APPLICATION OF THE METHOD OF MATCHED ASYMPTOTIC EXPANSIONS TO THE CALCULATION OF THE STATIONARY THERMAL PROPAGATION OF THE FRONT OF AN EXOTHERMIC REACTION IN A CONDENSED MEDIUM

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In this paper we use the method of matched asymptotic expansions to establish a two-term formula for the speed of propagation of the front of an exothermic reaction in a condensed medium whose thermophysical characteristics depend on the concentration of the reacting matter and the temperature. As the parameter of the expansion we use the ratio of the activation temperature to the adiabatic combustion temperature. The results are applied to the case of the combustion of nonvolatile condensed systems. We compare the approximate formula obtained with the results of a numerical integration.

1. Formulation of the Problem. Method of Solution. The problem concerning the stationary thermal propagation of the front of a one-stage exothermic reaction in a condensed phase may be formulated as follows (see, for example, [1, 3, 4]):

$$\frac{d}{dx}\left(\frac{\lambda}{c}\frac{dT}{dx}\right)-m\frac{dT}{dx}+\frac{h}{c}\rho^n(1-y)^n\Phi(T)=0 \tag{1.1}$$

$$m\frac{dy}{dx}-\rho^n(1-y)^n\Phi(T)=0 \tag{1.2}$$

$$T=T_-,\quad y=0,\qquad x=-\infty \tag{1.3}$$

$$dT/dx=0,\qquad y=1,\quad x=\infty \tag{1.4}$$

Here x is the spatial coordinate, T the temperature, y the concentration of the reaction product, h = const is the thermal reaction effect, m is the mass velocity of propagation of the reaction front, which is a characteristic value of the problem, c = const is the heat capacity, $\rho=\rho(T, y)$ is the density of the medium, $0<n<2$ is the order of the reaction, $\lambda=\lambda(T, y)$ is the coefficient of thermal conductivity of the medium, $\Phi(T)$ gives the dependence of the chemical reaction speed on the temperature, and T_- is the initial temperature.

The problem (1.1)-(1.4) has the first integral

$$\frac{\lambda}{c}\frac{dT}{dx}+m\left[T-T_--\frac{h}{c}(1-y)\right]=0,\quad T_+=T_-+\frac{h}{c} \tag{1.5}$$

The minus and plus subscripts refer to quantities at the cold and hot boundaries of the combustion zone, respectively.

Equation (1.5) will now be used instead of the equation (1.1).

We assume that the speed of the chemical reaction depends on the temperature according to the Arrhenius law

$$\Phi(T)=B\ \exp(-E/RT) \tag{1.6}$$

Here E is the activation energy, R the gas constant, and B is the factor multiplying the exponential term.

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It should be noted that for the existence of a solution of the problem (1.1)-(1.4) it is necessary to assume, just as in the theory of thermal flame propagation in a gas [2], that the function $\Phi(T)$ is not equal to zero and is defined by the formula (1.6) everywhere except for a small interval of temperatures near $T=T_-$ [3-5]. In the present paper we use an approximate form of the basic equations in which the need for an explicit use of this assumption does not arise.

In the problem (1.2)-(1.4) and (1.5) it is appropriate to introduce the new variable and unknown functions

$$\tau = \frac{c(T-T_-)}{h} \quad (0 \leqslant \tau \leqslant 1), \qquad P = \frac{\lambda}{c}\frac{d\tau}{dx} \tag{1.7}$$

From Eq. (1.5) we obtain

$$P = m(\tau - y) \tag{1.8}$$

Taking Eq. (1.8) into account, instead of the Eqs. (1.2)-(1.4) we can write

$$M^2(\tau - y)\frac{dy}{d\tau} = (1-y)^n K(\tau, y)\exp\frac{-\beta(1-\tau)}{\tau+\sigma} \tag{1.9}$$

$$K = B\rho^n\frac{\lambda}{c}, \qquad \beta = \frac{E}{RT_+}, \qquad \sigma = \frac{T_-}{T_+ - T_-}, \qquad M = m\exp\frac{\beta}{2}$$

