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ASYMPTOTIC ANALYSIS OF STATIONARY PROPAGATION OF THE FRONT OF PARALLEL EXOTHERMIC REACTION

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We develop an approximate theory of stationary propagation of the planar front of a two-stage parallel exothermic reaction in a condensed medium and in a gas. In constructing the solutions we use the method of matched asymptotic expansions. As parameter of the expansion we employ the ratio of the sum of the activation energies of the reactions to the terminal temperature, the latter being determined in the course of solution of the problem. We show the characteristic limiting modes corresponding to the various parameter values which appear in the problem. For each of these modes we obtain approximate analytical expressions for the wave velocity, the distribution of concentrations, and the terminal temperature.

1. Statement of the problem. The stationary propagation of the planar

front of the two-stage parallel exothermic reaction $A_2 \leftarrow A_0 \rightarrow A_1$ in a given medium can be described by the following system of equations and boundary conditions:

$$\frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - mc \frac{dT}{dx} + Q_{1}a_{0}\rho\Phi_{1}(T) + Q_{2}a_{0}\rho\Phi_{2}(T) = 0 \qquad (1.1)$$

$$\frac{d}{dx}\left(D\rho \frac{da_{1}}{dx}\right) - m \frac{da_{1}}{dx} + a_{0}\rho\Phi_{1}(T) = 0$$

$$\frac{d}{dx}\left(D\rho \frac{da_{2}}{dx}\right) - m \frac{da_{2}}{dx} + a_{0}\rho\Phi_{2}(T) = 0$$

$$\frac{d}{dx}\left(D\rho \frac{da_{0}}{dx}\right) - m \frac{da_{0}}{dx} - a_{0}\rho\left(\Phi_{1}(T) + \Phi_{2}(T)\right) = 0$$

$$\Phi_{1}(T) = K_{1}\exp\left(-\frac{E_{1}}{RT}\right), \quad \Phi_{2}(T) = K_{2}\exp\left(-\frac{E_{2}}{RT}\right)$$

$$x = -\infty, \quad a_{0} = 1, \quad T = T_{-}, \quad a_{1-} = a_{2-} = 0$$

$$T_{+} = T_{-} + c^{-1}\left(Q_{1}a_{1+} + Q_{2}a_{2+}\right)$$

$$x = +\infty, \quad a_{0+} = 0, \quad \frac{dT}{dx} = \frac{da_{1}}{dx} = \frac{da_{2}}{dx} = 0, \quad a_{1+} + a_{2+} = 1$$

Here a_0 , a_1 and a_2 are the mass fractions of the material A_0 , A_1 and A_2 ; ρ is the density; m is the mass combustion rate; c is the heat capacity; λ is the thermal conductivity; D is the diffusion coefficient; R is the gas constant; Q_1 and Q_2 are thermal reaction effects; K_1 and K_2 are exponential factors; and E_1 and E_2 are activation energies.

We assume that the density and all the thermophysical characteristics of the medium retain constant values and that the chemical reactions proceed in the first order, their rates being dependent on the temperature according to the law of Arrhenius.

The two-point boundary value problem (1.1) consists of determination of functions $a_1(x)$, $a_2(x)$, T(x) and eigenvalues m and a_{1+} For this problem to have a solution we assume that functions Φ_1 and Φ_2 differ from zero and are determined by the corresponding expressions in Eqs. (1.1) everywhere except for a small temperature interval $T_{-} \leqslant T < T_{\epsilon}$ where these expressions vanish [1].

The kinetic scheme assumed here approximates a reaction of the form

$$A_0 + B_1 \rightarrow A_1, \qquad A_0 + B_2 \rightarrow A_2$$

at an excess of the materials B_1 and B_2 ; it can also serve as a model for the reaction $A_2 \leftarrow A_0 \rightarrow A_1 \rightarrow A_2$, in which the stage $A_1 \rightarrow A_2$ proceeds slowly in an inductive mode. An experimental study was given in [2], for example, of a parallel two-stage reaction in a container.

The problem (1, 1) has the two first integrals

$$\frac{\lambda}{cm}\frac{dT}{dx} = T + \frac{Q_1}{c} \left(\frac{D\rho}{m}\frac{da_1}{dx} - a_1\right) + \frac{Q_2}{c} \left(\frac{D\rho}{m}\frac{da_2}{dx} - a_2\right) - T_- \quad (1.2)$$
$$a_1 + a_2 = 1 - a_0$$

We shall use the first of the equations (1, 2) in place of the first of the equations (1, 1). Taking the temperature T as the independent variable, we can write the initial value problem in the form

$$\frac{db_{1}}{d\tau} = L \frac{b_{1} - B_{1}}{\Delta}, \quad \frac{db_{2}}{d\tau} = L \frac{b_{2} - B_{2}}{\Delta}$$
(1.3)

$$a\mu \frac{dB_{1}}{d\tau} = \sigma_{k} \frac{1 - \alpha b_{1} - (1 - \alpha) b_{2}}{\Delta} \exp\left[-\beta \sigma_{E} \frac{1 + \sigma}{\tau + \sigma}\right]$$
(1.3)

