{\sigma + gy}{(\alpha V^2) - 1} \gamma, \qquad a_2 = \frac{\gamma}{(\alpha V)^2 - 1}$$

For $\nu \to 0$, (43) yields the equation

$$-U\frac{d\theta}{dX} + C(\theta)\frac{d\theta}{dX} = 0, \qquad C(\theta) = a_0 + a_1\theta + a_2\theta^2,$$

whose normal (non-self-similar) form is the nonlinear equation [generalization of (21)]

$$\frac{\partial\theta}{\partial\tau} + C(\theta)\frac{\partial\theta}{\partial\xi} = 0.$$
 (44)

Studying this equation, we can obtain the main properties of nonlinear hyperbolic waves.

For $F(\theta, y) = 0$, Eq. (43) yields a self-similar form of the shock-wave equation [generalization of (20)]:

$$\frac{\partial\theta}{\partial\tau} + C(\theta)\frac{\partial\theta}{\partial\xi} = \nu \frac{\partial^2\theta}{\partial\xi^2}.$$
(45)

As $\nu \to 0$, continuous solutions of Eq. (45) converge to discontinuous solutions of Eq. (44).

Apparently, as in the case of simpler models, for $\nu \neq 0$ and $F(\theta, y) \neq 0$, one can obtain solutions of Eq. (43) that describe a stationary wave of solid-phase detonation. Such a generalization is also possible for the coupled model of solid-phase combustion, taking into account failure in the reaction front [22, 23].

Conclusions. Thus, the regime of solid-phase transformation in the form of a solid-phase detonation wave is typical of a system capable of transformation, as well as the regime of slow solid-phase combustion. Yet, some issues remain unclear. For instance, under which conditions is this or that transformation regime realized and which fast (and slow) regimes are stable to two-dimensional disturbances? Some results of stability study can be found in [24, 25]. No analytical solutions have been found for most models proposed (except for the simplest variants). The kinetics of chemical reactions in the solid phase and the kinetics of the process of damage accumulation (failure) require further study; a detailed analysis of transformation models in inelastic media is also necessary.

Using coupled models of solid-phase combustion, one can describe transformations that can proceed in the solid phase in various regimes depending on reaction-initiation conditions and reagent structure. For instance, in two regimes (fast and slow), there can occur low-temperature radical reactions in polycrystalline matrices, solid-phase polymerization, solid-phase decomposition of the initiating explosives, etc. Experimental data obtained by various authors, which confirm the possibility of such phenomena, are analyzed in some papers cited above.

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