$$\tau = 0, \qquad y = 0 \tag{1.10}$$

$$\tau = 1, \qquad y = 1 \tag{1.11}$$

Equation (1.9) contains the parameter β, the values for which are usually of an order of magnitude larger than one. This permits us, in solving the problem, to use the method of matched asymptotic expansions [6, 7]. Taking into account the large size of β, we can decompose the interval of the independent variable $0 \leq \tau \leq 1$ into two regions. In the region adjacent to $\tau=0$ (exterior region) the right side of the equation is substantially less than the left. In the region adjacent to $\tau=1$ (interior region) the large size of β in the exponent compensates for the smallness of the factor $(1-\tau)$, and both sides of the equation become comparable in size. In the interior region we introduce the variable $\tau_* = \beta(1-\tau)$. In place of Eqs. (1.9) and (1.11) we obtain

$$M^2\left(y + \frac{\tau_*}{\beta} - 1\right)\beta\frac{dy}{d\tau_*} = K\left(y, 1 - \frac{\tau_*}{\beta}\right)(1-y)^n\exp\frac{-\tau_*}{\sigma + 1 - \beta^{-1}\tau_*} \tag{1.12}$$

$$\tau_* = 0, \qquad y = 1 \tag{1.13}$$

We seek an approximate solution of the problem in the form of expansions in powers of the small parameter β^{-1}. In the interior region

$$y(\tau_*) = F_0(\beta)\, y_0(\tau_*) + F_1(\beta)\, y_1(\tau_*) \tag{1.14}$$

In the exterior region

$$y(\tau) = f_0(\beta)\, y^{(0)}(\tau) + f_1(\beta)\, y^{(1)}(\tau) \tag{1.15}$$

The expansion for the characteristic value of the problem M is the same in both regions:

$$M = \alpha_0(\beta) M_0 + \alpha_1(\beta) M_1 \tag{1.16}$$

The coefficients in the expansions (1.14)-(1.16), which depend on β, must satisfy for $\beta \to \infty$ the conditions

$$\frac{F_1(\beta)}{F_0(\beta)} \to 0, \qquad \frac{f_1(\beta)}{f_0(\beta)} \to 0, \qquad \frac{\alpha_1(\beta)}{\alpha_0(\beta)} \to 0$$

The functions $y^{(0)}$, $y^{(1)}$ and y_0, y_1 are determined successively from Eqs. (1.9), (1.10) and Eqs. (1.12), (1.13), respectively. The terms of the series (1.16) for the characteristic value M, which remain to be determined, are then obtained from the condition of matching of the interior expansion (1.14) and the exterior expansion (1.15); this condition is expressed by requiring that corresponding terms of the expansions for $y(\tau_*)$ and $y(\tau)$ coincide when $\tau_* \to \infty$ and $\tau \to 1$, respectively. The form of the coefficients $F_{0,1}$ and $f_{0,1}, \alpha_{0,1}$ is established from the boundary conditions and the matching condition.

2. Two Approximations for m. We substitute the expansions (1.15) and (1.16) into Eq. (1.9). Since the following relations are satisfied when $\beta \to \infty$:

$$\exp(-\beta) / f_{0,1}(\beta) \to 0, \qquad \exp(-\beta) / \alpha_{0,1}(\beta) \to 0$$

it follows from Eqs. (1.9) and (1.10) that in the exterior region

$$y^{(0)}(\tau) = 0, \quad y^{(1)}(\tau) = 0 \tag{2.1}$$

From Eqs. (2.1) it is evident that the condition of matching of interior and exterior expansions amounts, in our case, to the requirement that

$$y_0(\tau_*) \to 0, \quad y_1(\tau_*) \to 0 \quad \text{for} \quad \tau_* \to \infty \tag{2.2}$$

From the boundary condition (1.11), which the expansion (1.14) must satisfy, it follows that

$$F_0(\beta) = 1, \quad y_0(0) = 1, \quad y_1(0) = 0 \tag{2.3}$$

We substitute the expansions (1.14) and (1.16) into Eq. (1.12). From an order of magnitude analysis of the individual terms we obtain, taking the conditions (2.2) and (2.3) into account,

$$\alpha^2_0(\beta) = \beta^{-1}$$

Grouping the terms of minimum order in β^{-1}, we obtain the equation for

$$M_0^2 \frac{dy_0}{d\tau_*} = -K(y_0, 1)(1-y_0)^{n-1} \exp\frac{-\tau_*}{1+\sigma} \tag{2.4}$$