$$(1 - \alpha)\mu \frac{dB_{2}}{d\tau} = (1 - \sigma_{K}) \frac{1 - \alpha b_{1} - (1 - \alpha) b_{3}}{\Delta} \exp\left[-\beta (1 - \sigma_{E}) \frac{1 + \sigma}{\tau + \sigma}\right]$$

$$\Delta = \tau - \gamma B_{1} - (1 - \gamma) B_{2}$$
(1.3)

$$\tau = 0, \ b_{1} = B_{1} = B_{2} = b_{2} = 0; \ \tau = 1, \ b_{1} = B_{2} = B_{1} = b_{2} = 1$$

$$b_{1} = \frac{a_{1}}{a_{1+}}, \ b_{2} = \frac{a_{2}}{a_{2+}}, \ \alpha = a_{1+}, \ \sigma_{E} = \frac{E_{1}}{E_{1} + E_{2}}$$

$$\tau = \frac{T - T_{-}}{T_{+} - T_{-}}, \ \mu = \frac{m^{2}c}{\lambda(K_{1} + K_{2})}, \ \sigma_{K} = \frac{K_{1}}{K_{1} + K_{2}}$$

$$\sigma_{Q} = \frac{Q_{1}}{Q_{1} + Q_{2}}, \ \sigma = \frac{T_{-}}{T_{+} - T_{-}}, \ L = \frac{\lambda}{D\rho c}, \ \beta = \frac{E_{1} + E_{2}}{RT_{+}}$$

Here b_1 , B_1 , b_2 and B_2 are the unknown functions and μ and α are eigenvalues of the problem.

We analyze this problem by the method of matched asymptotic expansions [3-6]. We assume that $\beta \gg 1$; for this to be true, it is sufficient to assume the simultaneous satisfaction of the inequalities

$$\frac{E_1+E_2}{R(T_-+Q_2/c)} \gg 1, \quad \frac{E_1+E_2}{R(T_-+Q_1/c)} \gg 1$$

2. Propagation of the front of a reaction in a condensed phase. Equations describing the propagation of the front of an exothermic reaction in a condensed phase are obtained from the Eqs. (1.3) by formally setting $L = \infty$. Then

$$b_{1} = B_{1}, \quad b_{2} = B_{2}$$

$$(2.1)$$

$$\alpha \mu \frac{db_{1}}{d\tau} = \sigma_{K} \frac{1 - \alpha b_{1} - (1 - \alpha) b_{2}}{\tau - \gamma b_{1} - (1 - \gamma) b_{2}} \exp\left[-\frac{\beta \sigma_{E}(1 + \sigma)}{\tau + \sigma}\right]$$

$$(1 - \alpha) \mu \frac{db_{2}}{d\tau} = (1 - \sigma_{K}) \frac{1 - \alpha b_{1} - (1 - \alpha) b_{2}}{\tau - \gamma b_{1} - (1 - \gamma) b_{2}} \exp\left[-\frac{\beta (1 - \sigma_{E})(1 + \sigma)}{\tau + \sigma}\right]$$

$$(2.2)$$

$$\tau = 0, \quad b_{1} = b_{2} = 0; \quad \tau = 1, \quad b_{1} = b_{2} = 1$$

$$(2.3)$$

It is necessary here to single out two regions with differing asymptotic behaviors of the solutions: a small neighborhood of the point $\tau = 1$ (interior region) and the remaining portion of the interval (0, 1). In the interior region we introduce in place of τ the variable $\tau^* = \beta (1 - \tau)$; we then seek solutions in each of these regions in the form of exterior and interior expansions.

$$b_{1}(\tau^{*}) = f_{0}(\beta) \ b_{10}(\tau^{*}) + f_{1}(\beta) \ b_{11}(\tau^{*})...$$

$$b_{1}(\tau) = F_{0}(\beta) \ b_{10}^{\circ}(\tau) + F_{1}(\beta) \ b_{11}^{\circ}(\tau) + ...$$

$$f_{1} / f_{0} \to 0, \quad F_{1} / F_{0} \to 0, \quad \beta \to \infty$$
(2.4)

$$b_{2}(\tau^{*}) = n_{0}(\beta) \ b_{20}(\tau^{*}) + n_{1}(\beta) \ b_{21}(\tau^{*}) + \dots$$

$$b_{2}(\tau^{*}) = N_{0}(\beta) \ b_{20}^{\circ}(\tau) + N_{1}(\beta) \ b_{21}^{\circ}(\tau) + \dots$$

$$n_{1} / n_{0} \to 0, \quad N_{1} / N_{0} \to 0, \quad \beta \to \infty$$

$$(2.5)$$

In both regions we seek expansions for the eigenvalues μ and α in the form

$$\mu = \varphi_0 (\beta) \mu_0 + \varphi_1 (\beta) \mu_1 + \dots, \quad \varphi_1 / \varphi_0 \to 0, \quad \beta \to \infty \quad (2.6)$$

$$\alpha = g_0 (\beta) \alpha_0 + g_1 (\beta) \alpha_1 + \ldots, \quad g_1 / g_0 \to 0, \quad \beta \to \infty$$
 (2.7)

The exterior expansions must satisfy the boundary conditions at $\tau = 0$ and the interior expansions at $\tau = 1$ ($\tau^{*}= 0$). A correspondence between the expansions in the exterior and interior regions is established from the matching condition, under which both expansions written in the same variables, are required to possess the same limiting behavior [3-5]. We limit ourselves to a determination of two terms in the expansions (2,4) - (2,7).

