

A CLASS OF SOLUTIONS OF NONSTATIONARY EQUATIONS OF THE THEORY
OF COMBUSTION OF CONDENSED SUBSTANCES

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A class of solutions of equations of the theory of condensed systems combustion that are defined by fairly simple ordinary differential equations and which in a number of cases can be completely integrated is considered. Certain particular cases of application of the obtained class of solutions to specific problems are presented. These solutions are interesting in themselves and can be used as standards for checking numerical and approximate methods of integration of nonstationary equations of the theory of combustion.

1. **Basic equations.** On a number of assumptions the problem of the course of a single-phase exothermic chemical reaction in a condensed medium can be defined by the system of dimensionless equations

$$\partial \theta / \partial t = \Delta \theta + y \Phi(\theta), \quad \partial y / \partial t = -y \Phi(\theta) \quad (1.1)$$

where t is the r -vector of space variables, $\Delta = \nabla^2$ is the Laplace operator, θ is the dimensionless temperature ($\theta \geq 0$), y is the concentration of the reagent ($0 \leq y \leq 1$), and $\Phi(\theta)$ defines the dependence of the chemical reaction rate on temperature. Usually $\Phi(\theta) \geq 0$ is a monotonically increasing function of θ . For example

$$\Phi(\theta) = \begin{cases} \Phi_1(\theta) \geq 0, & \theta_0 \leq \theta \\ 0, & 0 \leq \theta \leq \theta_0 \end{cases} \quad (1.2)$$

The problem of propagation of a stationary combustion wave in a space completely filled by the reacting medium is the most investigated analytically and numerically with the use of system (1.1). The unknown functions in that problem depend only on a single combination of independent variables $\eta = x + Vt$ (when propagation is along the x -axis), where V is the propagation velocity of the wave, and satisfy the boundary conditions

$$\theta(+\infty, t) = 1, \quad y(+\infty, t) = 0 \quad \text{и} \quad \theta(-\infty, t) = 0$$

with $y(-\infty, t) = 1$ (for waves propagating from right to left).

In the above formulas temperature and concentration for $x = -\infty$ correspond to the fully active substance, and for $x = +\infty$ to products of the reaction. The temperature $\theta = 1$ corresponds to the adiabatic combustion temperature.

The unknown functions $\theta(x, t) = \Theta(\eta)$ and $y(x, t) = Y(\eta)$ are the solutions of the system of ordinary differential equations

$$\frac{d^2 \Theta}{d\eta^2} - V \frac{d\Theta}{d\eta} + Y \Phi(\Theta) = 0 \quad (1.3)$$

$$V \frac{d\theta}{d\eta} + Y\Phi(\theta) = 0, \quad V > 0$$

$$\theta(+\infty) = 1, \quad Y(+\infty) = 0, \quad \theta(-\infty) = 0, \quad Y(-\infty) = 1$$

where V is the eigenvalue of problem (1.3).

This problem was analyzed in a number of works, for example [1-5], where several theorems about the existence and uniqueness of solution are proved and approximate solutions are derived. Thus for function $\Phi(\theta)$ of the form (1.2) for $\Phi_1 < \text{const}$ is the solution of problem (1.3) which exists and is unique. The typical form of solution is presented in Fig. 1.

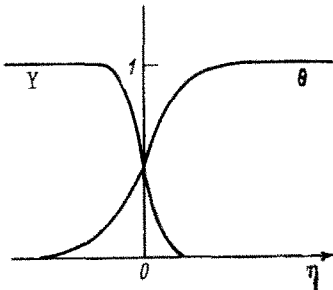


Fig. 1

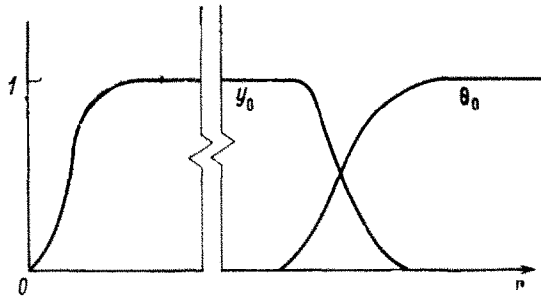


Fig. 2

Because the solution of problem (1.3) is invariant with respect to translation along the η -axis ($C = \text{const}$ when $\eta \rightarrow \eta + C$), we select the translational constant so that for $\eta = 0$ the quantity $\theta(0)$ corresponds to some specified quantity θ^* ($0 < \theta^* < 1$), for instance, $\theta^* = 1/2$. In what follows we assume that functions $\theta(\eta)$ and $Y(\eta)$ satisfy such normalization.