From Eq. (2.4) and the boundary condition (2.3) we find that

$$M_0^2 \int\limits_{y_0(\tau_*)}^{1} \frac{(1-z)^{1-n}}{K(z,1)} dz = (1+\sigma)\left[1 - \exp\left(-\frac{\tau_*}{1+\sigma}\right)\right] \tag{2.5}$$

The relation (2.5) determines the zeroth approximation for the function $y(\tau_*)$ in the interior region.

From Eq. (2.5) and the matching condition (2.2) we obtain a formula for calculating the zeroth approximation of the characteristic value of the problem:

$$M_0^2 = (1+\sigma)\left[\int\limits_0^1 \frac{(1-z)^{1-n}\, dz}{K(z,1)}\right]^{-1} \tag{2.6}$$

We find the following approximation. Substituting the Eqs. (1.14) and (1.16) into Eq. (1.12), we find, by matching orders of magnitudes of the individual terms, taking Eqs. (2.2), (2.3), and (2.4) into account, that $F_1 = \beta^{-1}$, $\alpha_1 = \beta^{-3/2}$. Then for the function $y_1(\tau_*)$ we obtain the equation

$$\frac{dy_1}{d\tau_*} = \frac{K^0}{M_0^2}(1-y_0)^{n-1}\exp\left(-\frac{\tau_*}{1+\sigma}\right)\left\{\left[\frac{n-1}{1-y_0} - \left(\frac{\partial \ln K}{\partial y}\right)^0\right] y_1 + \right.$$
$$\left. + \frac{2M_1}{M_0} + \tau_*\left(\frac{\partial \ln K}{\partial \tau}\right)^\circ + \frac{\tau_*^2}{(1+\sigma)^2} - \frac{\tau_*}{1-y_0}\right\} \tag{2.7}$$

Here the function $y_0(\tau_*)$ and the quantity M_0 are determined by Eqs. (2.5) and (2.6); the arguments of the functions marked with a degree superscript are equal to

$$y = y_0(\tau_*), \quad \tau = 1$$

The solution of Eq. (2.7), satisfying the boundary condition (2.3), may be written in the form

$$y_1(\tau_*) = \frac{(1-y_0)^{n-1}}{M_0^2} e^{F(\tau_*)} \int\limits_0^{\tau_*} K^\circ \left[\frac{2M_1}{M_0} + \frac{x^2}{(1+\sigma)^2} + x\left(\frac{\partial \ln K}{\partial \tau}\right)^\circ - \frac{x}{1-y_0}\right] \exp\left[\frac{-x}{1+\sigma} - F(x)\right] dx$$

$$F(x) \equiv \int\limits_0^{y_0(x)} \left(\frac{\partial \ln K}{\partial y}\right)^\circ dy \tag{2.8}$$

Using the matching condition (2.2), we obtain from Eq. (2.8) an expression for the first term of the expansion of the characteristic value:

$$\frac{2M_1}{M_0} = -\int\limits_0^\infty K^\circ \left[\frac{x^2}{(1+\sigma)^2} + x\left(\frac{\partial \ln K}{\partial \tau}\right)^\circ - \frac{x}{1-y_0}\right] \exp\left[\frac{-x}{1+\sigma} - F(x)\right] dx \left[\int\limits_0^\infty K^\circ \exp\left[\frac{-x}{1+\sigma} - F(x)\right] dx\right]^{-1} \tag{2.9}$$

Thus the two-term expansion in β^{-1} of the mass velocity of propagation of an exothermic reaction front in a condensed phase has the form

$$m = M_0 e^{-\beta/2} \beta^{-1/2}\left(1 + \beta^{-1}\frac{M_1}{M_0}\right) \tag{2.10}$$

where the quantities M_0 and M_1 are given by Eqs. (2.6) and (2.9).