Consider first the case
$$\sigma_E = \frac{1}{2}$$
. Dividing (2.2) by (2.1) and integrating, we obtain
 $b_1 \equiv b_2, \ \alpha = \sigma_K$ (2.8)

After changing over to the variable τ^* and substituting into the relations (2, 1), (2, 4), (2, 6) - (2, 8), we obtain, to within terms of the highest order of smallness in β ,

$$-\beta \varphi_0 \mu_0 \frac{db_{10}}{d\tau^*} = \exp\left[-\frac{\tau}{2(1+\tau)} - \frac{\beta}{2}\right], \quad b_{10}(0) = 1 \quad (2.9)$$

Here we have used the equation $f_0 = 1$ which follows from the boundary conditions at $\tau^* = 0$. It is evident from (2.9) that we must choose

$$\varphi_0 = \beta^{-1} \exp(-\beta/2) \tag{2.10}$$

It then follows from (2.9) that

$$b_{10} = 1 - 2 \frac{1+\sigma}{\mu_0} + 2 \frac{1+\sigma}{\mu_0} \exp\left[-\frac{\tau^*}{2(1+\sigma)}\right]$$
(2.11)

Taking the expression (2, 10) into account, we see that the solutions for b_1 in the exterior region are exponentially small. Therefore, in the exterior expansions (2, 4) and (2, 5)

$$b_{20}^{\circ} = b_{10}^{\circ} = b_{21}^{\circ} = b_{11}^{\circ} = 0$$

The matching condition then reduces to the requirement that

$$b_{10} \rightarrow 0, \ b_{11} \rightarrow 0, \ \tau^* \rightarrow \infty$$
 (2.12)

Applying (2, 12) to Eq. (2, 11), we find

$$\mu_0 = 2(1 + \sigma), \quad b_{10} = \exp\left[-\frac{\tau^*}{2(1 + \sigma)}\right]$$
 (2.13)

Proceeding now to obtain two-term expansions (2.4) and (2.6), we obtain, from Eq. (2.1) in the variable τ^* $\varphi_1 = \varphi_1 / \beta = \beta^{-2} \exp(-\beta / 2), \ n_1 = f_1 = \beta^{-1}$ (2.14)

$$\frac{db_{11}}{d\tau^*} = \frac{1}{2(1+\sigma)} \left[\frac{\mu_1}{2(1+\sigma)} + \frac{\tau^{*2}}{2(1+\sigma)} - \frac{\tau^*}{1-\exp\left[-\frac{\tau^*}{2(1+\sigma)}\right]} \right] \times (2.15)$$
$$\exp\left[-\frac{\tau^*}{2(1+\sigma)}\right], \quad b_{11}(0) = 0, \quad b_{11}(\tau^* \to \infty) = 0$$

From (2.15) we find

$$\mu_1 = 2 \left(1 + \sigma\right) \left[\frac{\pi^2}{3} \left(1 + \sigma\right) - 4\right]$$

We write in dimensional variables a two-term expansion for the mass rate of propagation of combustion

$$m = \left[\lambda \frac{K_1 + K_2}{c} \frac{RT_+}{E_1} \frac{T_+}{T_+ - T_-}\right]^{1/s} \left[1 + \frac{RT_+}{E_1} \frac{T_+}{T_+ - T_-} \left(\frac{\pi^2}{6} \frac{T_+}{T_+ - T_-} - 2\right)\right] \times (2.16)$$

$$\exp\left(-\frac{E_1}{2RT_+}\right), \quad T_+ = T_- + c^{-1} \left[Q_1 \sigma_K + (1 - \sigma_K) Q_2\right]$$

We note that the rate is determined by the sum of the factors multiplying the exponential.

Consider now the case $0 < \sigma_E < V_s$. Then, introducing as before the variable τ^* , we obtain from (2.1) and (2.2)

$$-\alpha\mu\frac{\beta db_1}{d\tau^*} = \sigma_K \frac{1-\alpha b_1-(1-\alpha)b_2}{1-\tau^*/\beta-\gamma b_1-(1-\gamma)b_2} \exp\left[-\sigma_E\beta - \frac{\tau^*\sigma_E}{1+\sigma}\right]$$
(2.17)

$$-(1-\alpha)\mu\beta \frac{ab_{2}}{d\tau^{*}} = (1-\sigma_{K})\frac{1-\alpha b_{1}-(1-\alpha)b_{2}}{1-\tau^{*}/\beta-\gamma b_{1}-(1-\gamma)b_{2}} \times \qquad (2.18)$$
$$\exp\left[-\beta(1-\sigma_{E})-\frac{\tau^{*}(1-\sigma_{E})}{1+\sigma}\right]$$

As before, it then follows from (2.3) that $n_0 = f_0 = 1$. Dividing Eq. (2.17) by (2.18), we can obtain the estimate

$$\frac{\alpha}{1-\alpha} = O\left(\exp\left[-\left(1-2\sigma_E\right)\beta\right]\right)$$