Besides the solution of the kind of stationary running wave derived above, it is possible to construct for system (1.1) a wider class of solutions. For this we shall seek a solution of system (1.1) of the form

$$\theta(\mathbf{r}, t) = z(\xi), \quad y(\mathbf{r}, t) = f(\mathbf{r})\varphi(\xi), \quad \xi = at + g(\mathbf{r}) \quad (1.4)$$

where functions $z(\xi)$, $f(\mathbf{r})$, φ and $y(\mathbf{r})$ are determined below, and a is an arbitrary constant ($a \neq 0$).

Substituting (1.4) into (1.1) we obtain

$$\frac{d^2z}{d\xi^2} |\nabla g|^2 + \frac{dz}{d\xi} (\Delta g - a) + f(\mathbf{r}) \varphi(\xi) \Phi(z(\xi)) = 0 \quad (1.5)$$

$$a \frac{d\varphi}{d\xi} + \varphi(\xi) \Phi(z(\xi)) = 0$$

If the solution of system (1.1) is to be of the form (1.4), it is necessary to set

$$\Delta g - a = b |\nabla g|^2, \quad f(\mathbf{r}) = d |\nabla g|^2 \quad (1.6)$$

where b and d are arbitrary constants. Since the problem contains only the product $f(r)\varphi(\xi)$ hence without loss of generality we can set $d = 1$. Then with allowance for (1.6) from (1.5) we have

$$\frac{d^2z}{d\xi^2} + b\frac{dz}{d\xi} + \varphi\Phi(z) = 0, \quad u\frac{d\varphi}{d\xi} + \varphi\Phi(z) = 0 \quad (1.7)$$

Thus any solution of Eqs. (1.6) and (1.7) yields the solution of the input system (1.1).

When $b \neq 0$ the first of Eqs. (1.6) is nonlinear, hence it is convenient to introduce a new unknown function. We have

$$\Delta u = -abu \quad (g(r) = -b^{-1} \ln |u(r)|) \quad (1.8)$$

The first integral of Eqs. (1.7) is

$$dz/d\xi + bz - a\varphi = c$$

with the use of which from (1.7) we obtain

$$\frac{dp}{dz} = p^{-1}[(c - bz - p)\Phi(z) - abp], \quad \frac{dz}{d\xi} = p(z) \quad (1.9)$$

Note the substantial difference between systems (1.7) and (1.3) in that in the former the variable ξ can vary in a semibounded interval and the constants a , b and c are, in the general case, not interconnected quantities.

2. Particular cases. Let us consider some problems whose solutions can be constructed in the form (1.4).

We assume that the constants a , b and c are chosen so that

$$a = -b = -c = V > 0 \quad (2.1)$$

The solution of system (1.7) is then of the form

$$z(\xi) = \Theta(\xi), \quad \varphi(\xi) = Y(\xi) \quad (2.2)$$

For a centrally symmetric function $u(r)$, we have from (1.8)

$$r^{-n} \frac{d}{dr} \left(r^n \frac{du}{dr} \right) = V^2 u \quad (2.3)$$

The values of n equal to 0, 1, 2, relate to plane, cylindrical and spherical symmetry. From (1.4), (1.6), (1.8) and (2.3) we have

$$\xi = Vt + V^{-1} \ln \operatorname{ch}(Vr) + A, \quad f(r) = \operatorname{th}^2(Vr) \quad (n=0) \quad (2.4)$$

$$\xi = Vt + V^{-1} \ln I_0(Vr) + A, \quad f(r) = I_1^2(Vr)I_0^{-2}(Vr) \quad (n=1) \quad (2.5)$$

$$\xi = Vt + V^{-1} \ln [r^{-1} \operatorname{sh}(Vr)] + A \quad (2.6)$$

$$f(r) = [\operatorname{cth}(Vr) - V^{-1}r^{-1}]^2 \quad (n=2)$$

where $I_i(r)$ ($i = 0, 1$) are Bessel functions of imaginary argument and A is an arbitrary constant.