3. Particular Cases. We now apply the results obtained to describing the combustion of nonvolatile condensed systems with strong dispersion, wherein the formation of gaseous products and change in vol-

ume and thermal conductivity of the condensed medium may, in the course of the chemical reaction, be described within the scope of the model presented in [8, 9]. In accord with [8, 9] we assume that the density and the thermal conductivity of the condensed medium vary with a change in the mass fraction of the reaction products and the temperature according to the laws

$$\frac{\rho}{\rho_0} = \left[1 + yz\left(\rho_0 \frac{RT}{\mu p} - 1\right)\right]^{-1}, \quad \frac{\lambda}{\lambda_1} = \left[1 + yz\left(\frac{\lambda_2}{\lambda_1}\frac{\rho_0 RT}{\mu p} - 1\right)\right]\left[1 + yz\left(\frac{\rho_0 RT}{\mu p} - 1\right)\right]^{-1} \tag{3.1}$$

Here λ_1 and λ_2 are, respectively, the coefficients of thermal conductivity of the condensed phase and of the gaseous reaction products; ρ_0 is the initial density of the condensed phase; R is the gas constant; μ is the molecular weight of the gaseous reaction products; p is the pressure; and z is the fraction of gas in the reaction products.

We assume that in the condensed system a chemical reaction of the first order (n = 1) takes place. The expression for the function $K^\circ \equiv K(y_0, 1)$ assumes the form

$$K^\circ = \frac{B\lambda_1\rho_0}{c}\frac{(1 + by_0)}{(1 + ay_0)^2}, \quad a \equiv z\left(\frac{\rho_0 RT_+}{\mu p} - 1\right), \quad b \equiv z\left(\frac{\lambda_2}{\lambda_1}\frac{\rho_0 RT_+}{\mu p} - 1\right) \tag{3.2}$$

Substituting the expressions (3.2) into the relations (2.5) and (2.6), we find, after integrating, for n = 1

$$1 - \frac{I(y_0)}{I(0)} = \exp\frac{-\tau_*}{1+\sigma}, \quad M_0^2 = \frac{B\lambda_1\rho_0(1+\sigma)}{cI(0)} \tag{3.3}$$

$$I(y_0) = \frac{(b-a)^2}{b^3}\ln\frac{1+b}{1+by_0} + 2\frac{a}{b}(1 - y_0) - \frac{a^2}{b^3}\frac{(1+by_0)(by_0-3)}{2} + \frac{a^2}{b^3}\frac{(1+b)(b-3)}{2}$$

The relations (3.3) determine the function $y_0(\tau_*)$ and the zeroth approximation M_0 for the characteristic value of the problem.

The expression for m may be written in the form

$$m^2 = \frac{B\rho_0\lambda_1}{h}\frac{RT_+^2}{E}\left[\frac{(b-a)^2}{b^3}\ln(1+b) + \frac{a}{b}\left(2 - \frac{a}{b} + \frac{a}{2}\right)\right]^{-1}\exp\frac{-E}{RT_+} \tag{3.4}$$

Equation (3.4), which determines the stationary combustion front propagation velocity, coincides with the formula given in [8, 9], obtained by the Zel'dovich–Frank-Kamenetskii method.

For the second term of the expansion of the characteristic value of the problem we obtain from Eq. (2.9) for the case considered

$$\frac{M_1}{M_0} = -1 + \frac{1}{2}\int_0^1 \frac{M_0^2}{K^\circ}\left[\left(\frac{\partial \ln K}{\partial \tau}\right)^\circ - \frac{1}{1-y_0}\right]\ln\left[1 - \frac{I(y_0)}{I(0)}\right]dy_0 \tag{3.5}$$

$$\left(\frac{\partial \ln K}{\partial \tau}\right)^\circ \equiv \frac{zy_0}{1+\sigma}\left[\frac{b+z}{1+by_0} - \frac{2(a+z)}{1+ay_0}\right]$$

If the thermal conductivity coefficients of the condensed and gaseous phases are equal to each other, the Eq. (3.5) simplifies.