From this it follows that in the expansions (2, 6) and (2, 7) we must set

$$g_0 = 1, \alpha_0 = 1, g_1 = \exp [-(1-2\sigma_E)\beta], \varphi_0 = \beta^{-1}\exp [-\sigma_E / \beta]$$

Taking into account the dependence of γ and α , we obtain from (2.17) and (2.18)

$$-\mu_0 \frac{db_{10}}{d\tau^*} = \sigma_K \exp\left[-\frac{\tau^* \sigma_E}{1+\sigma}\right], \quad b_{10}(0) = 1$$
(2.19)

$$\alpha_{1}\mu_{1}\frac{db_{20}}{d\tau^{*}} = (1 - \sigma_{K})\exp\left[-\frac{\tau^{*}(1 - \sigma_{E})}{1 + \sigma}\right], \quad b_{20}(0) = 1 \quad (2.20)$$

In analogy to the previous case, the condition (2.12) holds and we also have $b_{20} \rightarrow 0$, $b_{21} \rightarrow 0$ and $\tau^* \rightarrow 0$. Then from Eqs. (2.19) and (2.20) we obtain, respectively.

$$\mu_{0} = (1 + \sigma) \frac{\sigma_{K}}{\sigma_{E}}, \quad b_{10} = \exp\left[-\frac{\tau^{*}\sigma_{E}}{1 + \sigma}\right]$$
$$\sigma_{1} = -\frac{1 - \sigma_{K}}{\sigma_{K}} \frac{\sigma_{E}}{1 - \sigma_{E}}, \quad b_{20} = \exp\left[-\frac{\tau^{*}(1 - \sigma_{E})}{1 + \sigma}\right]$$

In determining the successive terms of the expansion we must set

 $g_1 = \beta \varphi_1 = \beta^{-1} \exp \left[-(1-2\sigma_E) \beta\right], \ n_1 = f_1 = \beta^{-1}$

Then

$$\frac{db_{11}}{d\tau^*} = \frac{\sigma_K}{\mu_0} \left\{ \frac{\mu_1}{\mu_0} + \frac{\tau^{*2}\sigma_E}{(1+\sigma)^2} - \frac{\tau^*}{1-\exp\left[-\tau^*\sigma_E/(1+\sigma)\right]} \right\} \exp\left[-\frac{\tau^*\sigma_E}{1+\sigma}\right]$$

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$$\frac{db_{21}}{d\tau^*} = \frac{1 - \sigma_K}{\mu_0 \alpha_1} \left\{ \frac{\tau^*}{1 - b_{10}} - \tau^{*2} \frac{1 - \sigma_E}{(1 + \sigma)^2} - \frac{\mu_1}{\mu_0} - \frac{\alpha_2}{\alpha_1} \right\} \exp\left[-\frac{\tau^* (1 - \sigma_E)}{1 + \sigma} \right]$$

$$b_{11}(0) = b_{21}(0) = b_{11}(\infty) = b_{21}(\infty) = 0$$

From this we obtain

$$\mu_{1} = (1 + \sigma) \frac{\sigma_{K}}{\sigma_{E}^{2}} \left[\frac{\pi^{2}}{6} (1 + \sigma) - 2 \right]$$

$$\alpha_{2} = \alpha_{1} \left[-\frac{\mu_{1}}{\mu_{0}} - \frac{4}{1 - \sigma_{E}} + \frac{1 + \sigma}{1 - \sigma_{E}} J_{2}(\infty) \right]$$

$$J_{2}(y) = \int_{0}^{y} \frac{y e^{-y} dy}{1 - \exp\left[-\frac{y \sigma_{E}}{1 - \sigma_{E}} \right]}$$

In dimensional form the two-term expansion for the mass combustion rate has the form

$$m = \left[\lambda \frac{K_1}{c} \frac{RT_+}{E_1} \frac{T_+}{T_+ - T_-}\right]^{1/2} \left\{1 + \frac{RT_+}{E_1} \left[\frac{\pi^2}{12} \frac{T_+}{T_+ - T_-} - 1\right]\right\} \times \qquad (2.21)$$

$$\exp\left(-\frac{E_1}{2RT_+}\right), \quad T_+ = T_- + \frac{Q_1}{c} \alpha + \frac{Q_2}{c} (1 - \alpha)$$

We note that the expression (2, 16) cannot be obtained from Eq. (2, 21). There is no need to treat the case $1/2 < \sigma_E < 1$ separately since it is completely analogous to the case considered.

3. Propagation of the reaction front in gas. In this case L is finite. Side by side with the expansions (2,4) - (2,7) we seek a solution for B_1 and B_2 in the form of exterior and interior expansions

$$B_{1}(\tau^{*}) = \delta_{0}(\beta) B_{10}(\tau^{*}) + \delta_{1}(\beta) B_{11}(\tau^{*}) + \delta_{2}(\beta) B_{2}(\tau^{*}) + \dots (3.1)$$

$$B_{1}(\tau) = D_{0}(\beta) B_{10}^{\circ}(\tau) + D_{1}(\beta) B_{11}^{\circ}(\tau) + \dots$$

$$\frac{\delta_{1}}{\delta_{0}} \rightarrow 0, \quad \frac{D_{1}}{D_{0}} \rightarrow 0, \quad \beta \rightarrow \infty$$

$$B_{2}(\tau^{*}) = \rho_{0}(\beta) B_{20}(\tau^{*}) + \rho_{1}(\beta) B_{11}(\tau^{*}) + \rho_{2}(\beta) B_{2}(\tau^{*}) + \dots (3.2)$$

$$B_{2}(\tau) = S_{0}(\beta) B_{20}^{\circ}(\tau) + S_{1}(\beta) B_{21}^{\circ}(\tau) + \dots$$

$$\rho_{1} / \rho_{0} \rightarrow 0, \quad S_{1} / S_{0} \rightarrow 0, \quad \beta \rightarrow \infty$$

