MULTIZONE COMBUSTION OF CONDENSED SYSTEMS

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In the general case the combustion of condensed systems is of a stage-wise character and the combustion front is multizone [1, 2]. Following the investigation of two-zone models [3-5] it became clear that, during multizone combustion, one of the zones of heat evolution is the controlling zone. The velocity of the front is equal to the velocity of the controlling zone; however, with a change in the parameters of the system, there is the possibility of a transition of the controlling role from one zone to another, as well as of the coalescence and splitting of zones. This paper discusses a generalization of the two-zone problem which makes it possible to go over to the analysis of a complex, multizone front and shows that, for a front with two reactions (in the condensed phase and in the gas) and with dispersion, there are in all three possible arrangements of the zones of heat evolution (two three-zone variants and one two-zone variant). All possible types of dependence of the combustion rate on the depth of the dispersion are found.

Combustion Model. We shall consider a model of a multizone front which, obviously, describes the principal special characteristics of the combustion of many condensed systems. Let a reaction take place in the c-phase (the condensed phase) with a heat effect $Q_1$ and an activation energy $E_1$ (pre-exponential $k_1$). The gaseous products enter the second reaction with the parameters $Q_2$, $E_2$, $k_2$. As a result of dispersion, a part $\eta_d$ of the condensed substance breaks away from the hot surface. Since the density of the heat evolution for the first reaction falls sharply with dispersion, it terminates in the c-phase (in the fumes) at a certain distance from the surface at a higher temperature. Therefore, the second reaction also may take place in two stages. At the same time, different variants of the coalescence of these zones are possible.

The investigation of the above-described complex front was based essentially on results which refer to two-zone models, which have been previously calculated numerically and analyzed [3-5]. We shall evaluate here the problem of two-zone combustion from the point of view of the mechanism of the restructuring of the front.

Control, Coalescence, and Breakaway Conditions. The exponential dependence of the rate of the chemical processes on the temperature makes it possible to divide a front with a single reaction into two zones, i.e., heat-evolution and heating zones. However, for the same reason, in a front with several reactions, several heat-evolution zones are possible. Each zone occupies a narrow temperature interval ($\sim RT_i^2/E_i$, where $T_i$ is the temperature in the i-th zone, and $E_i$ is the activation energy of the i-th reaction), in comparison with the total change over the front. At a higher temperature, the reaction does not proceed, since the starting substances (for this reaction) have been expended, while at a lower temperature the rate of the reaction is negligibly slow.

In the intervals between the heat-evolution zones, the heat flux is connected with the temperature linearly (Michelson's law), while in the zones themselves it varies sharply. The jump in the heat flux in the i-th reaction zone is equal to $Q_iU$, where $Q_i$ is the heat of the reaction, and $U$ is the mass flux (the mass combustion rate). The large curvature of the temperature profile permits an approximate integration of the heat-conductivity equation in the reaction zone, with the convective term dropped [6]. We write the integral in the form

$$ (Q_iU + q_i^a)^2 - q_i^b = (Q_i^a)^2(\eta_d^a - \eta_d^b) $$

(1)

Here $q_i$ is the heat flux flowing into the reaction zone; $T_i$ is the temperature in the zone; $\rho_i$ is the density; $a_i$ is the thermal diffusivity. The dimensionless quantity $F_i$, which takes on small values, was introduced by D. A. Frank-Kamenetski [7] in a description of single-zone combustion. The smallness of $F_i$ is connected with the smallness of the parameter $\gamma_i = (RT_i^2/E_i) (c/Q_i)$. Accurate determination of all values of $F_i$ is possible only with the solution (for the whole front) of a system made up of the thermal-conductivity equations and equations describing the (multicomponent) diffusion of the starting substances, the products, and the intermediate products. For a single-zone front in a gas with a reaction of the $n$-th order

$$F = 2n! \gamma^{n+1}$$

Since the temperature dependence of $F_i$ is of an exponential character and, consequently, weak compared with the Arrhenius factor $\exp(-E_i/RT_i)$, a qualitative investigation of the front can be made without taking changes in these quantities into account.

The unknowns in (1) are $U$, $q_i$, and $T_i$. For $N$ reaction zones we have $N$ equalities of the type of (1) and $N$ relationships of the type

$$(Q_i U + q_i) - q_{i-1} = Uc (T_i - T_{i-1})$$

which determine the changes in the heat flux in the intervals between the heat-evolution zones. Together with the condition $q_N = 0$, they completely determine the structure of the front, i.e., $U$ and all the values of $q_i$ and $T_i$. It can be shown that, to calculate the reaction rate $U$, relationships (1) for the last zone are sufficient, since $q_N = 0$, while $T_N$ is obviously the combustion temperature. Under these circumstances, the other (low-temperature) zones have no effect on the combustion temperature, a fact already noted by Ya. B. Zel'dovich in 1942 [8]. Nevertheless, a detailed examination has not yet made it possible to determine either the actual structure of the front or the combustion rate.

The dependence of the heat flux $q$ on the temperature $T$ for a two-zone front is shown on Fig. 1. The temperature of the first zone $T_1$, in distinction from $T_2$ (the combustion temperature), cannot be found by a thermodynamic calculation. With a given value of $U$, the value of $T_1$, which determines the rate of the first reaction, must be such that the rates of both reactions will be equal, which is required under steady-state conditions. The fully developed distance $l$ between the zones is thus given by a determined value of the temperature $T_1$ and of the uniquely related value of the flux $q_1$. These values are determined using equations of the type (1), (2). With an increase in the inter-zone distance $l$, the temperature, and of course also the rate of the first zone, decrease, and the zones again approach one another. With a decrease in $l$, a rise in the value of $T_1$ accelerates the first zone and re-establishes the previous value of the distance, so that the described structure of the front is stable. The combustion rate is the "normal rate" of the second (controlling) zone

$$U_2(T_2) = \rho_2 (a_2 k_2 e^{-E_2/RT_2} F_2)^{1/4}, \quad T_2 = T_0 + Q_1 + Q_2/c$$

The first zone also must move at the same rate. Its "normal rate" due to the "inherent" heat effect is

$$U_1(T_{10}) = \rho_1 (a_1 k_1 e^{-E_1/RT_1} F_1)^{1/4}, \quad T_{10} = T_0 + Q_1/c$$

If $U_1(T_{10}) < U_2(T_2)$, the second zone heats the first up to a temperature $T_1 > T_{10}$, by the same token increasing its own rate up to $U_2(T_2)$. However, at $U_1(T_{10}) > U_2(T_2)$, control of the first zone is no longer