If in Eq. (3.5) we put $\lambda_1 = \lambda_2$, i.e., $b = a$, we find, after integrating,

$$\frac{M_1}{M_0} = -1 + \frac{a+z}{a+2}\left(\frac{1}{2} - \frac{1}{a} + \frac{2}{a^2}\ln\frac{a+2}{2}\right) + \frac{1+\sigma}{a+2}\left[(1+a)\frac{\pi^2}{3} - 2a + 2\ln\frac{a+2}{2} + (1+a)J\left(\frac{2}{2+a}\right)\right]$$

$$J(\alpha) = \int_0^\alpha \frac{\ln t\, dt}{1-t}, \quad J(1) = -\frac{\pi^2}{6} \tag{3.6}$$

In the particular case involving propagation of an exothermic reaction front in a medium with constant thermophysical characteristics, we find from Eqs. (3.3) and (3.6), putting z = 0 ($b = a = 0$), that

$$M_0 = \left[\frac{B\lambda_1\rho_0(1+\sigma)}{c}\right]^{1/2}, \quad \frac{M_1}{M_0} = (1+\sigma)\frac{\pi^2}{12} - 1 \tag{3.7}$$

Here the first equation determines the zeroth approximation for the stationary reaction front propagation velocity; it agrees with that found in [1, 4]. The second equation determines the first correction to the zeroth approximation.

Let us compare the results obtained in calculating the speed of combustion of a condensed system using the two-term formula defined by Eqs. (2.10), (3.3), and (3.6) with the exact solution of the problem concerning the stationary propagation speed of the combustion front [8, 9]. The calculations in [8, 9] were made for $b = a$ (z = 1) and for large numerical values of the parameter a; therefore, in place of the Eqs. (3.3) and (3.6), it is appropriate to use the limiting expressions for M_0 and M_1/M_0, valid for large a.

TABLE 1

a	β	σ	Δ_0	Δ_1
734	19.37	0.337	6.167	0.26
735	19.37	0.337	6.983	1.1
72.5	19.37	0.337	4.493	−1.3
1387	10.3	0.258	11.53	1.9
468	30.3	1.564	11.6	3.44
325	43.85	0.776	1.14	−2.87
6.4	19.37	0.337	1.18	−2.8
1246	11.46	0.13	11	3.4
$1.47 \cdot 10^8$	9.688	0.337	12	0.4
$5.5 \cdot 10^6$	25.76	2.02	19	8
29	19.42	0.837	7	1.1
106	13.4	0.937	6.5	−9

From Eq. (3.3), putting $b = a$, we obtain for $a \gg 1$

$$M_0^2 = 2B\lambda_1\rho_0 (1 + \sigma)/ca \tag{3.8}$$

From Eq. (3.6) for $a \gg 1$, we find

$$M_1 / M_0 = -1/2 + (1 + \sigma)(1/3\,\pi^2 - 2) \tag{3.9}$$

The two-term approximation for the stationary combustion speed in the limiting case considered is given by the Eqs. (2.10), (3.8), and (3.9).

The results are shown for comparison in Table 1.

In this table Δ_0 denotes the deviation in per cent of the mass combustion velocity, obtained from the zeroth approximation formula, from the value obtained from a numerical solution of the problem; Δ_1 denotes the deviation in percent of the mass velocity, calculated from the two-term approximate formula, from the value obtained from the numerical solution. It is evident that the zeroth approximation always gives a lowered value of the stationary combustion speed. The second term in the two-term formula is always positive. In the majority of cases, by taking account of the second approximation, we obtain a substantial decrease in the deviation of the speed, obtained by the approximate analytical method, from that obtained by numerical integration.

We remark that various approximate methods of calculating the stationary propagation speed of an exothermic reaction front in a condensed medium were proposed in a series of papers (for example, [1, 4, 10, 11]).

The method of matched asymptotic expansions, favored in many problems of mechanics, makes it possible, with the help of a standard procedure, to obtain an approximate analytical solution of the problem which guarantees good agreement with the exact solution. By analogy with other problems of mechanics, for example, with the problem of laminar flow around a sphere [6], it may be assumed that the results obtained will be sufficiently close to the exact solution providing the values of the parameter of the expansion are not too large.

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