We consider first the case $\sigma_E = \frac{1}{2}$. Dividing the third equation of (1.3) by the fourth one and integrating, we have $B_1 \equiv B_2, \ b_1 \equiv b_2, \ \alpha = \sigma_K$ (3.3)

The problem then reduces then to the following

$$\frac{db_1}{d\tau} = L \frac{b_1 - B_1}{\tau - B_1}, \quad \mu \frac{dB_1}{d\tau} = (\tau - B_1)^{-1} (1 - b_1) \exp\left[-\frac{\beta(1 + \sigma)}{2(\tau + \sigma)}\right] \quad (3.4)$$

$$\tau = b_1 = B_1 = 0, \ \tau = b_1 = B_1 = 1 \tag{3.5}$$

From the conditions at the hot boundary and from (3, 4) it follows that

$$\delta_0 = f_0 = 1, f_1 = \beta^{-1}, \phi_0(\beta) = \beta^{-2} \exp[-\beta/2]$$
 (3.6)

Similar to what was done in Sect. 2, we have

$$\frac{db_{10}}{d\tau^*} = 0, \ b_{10}(0) = 1, \ b_{10} = 1$$

$$\frac{db_{11}}{d\tau^*} = -L, \ \mu_0 \frac{dB_{10}}{d\tau^*} = \frac{b_{11}}{1 - B_{10}} \exp\left[-\frac{\tau^*}{2(1 + \sigma)}\right], \ B_{10}(0) = 1$$
(3.7)

then

$$b_{11} = L\tau^*, \quad B_{10} = 1 - \left\{ 8L \frac{(1+\sigma)^2}{\mu_0} \left[1 - \exp\left[-\frac{\tau^*}{2(1+\sigma)} \right] \right\}^{1/2} \left(1 + \frac{\tau^*}{2(1+\sigma)} \right) \right\}^{1/2}$$

In the exterior region we have, from the matching condition, upon taking the relations (3.6) into account, $F_0(\beta) = 1$, $\delta_0 = 1$, $B_{10}^{\circ} = B_{20}^{\circ} = 0$ (3.9)

It then follows from Eq. (1, 9) that

$$b_{10} (\tau) = C_1 \tau^L, \ C_1 = \text{const}$$
 (3.10)

From the combination of the relations (3, 9) and (3, 10) with (3, 8), we obtain

$$C_{1} = \mathbf{1}, \ \mu_{0} = 8L \ (1 + \sigma)^{2}$$

$$B_{10} = \mathbf{1} - \sqrt{1 - \exp\left[-\frac{\tau^{*}}{2(1 + \sigma)}\right] \left(1 + \frac{\tau^{*}}{2(1 + \sigma)}\right)}$$
(3.11)

Continuing the calculation of the successive terms of the expansion it is necessary to set

$$\varphi_1 = \varphi_0 / \beta, \quad F_1 = \beta^{-2}, \quad f_2 = \beta^{-2}$$
 (3.12)

then

$$-\frac{db_{12}}{d\tau^*} = L\tau^* \frac{1-L}{1-B_{10}}, \quad b_{12}(0) = 0$$

$$\frac{dB_{11}}{d\tau^*} = \frac{b_{11}}{\mu_0} (1-B_{10})^{-1} \left[\frac{b_{12}}{b_{11}} - \frac{\tau^{*2}}{2(1+\sigma)^2} - \frac{\tau^* + B_{11}}{1-B_{10}} - \frac{\mu_1}{\mu_0} \right] \times$$

$$\exp\left[-\frac{\tau^*}{2(1+\sigma)} \right]$$

$$B_{11}(0) = 0$$

$$b_{12} = J_3(x) (1+\sigma)^2 L (L-1), \quad \int_0^x \frac{xdx}{\sqrt{1-e^{-x}(1+x)}} = J_3(x) \quad (3.14)$$

$$x = \frac{\tau^*}{2(1+\sigma)}$$

$$B_{11}(\tau^*) = \frac{-L}{\mu_0(1-B_{10})} \int_0^{\tau^*} x \exp\left(-\frac{x}{2(1+\sigma)}\right) \times$$

$$\left[\frac{b_{12}}{b_{11}} - \frac{x^2}{2(1+\sigma)^2} - \frac{\mu_1}{\mu_0} + \frac{x}{1-B_{10}(x)} \right] dx$$

From the condition of matching with B_{11}° we obtain

$$\frac{\mu_1}{\mu_0} = 2(1+\sigma)J_4(\infty) - 12 - 4(1+\sigma)(L-1), J_4(x) = \int_0^x \frac{t^2 e^{-t} dt}{\sqrt{1-e^{-t}(1+t)}}$$
(3.15)
$$J_4(\infty) = 2.688$$