We assume that $0 \leq r \leq \infty$. First, we consider the case of $n = 0$, then setting $t = 0$, we find that solution (1.7) defines the evolution of initial distribution

$$\begin{aligned} \theta_0 &= \theta(r, 0) = \Theta(V^{-1} \ln \operatorname{ch}(Vr) + A) \\ y_0 &= y(r, 0) = \operatorname{th}^2(Vr) Y(V^{-1} \ln \operatorname{ch}(Vr) + A) \end{aligned} \tag{2.7}$$

whose pattern is shown in Fig. 2

To determine the variation of concentration and temperature profiles in time we observe the motion of the isotherm $\theta(\xi, t) = \theta_i$. From (2.4) we then have

$$\begin{aligned} r_i(t) &= V^{-1} \ln(E + \sqrt{E^2 - 1}), \quad E(t) = B_i e^{-Vt} \\ \frac{dr_i(t)}{dt} &= -V \frac{E}{\sqrt{E^2 - 1}}, \quad E \geq 1 \end{aligned} \tag{2.8}$$

where B_i are constants that are different for different isotherms.

It is seen from (2.8) that when $t \rightarrow -\infty$, all isotherms move at constant velocity V . With increasing t the isotherm velocity increases and becomes different for different isotherms. When $t_i = V^{-2} \ln B_i$ the velocity of motion becomes infinite, and for $t > t_i$ temperature $\theta(r, t) > \theta_i, 0 \leq r \leq \infty$.

The problem whose solution is defined by formulas (2.2), (2.4), (2.7) and (2.8) corresponds in the physical sense to the propagation of a combustion wave in the half-space bounded on the left ($r = 0$) by the adiabatic wall ($\partial\theta(0, t) / \partial r = 0$). In the wall neighbourhood up to distances of order V^{-1} the concentration of the reagent differs from that in the unreacted media and is of the form $\operatorname{th}^2(Vr)$. It is seen from (2.7) that when $(-A) \gg 1$

$$\begin{aligned} \theta(r, 0) &\approx 0, \quad y(r, 0) \approx \operatorname{th}^2(Vr) \quad \text{for } Vr \sim 1 \\ \theta(r, 0) &= \theta(A + r - \ln 2) \text{ and } y(r, 0) = Y(A + r - \ln 2) \\ &\text{for } Vr \gg 1 \end{aligned}$$

Thus the initial distribution is a perturbed stationary wave. When $A = \text{const}$ and $-\infty \leq t \leq +\infty$ solution (2.2), (2.4) corresponds to "interaction" between the adiabatic wall and the stationary (when $t \rightarrow -\infty$), combustion wave propagating from right to left in the half-space with concentration $\operatorname{th}^2(Vr)$ (or, what is the same, to two combustion waves moving against each other).

Solutions for converging cylindrical (2.5) and spherical (2.6) combustion waves in a condensed substance with initial concentration distribution $f(r)$ and temperature $\theta = 0$ are derived in the same manner. The question of stability of the obtained nonstationary solution remains open. However, since this solution defines a physically correct concentration and temperature distribution when $t \rightarrow +\infty$, respectively, $\theta(r, +\infty) = 1$ and $y(r, +\infty) = 0$, one should expect

this solution to be stable.

Solution of the kind (1.4) may also be derived with the use of other solutions of Eq. (1.8).

Such solutions ($ab = 0$) can be obtained by setting $b = 0$, $a = 1$ and $c = 0$ and seeking a univariate symmetric solution for $n = 0$ that satisfies conditions

$$\theta(\pm \infty, t) = 1, \quad y(\pm \infty, t) = 0$$

In that case from (1.6) and (1.7) we obtain

$$-\frac{dz}{d\xi} = \int_1^z \Phi(z') dz', \quad \varphi = -\int_1^z \Phi(z') dz', \quad g(r) = 1/2 r^2 + A \quad (2.9)$$

where A is an arbitrary constant. Setting for simplicity $\Phi(z) = z$ from (2.9) we have

$$\theta(r, t) = \operatorname{th} \frac{\xi}{2}, \quad \xi = t + \frac{r^2}{2} + A \quad (A \geq 0), \quad y(r, t) = \frac{r^2}{2} \operatorname{ch}^{-2} \frac{\xi}{2}$$

Now setting $ab = \gamma^2 \geq 0$ (e.g., $b = a = \gamma > 0$) in the one-dimensional case ($n = 0$) we take ξ in the form

$$\xi = \gamma t - \gamma^{-1} \ln |\cos(\gamma r)| + A, \quad f(r) = \operatorname{tg}^2(\gamma r) \quad (2.10)$$

where A is an arbitrary constant related to the selection of the time reference point. It is then possible to define the course of the chemical reaction (1.1) in an infinite plane vessel whose walls are $2l$ apart and at temperature θ_s which is maintained constant. For this it is necessary to set

$$\gamma(k) = \pi(1/2 + k) l^{-1}, \quad k = 0, 1, 2, \dots \\ z(+\infty) = \theta_s, \quad c = \gamma \theta_s$$

