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DISTINCTIVE FEATURES OF TEMPERATURE PROFILES IN FILTRATION-COMBUSTION WAVES RELATED TO THE TEMPERATURE DEPENDENCES OF THE HEAT CAPACITIES OF A GAS MIXTURE AND A SOLID PHASE

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In most publications devoted to filtration-combustion waves, the temperature dependences of the heat capacity of gas and solid phases have not been considered at all. In those cases where such dependences are included in the models (numerical ones, as a rule) the authors put emphasis on certain interesting features of such systems. This work is devoted to consideration of special cases related to the temperature dependences of the heat capacities.

In the first stages of analytical study of the limits of propagation of a flame and subsequently filtration-combustion waves [1–7], the properties of media (heat conduction, heat capacity, heat of reaction) were assumed to be constant, i.e., it was agreed that one can employ the average values. It is precisely at that time that the terminology of this area of study began to include such notions as the thermal velocity u_{th} and the adiabatic thermal effect of reaction ΔT_{ad}, which were considered to be constants for the problem in question. The classical formula relating the maximum temperature $T_{\max}$ in a filtration-combustion wave to its velocity u_{w} and other parameters of the process is given (in one form or another) or employed almost in all the works on this subject:

$$T_{\max} = T_0 + \frac{\Delta T_{\text{ad}}}{1 - \dfrac{u_{\text{w}}}{u_{\text{th}}}}\,, \tag{1}$$

where u_{th} is determined in terms of the specific mass flow rate of the gases G, the heat capacity of the gases c_{g}, the bulk density of a porous charge $\rho_{\text{s.bulk}}$, and the heat capacity of the charge material c_{s} as follows: $u_{\text{th}} = Gc_{\text{g}}(c_{\text{s}}\,\rho_{\text{s.bulk}})$.

In the initial works and for a long time thereafter, much research effort went into the development of a means for calculating the basic characteristics of a filtration-combustion wave u_{w} and $T_{\max}$. Condition (1), which is an energy balance, includes these two unknown quantities. Another equation which will supplement the definition of the problem must contain all the remaining characteristics of the process, such as the kinetics of oxidation, the thermal conductivity of the charge, and the intensity of interphase heat exchange. Different modifications of closing relations exist (for example, [5, 7–10]), but, in our opinion, it is not quite correct to single out any of them as the best one. In comparing the "accuracy" of such approaches, one usually orients oneself to numerical solution of the problem in the analogous formulation but without the simplifications required for obtaining analytical expressions. However, all these approximations employ the description of the combustion kinetics by one exponent, but this simplification is so rough that the comparison of the accuracy within this approximation is not extended to the comparison with experimental data.

In recent years, in developing chemical reactors that employ filtration combustion, one has begun to include real kinetic schemes, which take into account tens of components and hundreds of reactions, into numerical models [11–16]. Correct temperature dependences of c_{g} taking into account changes in both the temperature and the composition were naturally used in such calculations, and it was unnecessary to use the quantity ΔT_{ad} since the formulation of the problem became thermodynamically consistent and included the heat of formation of the components. The incorporation of the real temperature dependence of c_{s} into such a model complicated it in no way and also became a norm of modeling.

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To accelerate the process of computations one frequently carries out calculations in the approximation of a steady-state traveling wave, which is much faster than nonstationary modeling and provides all important information [13, 15, 16]. In such an approach, the solution is found from the targeting of the parameter u_w. Among the large number of variants of the systems of filtration combustion calculated without difficulties, one sometimes came across such variants for which the targeting failed. The analysis of "poor" sets of the initial parameters led us to a simple explanation of the reason why the targeting is impossible and to the algorithm of finding a solution of the traveling-wave type for such cases.

To demonstrate the arising problem and its cause and a means for solving it we direct our attention to the traditional nonstationary formulation of the problem of filtration combustion in enthalpy form:

$$G \frac{dE_\mathrm{g}}{dx} = \alpha_\mathrm{vol} (\Theta - T_\mathrm{g}) \, , \tag{2}$$

$$E_\mathrm{g} = \sum_{k=1}^{K} h_k (T_\mathrm{g}) \, Y_k \, , \tag{3}$$

$$c_\mathrm{s} \, \rho_\mathrm{s.bulk} \frac{\partial \Theta}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_\mathrm{ef} \frac{\partial \Theta}{\partial x} \right) - \alpha_\mathrm{vol} (\Theta - T_\mathrm{g}) \, , \tag{4}$$

$$\frac{G}{\varepsilon_\mathrm{p}} \frac{dY_k}{dx} = \dot{\omega}_k W_k \quad (k = 1, ..., K) \, . \tag{5}$$