We have here used the fact that in the exterior expansion

$$b_{11}(\tau) = C_1 \tau^L, \quad C_2 = 4 (1 + \sigma)^2 L (L - 1) \int_0^\infty \left[\frac{x}{\sqrt{1 - e^{-x} (1 + x)}} - x \right] dx \quad (3.16)$$

In dimensional form the expression for the mass combustion rate is given by

$$m = \left[2\lambda \frac{K_1 + K_2}{c} L\left(\frac{RT_+}{E_1}\right) \left(\frac{T_+}{T_+ - T_-}\right) \left\{ 1 + \frac{RT_+}{E_1} \left[\frac{T_+}{T_+ - T_-} - 3\right] \right\} \times (3.17)$$
$$\exp\left(-\frac{E_1}{2RT_+}\right) \right], \quad T_+ = T_- + c^{-1} \left[Q_1 \sigma_K + Q_2 \left(1 - \sigma_K\right)\right]$$

We consider now the case $0 < \sigma_E < 1/_2$. As in the case of the condensed medium, we assume $\alpha = 1 + \exp \left[-(1 - 2\sigma_E) \beta \right] \left[\alpha + \sigma_E - (\beta - 1) \beta \right]$

$$\alpha = 1 + \exp\left[-(1-2\sigma_E)\beta\right] \left[\alpha_1 + \alpha_2 / \beta\right] \qquad (3.18)$$

Then, for a two-term expansion in the interior region we can obtain

$$f_{0} = 1, f_{1} = \beta^{-1}, f_{2} = \beta^{-2}, \rho_{0} = \delta_{0} = 1, \rho_{1} = \delta_{1} = \beta^{-1} \qquad (3.19)$$

$$b_{10} = b_{20} = 1, \varphi_{0} = \beta^{-2} \exp(-\sigma_{E}\beta), \varphi_{1} = \varphi_{0}\beta^{-1}$$

$$-\frac{db_{11}}{d\tau^{*}} = L, \quad -\frac{db_{21}}{d\tau^{*}} = L\frac{1-B_{20}}{1-B_{10}}, \quad b_{11}(0) = 0, \quad b_{21}(0) = 0 \qquad (3.20)$$

$$\mu_{0} - \frac{dB_{10}}{d\tau^{*}} = \sigma_{K}b_{11}\frac{\exp\left(-\frac{\sigma_{E}\tau^{*}}{1+\sigma}\right)}{1-B_{10}}, \quad B_{10}(0) = 1$$

$$\alpha_{1}\mu_{0}\frac{dB_{20}}{d\tau^{*}} = -b_{11}\frac{1-\sigma_{K}}{1-B_{10}}\exp\left[-\frac{(1-\sigma_{E})\tau^{*}}{1+\sigma}\right], \quad B_{20}(0) = 1$$

In the exterior region we seek a solution in the form

$$N_{0} = F_{0} = 1, \ b_{10} = C_{3}\tau^{L}, \ N_{1} = F_{1} = \beta^{-2}, \ b_{11} = C_{4}\tau^{L}$$
(3.21)
$$B_{10}^{\circ} = B_{20}^{\circ} = B_{11}^{\circ} = B_{21}^{\circ} = 0, \ b_{20}^{\circ} = C_{5}\tau^{L}, \ b_{21}^{\circ} = C_{6}\tau^{L}$$

Integrating Eq. (3, 20) and matching with (3, 21), we obtain

$$b_{11} = -L\tau^{*}, \quad B_{10} = 1 - \sqrt{1 - \exp\left(\frac{-\tau^{*}\sigma_{E}}{1 + \sigma}\right)\left(1 + \frac{\sigma_{E}\tau^{*}}{1 + \sigma}\right)} \quad (3.22)$$

$$\mu_{0} = 2L\sigma_{K} \frac{(1 + \sigma)^{2}}{\sigma_{E}^{2}}$$

$$B_{20} = 1 - \frac{1 - \sigma_{K}}{2\sigma_{K}\alpha_{1}} J_{5}\left(\frac{\tau^{*}\sigma_{E}}{1 + \sigma}\right), \quad J_{5}(x) = \int_{0}^{x} \exp\left(-\frac{x\left(1 - \sigma_{E}\right)}{\sigma_{E}}\right) \times$$

$$\frac{xdx}{\sqrt{1 - e^{-x}\left(1 + x\right)}}, \quad b_{21} = -\frac{1 + \sigma}{\sigma_{E}} \frac{L}{J_{5}(\infty)} \int_{0}^{\tau^{*}\sigma_{E}/1 + \sigma} \frac{J_{5}(x)}{\sqrt{1 - e^{-x}\left(1 + x\right)}} dx$$

$$\alpha_{1} = \frac{1 - \sigma_{K}}{2\sigma_{K}} J_{5}(\infty), \quad C_{3} = 1, \quad C_{5} = 1$$