Let us consider the simplicity function $\Phi(\theta)$ of the form (1.2) with $\Phi_1 = 1$. From (1.7) we then have

$$z(\xi) = A_1 + A_2 \exp(-\gamma \xi) \\ \varphi(\xi) = A_1 - \theta_s \quad \text{for } z < \theta_0 \\ z(\xi) = \theta_s + A_3 \exp(-\gamma \xi) - A_4(1 - \gamma^{-2}) \exp(-\xi \gamma^{-1}) \\ \varphi(\xi) = A_4 \exp(-\xi \gamma^{-1}) \quad \text{for } z > \theta_0$$

where A_i ($i = 1, 2, 3, 4$) are arbitrary constants. From the condition of continuity of the temperature field $\theta(r, t)$ and of the heat flux $\partial \theta(r, t) / \partial r$ we obtain along the isotherm $z(\xi) = 0$ the following three relationships:

$$\begin{aligned} \theta_0 &= A_1 + A_2 \exp(-\gamma \xi_0) = \theta_s + A_3 \exp(-\gamma \xi_0) - \\ & A_4 (1 - \gamma^{-2}) \exp(-\xi_0 \gamma^{-1}) \\ A_2 \exp(-\gamma \xi_0) &= A_3 \exp(-\gamma \xi_0) - A_4 \gamma^{-2} (1 - \gamma^{-2}) \exp(-\xi_0 \gamma^{-1}) \end{aligned}$$

where ξ_0 is the coordinate which defines the position of isotherm $z(\xi) = \theta_0$.

Owing to the arbitrariness of the selection of A in (2.10), we can set without loss of generality, $\xi = 0$. Then

$$\begin{aligned} z(\xi) &= A_1 + (\theta_0 - A_1) \exp(-\gamma \xi) \\ \varphi(\xi) &= A_1 - \theta_s \quad \text{for } z < \theta_0 \\ z(\xi) &= \theta_s + [(\theta_0 - \theta_s) + (\theta_s - A_1) (1 - \gamma^{-2})^{-1}] \exp(-\gamma \xi) - \\ & (\theta_s - A_1) (1 - \gamma^{-2})^{-1} \exp(-\xi \gamma^{-1}), \\ \varphi(\xi) &= (A_1 - \theta_s) \exp(-\xi \gamma^{-1}) \quad \text{for } z(\xi) > \theta_0 \end{aligned} \tag{2.11}$$

where A_1 is a free parameter. The physical requirement that $0 \leq y(r, t) \leq 1$ implies this condition

$$l \geq \sqrt{2\pi} (1/2 + k), \quad \gamma^{-2} \geq 2 \tag{2.12}$$

It is, thus, possible to derive for a given k a solution of the form (1.4) where ξ and $f(r)$ are determined in (2.10), however, only for vessels for which formula (2.12) is valid.

Note that solution similar to (2.10) and (2.11) can be also derived for vessels of other shapes. In that case functions $u(r)$ and parameters γ are, respectively, eigenfunctions and eigenvalues of the problem

$$\Delta u = -\gamma^2 u, \quad u|_S = 0$$

where S is the vessel surface area.

When $t \rightarrow \infty$ the temperature distribution in the vessel becomes uniform: $\theta(r, +\infty) = \theta_s$ and $y(r, +\infty) = 0$, which is in agreement with the physical sense of the problem.

The solution of the problem under conditions of heat insulation can be similarly solved: $\nabla \theta \cdot \nabla S = 0$. Function $u(r)$ and parameter γ must then correspond to eigenfunctions and eigenvalues of the problem

$$\Delta u = -\gamma^2 u, \quad \nabla u \cdot \nabla S = 0$$

We note in concluding that solution of the form (1.4) can be constructed for other problems of the theory of combustion of condensed substances, that are defined by more complex kinetics, for example,

$$\frac{\partial \theta}{\partial t} = \Delta \theta + \sum_{j=1}^N A_j \prod_{i=1}^N y_i^{\beta_{ij}} \Phi_j(\theta) \quad \left(\sum_{i=1}^N \beta_{ij} = 1 \right)$$

$$\frac{\partial y_i}{\partial t} = \sum_{j=1}^N B_j \prod_{i=1}^N y_i^{\beta_{ij}} \Phi_j(\theta), \quad i = 1, 2, \dots, N$$

where A_i , B_i and β_{ij} are constants and N is the number of reagents taking part in the reaction.

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