When the approximation of a steady-state traveling wave is employed a change to a coordinate system moving with a velocity u_w is carried out, which results in the appearance, in Eqs. (2), (4), and (5), of the convective terms

$$G \frac{dE_\mathrm{g}}{dx} - u_\mathrm{w} \, \rho_\mathrm{g} \frac{dE_\mathrm{g}}{dx} = \alpha_\mathrm{vol} (\Theta - T_\mathrm{g}) \, , \tag{6}$$

$$c_\mathrm{s} \, \rho_\mathrm{s.bulk} \frac{\partial \Theta}{\partial t} - u_\mathrm{w} c_\mathrm{s} \, \rho_\mathrm{s.bulk} \frac{d\Theta}{dx} = \frac{\partial}{\partial x} \left(\lambda_\mathrm{ef} \frac{\partial \Theta}{\partial x} \right) - \alpha_\mathrm{vol} (\Theta - T_\mathrm{g}) \, , \tag{7}$$

$$\frac{G}{\varepsilon_\mathrm{p}} \frac{dY_k}{dx} - u_\mathrm{w} \, \rho_\mathrm{g} \frac{dY_k}{dx} = \dot{\omega}_k W_k \quad (k = 1, ..., K) \, . \tag{8}$$

The next step of transformation of the equations of the model is rejection of the terms $u_\mathrm{w}\rho_\mathrm{g} \frac{dE_\mathrm{g}}{dx}$ and $u_\mathrm{w}\rho_\mathrm{g} \frac{dY_k}{dx}$ in (6) and (8), which are 2 to 3 orders of magnitude smaller than the other terms of the equations. Authors often disregard these transport components related to the motion of the wave without mention in their papers, since this disregard is used as an approximation that is usual for everyone. For the case of combustion of atmospheric-pressure gases in ordinary solid charges such a simplification is sure to work, but upon a change to high pressures and charges of hollow spheres it is necessary to carefully analyze the possibility of using it. In the case of combustion of liquid fuels in porous media these quantities cannot be disregarded at all.

Analogously to the rejection of the transport terms in (6) and (8), one treats the nonstationary term $c_\mathrm{s} \, \rho_\mathrm{s.bulk} \frac{\partial \Theta}{\partial t}$ in Eq. (7) in the same manner, since the steady-state (i.e., stationary in a moving coordinate system) solution is sought. It is precisely at this step that an error leading to the impossibility of targeting is introduced, and this error is of fundamental character. The fact is that without analyzing the conditions of existence of the stationary solution

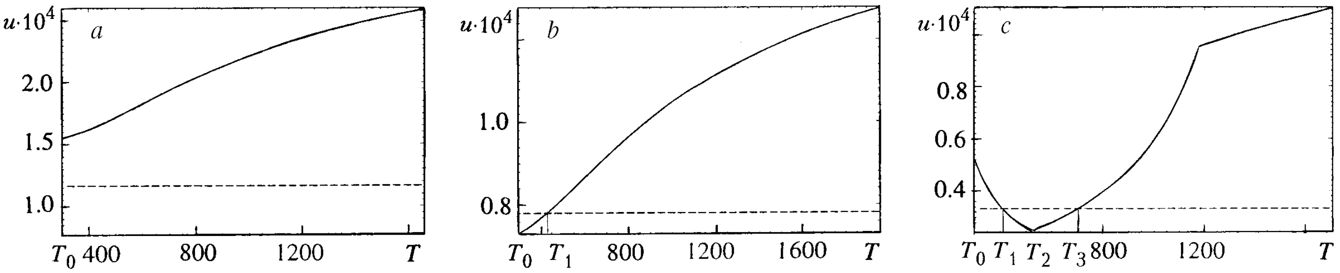

Fig. 1. Thermal-wave velocities (solid curve) vs. temperature for three characteristic cases (the quantity u_w is denoted by the dashed curve): $u_w < u_{th}(T)$ for the entire interval of temperatures $T_0 \le T \le T_{max}$ (a); $u_w > u_{th}(T)$ for $T_0 \le T < T_1$ and $u_w < u_{th}(T)$ for $T_1 < T \le T_{max}$ (b); $u_w < u_{th}(T)$ for $T_0 \le T < T_1$, $u_w > u_{th}(T)$ for $T_1 < T < T_3$, and $u_w < u_{th}(T)$ for $T_3 < T \le T_{max}$ (c).

which is then sought at $-\infty$ one employs the supplied-gas temperature T_0 as the asymptotic condition. However, situations exist where the temperature dependences of the heat capacities c_g and c_s are such that for the wave moving with a velocity u_w the stationary portion of the temperature profile is possible only for temperatures higher than a certain T_{min}, which is in turn higher than T_0. To demonstrate such a situation we transform (7), having added it and (6), in which we have previously rejected the term $u_w \rho_g \frac{dE_g}{dx}$:

$$c_s \rho_{s.bulk} \frac{\partial \Theta}{\partial t} + G \frac{dE_g}{dx} - u_w c_s \rho_{s.bulk} \frac{d\Theta}{dx} = \frac{\partial}{\partial x}\left(\lambda_{ef} \frac{\partial \Theta}{\partial x}\right). \tag{9}$$