For the successive terms of the expansion we obtain

$$\frac{db_{12}}{d\tau^*} = \frac{L-1}{1-B_{10}} L\tau^*, \quad b_{12}(0) = 0$$
(3.23)

$$\begin{aligned} \frac{db_{22}}{d\tau^*} &= -\frac{L}{(1-B_{10})^2} \left[(b_{21}-B_{21}) \left(1-B_{10}\right) + (\tau^*+B_{11}) (1-B_{20}) \right], \\ b_{22}(0) &= 0 \\ \frac{dB_{11}}{d\tau^*} &= -\frac{\sigma_K}{\mu_0 \left(1-B_{10}\right)} L \tau^* \left[\frac{b_{12}}{b_{11}} - \frac{\tau^{*2}\sigma_E}{(1+\sigma)^2} + \frac{\tau^*}{1-B_{10}} + \frac{B_{11}}{1-B_{10}} - \frac{\mu_1}{\mu_0} \right] \times \\ \exp \left[-\frac{\sigma_E \tau^*}{1+\sigma} \right] \\ \frac{dB_{21}}{d\tau^*} &= -\frac{1-\sigma_K}{\mu_0 \sigma_1 \left(1-B_{10}\right)} L \tau^* \left[\frac{b_{12}}{b_{11}} - \tau^{*2} \frac{1-\sigma_E}{(1+\sigma)^2} + \frac{\tau^*}{1-B_{10}} + \frac{B_{11}}{1-B_{10}} - \frac{\mu_1}{1-B_{10}} - \frac{\mu_1}{1-B_{10}} \right] \\ \frac{\mu_1}{\mu_0} - \frac{\alpha_2}{\alpha_1} \right] \exp \left[-\frac{\tau^* \left(1-\sigma_E\right)}{1+\sigma} \right] \end{aligned}$$

After integrating, we have

$$b_{12} = J_3 \left(\frac{\tau^* \sigma_E}{1 + \sigma} \right) L \left(L - 1 \right) \frac{(1 + \sigma)^2}{\sigma_E^2}$$
(3.24)
ds

Matching with (3,21) yields

$$C_4 = L(L-1) \frac{(1+\sigma)^2}{\sigma_E^2} \int_0^{\infty} \left[\frac{x}{\sqrt{1-e^{-x}(1+x)}} - x \right] dx \qquad (3.25)$$

$$C_{6} = \int_{0}^{\infty} \left\{ -\frac{L}{(1-B_{10})^{2}} \left[(b_{21}-B_{21})(1-B_{10}) + (x+B_{11})(1-B_{20}) \right] - L(L-1)x \right\} dx$$

$$B_{11} = -\frac{\sigma_{K}}{\mu_{0}(1-B_{10})}L\int_{0}^{1} x \exp\left(-\frac{x\sigma_{E}}{1+\sigma}\right)\left[-\frac{\mu_{1}}{\mu_{0}} + \frac{x}{1-B_{10}(x)} - (3.26)\right]$$
$$\frac{x^{2}\sigma_{E}}{(1+\sigma)^{2}} + \frac{b_{12}(x)}{b_{11}(x)}dx$$

$$B_{21} = \frac{1 - \sigma_K}{\mu_0 \alpha_1} L \int_0^{\tau^*} \left[\frac{b_{12}}{b_{11}} - x^2 \frac{1 - \sigma_E}{(1 + \sigma)^2} + \frac{x}{1 - B_{10}} + \frac{B_{11}}{1 - B_{10}} - \frac{\mu_1}{\mu_0} - \frac{\alpha_3}{\alpha_1} \right] \times \exp\left[-\frac{1 - \sigma_E}{1 + \sigma} x \right] \frac{dx}{1 - B_{10}(x)}$$

Assuming $\tau_* \rightarrow \infty$, we have

$$\frac{\mu_{1}}{\mu_{0}} = \frac{1+\sigma}{\sigma_{E}} J_{4}(\infty) - \frac{6}{\sigma_{E}} - \frac{2(1+\sigma)}{\sigma_{E}} (L-1)$$

$$\frac{\alpha_{2}}{\alpha_{1}} = \left[\int_{0}^{\infty} \frac{\exp\left[-\frac{x(1-\sigma_{E})}{1+\sigma}\right]}{1-B_{10}(x)} dx \right]^{-1} \int_{0}^{\infty} \left[\frac{b_{12}}{b_{11}} - x^{2} \frac{1-\sigma_{E}}{(1+\sigma)^{2}} + \frac{x+B_{11}}{1-B_{10}} - \frac{\mu_{1}}{\mu_{0}} \right] \exp\left[-\frac{x(1-\sigma_{E})}{1+\sigma}\right] dx$$
(3.27)

In a dimensional form the two-term expression for the mass combustion rate of the gas is written as follows:

$$m = \left[2\lambda \frac{K_1}{c} L \exp\left(-\frac{E_1}{RT_+}\right) \right]^{t/*} \left(\frac{T_+}{T_+ - T_-} \right) \frac{RT_+}{E} \left\{ 1 + \frac{RT_+}{E} \times (3.28) \left[\frac{T_+}{T_+ - T_-} (2.344 - L) - 3 \right] \right\}$$

4. Discussion of the results. We have found two-term expansions for the combustion rate and the terminal combustion temperature. It is very important to take into account several terms in the expansion for the combustion temperature. Thus, if we take into account only the first term in the expansion for α , we have

$$T_{+}^{(0)} = T_{-} + Q_{i} / c$$

The final temperature is equal to the adiabatic combustion temperature for the first reaction. Upon taking into account two terms in the expansion, we have, in the case of a condensed phase. $T_{+}^{(1)} = T_{-} + \frac{Q_{1}}{c} + \frac{K_{2}}{K_{1}} \frac{E_{1}}{E_{2}} \exp\left[-\frac{E_{2} - E_{1}}{RT_{+}^{(1)}}\right] \left(\frac{Q_{2} - Q_{1}}{c}\right)$ (4.1)

and, in the case of a gas.

$$T_{+}^{(1)} = T_{-} + \frac{Q_{1}}{c} + \frac{K_{2}}{2K_{1}} J_{5}(\infty, \sigma_{E}) \exp\left[-\frac{E_{2} - E_{1}}{RT_{+}^{(1)}}\right] \left(\frac{Q_{2} - Q_{1}}{c}\right) \quad (4.2)$$

As was shown in [6], the asymptotic expansions, obtained for $\beta \to \infty$, describe the solution with sufficient accuracy even for $\beta = O$ (1). The value $\beta = 10$ is typical. We note that in carrying out the expansions, β was considered to be large but still unknown, and σ_K , σ_Q , $\sigma_E \sim O(1/2)$.

As an example we consider a reaction taking place in a condensed phase with the following physicochemical parameters: $E_1 = 20 \text{ kcal/mole}$, $E_2 = 25 \text{ kcal/mole}$, $(\sigma_E = 4/9)$, $T_- = 300$ °K, $c = 0.25 \text{ cal/g} \cdot \text{deg } K^\circ$, $Q_1 = 125 \text{ cal/g}$, $Q_2 = 250 \text{ cal/g}$ $(\sigma_Q = 1/3)$, $K_2 / K_1 = 3.4$ ($\sigma_K \approx 0.23$). Then $T_+(0) = 800$ °K, $T_+(1) = 880$ °K, $m(T_+(0))/m(T_+(1)) = 0.55$. Similar results can be obtained also for the case of an exothermic reaction in a gas. We point out here that for $\sigma_E < 1/2$ the expressions (2.21) and (3.28) for the mass rate have a form similar to that for the mass rate in the case of the occurrence of only a single first reaction, the effect of a second reaction being manifested in terms of the quantity T_+ .

In the general case, when K_1 and K_2 are distinct functions of the pressure, the final concentration a_{1+} and the temperature T_+ are also functions of the pressure. The adiabatic combustion temperature $T_+^{(1)}$ is a root of Eqs. (4.1) and (4.2). These equations can be solved iteratively, for example, using $T_+^{(0)}$ from (4.1) as the initial value.

Thus, when $K_1 = K_{10}p^{\nu_1}$ and $K_2 = K_{20}p^{\nu_2}$, we have $\sigma_K = K_{10}p^{\nu_1} / K_{10}p^{\nu_1} + K_{20}p^{\nu_2}$. An important characteristic of the process is the coefficient giving the variation of the combustion rate with the pressure, namely, $\nu = \partial \ln m / \partial \ln p$. It follows from the relations (2, 21) and (3, 28) that when $0 < \sigma_E < 1/2$

$$\mathbf{v} = \mathbf{v}_{\mathbf{i/s}} + \frac{\partial \ln m}{\partial T_+} \frac{\partial T_+}{\partial \ln p}$$

Usually, $\partial m / \partial T_+ > 0$ and the sign of $\partial T_+ / \partial \ln p$, depending on the values of the quantities p, σ_K , E_1 and E_2 , can be either positive or negative. As a consequence, the coefficient ν can be larger or smaller than it is in the case of the occurrence of only a single first reaction.

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FLUIDIZATION IN THE PRESENCE OF AN OBSTACLE

PMM Vol. 39, № 2, 1975, pp. 316-323 Iu. P. GUPALO and G. P. CHEREPANOV (Moscow) (Received December 24, 1974)

The problem of transition of a friable medium layer into a suspended state in the presence in it of an internal obstacle is considered. Problems of this kind are frequently encountered in practice in connection with heterogeneous catalytic reactions in reactors with suspended catalyst layer, heat exchangers, surface coating operations which involve the immersion of articles in a fluidized layer, etc. Critical regions of the onset of fluidized state and the critical velocity of the stream are determined by the general method described in [1, 2]. Results of experiments on the fluidization of a layer with a cylindrical obstacle are presented. Comparison of theoretical and experimental data shows a good agreement.

1. The problem considered here is a particular case of the general problem of fluidization onset [1, 2]. The latter reduces to the problem of the limit equilibrium of a body whose resistance to tensile stress does not exceed a certain limit σ_s which is constant for a particular friable medium and, generally, nonzero.

It was shown earlier [1, 2] that in the case of the plane problem the lines of principal stress along which normal stress components at small areas tangent to these attain their maximum σ_s , while all shear stresses are zero, coincide with the integral curves $x = x_1$ (ξ , η), $y = x_2$ (ξ , η) of equation

$$adx_2 = bdx_1 \tag{1.1}$$

(Condition $\eta = \text{const}$ separates one line of the set, x and y are Cartesian coordinates, and the ξ -coordinate is measured along the line $\eta = \text{const}$). Here a and b are components of the body force vector acting on the friable body in directions x_1 and x_2 and taken with the opposite sign. The body force is