For the asymptotic side of the solution the temperatures of the gas and the solid phase virtually coincide and (9) can be rewritten in the form

$$c_s \rho_{s.bulk} \frac{\partial \Theta}{\partial t} + (G c_g - u_w c_s \rho_{s.bulk}) \frac{d\Theta}{dx} = \frac{\partial}{\partial x}\left(\lambda_{ef} \frac{\partial \Theta}{\partial x}\right) \tag{10}$$

or

$$c_s \rho_{s.bulk} \left[\frac{\partial \Theta}{\partial t} + (u_{th} - u_w) \frac{d\Theta}{dx}\right] = \frac{\partial}{\partial x}\left(\lambda_{ef} \frac{\partial \Theta}{\partial x}\right). \tag{11}$$

The hyperbolic operator on the left-hand side of (11) has the difference $u_{th} - u_w$ (in which u_w is a constant and the u_{th} is a function of temperature) as the velocity. If $u_{th} - u_w > 0$, the characteristics of the hyperbolic operator are directed from left to right and, conversely, from right to left, for $u_{th} - u_w < 0$. The temperature dependence $c_g(T_g)$ can be complex since it is determined by the chemical process with the resulting change not only in the type of molecules but in their number as well. Moreover, it can change nonmonotonically, for example, first increase and then decrease. The heat capacity of the solid material of the charge $c_s(\Theta)$ increases monotonically with temperature, as a rule. It is clear that the velocity of the filtration-combustion wave, dependent as it is on all the parameters of the problem, is mainly determined by the high-temperature region of the solution but in no way by just the thermal velocity u_{th} at the initial temperature T_0. It is obvious that if $u_{th}(T_0) - u_w < 0$ the problem cannot be solved by targeting from T_0, but this by no means implies that a filtration-combustion wave does not exist. It is necessary to separate the cases where the thermal-wave velocity $u_{th}(T, \Theta)$ calculated from the real solution, i.e., for all the temperatures of this solution and their attendant compositions of the gases, is higher than the velocity of the filtration-combustion wave u_w (see Fig. 1a) and the cases where the temperature interval exists in which $u_w > u_{th}(T, \Theta)$ (see Fig. 1b). The first variant corresponds to a filtration-combustion wave in which the temperature profile becomes stationary in the entire interval of the existing temperatures from T_0 to T_{max}, i.e., the entire profile is localized on a finite portion of space. For the second case (Fig. 1b), the distribution (localized in space) rapidly becomes stationary only in the interval from T_1 to T_{max} while the por-

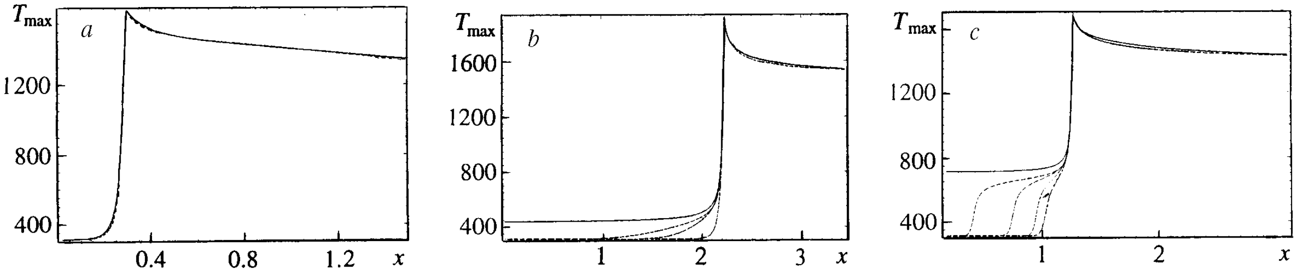

Fig. 2. Temperature profiles calculated using the nonstationary model (dashed curves) and the traveling-wave model (solid curve) for the three cases presented in Fig. 1: the entire profile $T_0 \le T \le T_{\max}$ is totally localized in space (a); part of the profile for $T_0 \le T < T_1$ is nonstationary and is extended to infinity, whereas the profile localized in space has been formed for $T_1 < T < T_{\max}$ (b); $u_w < u_{th}(T)$ for $T_0 \le T < T_1$, $u_w > u_{th}(T)$ for $T_1 < T < T_3$, and $u_w < u_{th}(T)$ for $T_3 < T \le T_{\max}$ (c).

tion of the temperatures from T_0 to T_1 will constantly change, extending in space. From the viewpoint of the steady-state profile (from T_1 to $T_{\max}$), the picture at long times from the beginning of the process will appear as if this stationary solution has the asymptote T_1 rather than T_0 on the left-hand side (it is precisely the temperature T_1 that is transferred from right to left along the characteristic).

Figure 2 compares the solutions obtained in nonstationary modeling and using the model in the approximation of a traveling wave. For case *b* the asymptote T_1 was employed in the traveling-wave model. It is obvious that a correct assignment of the left-hand asymptote enables us to obtain all the important characteristics of the filtration-combustion wave for both the "normal" situation (case *a*) and for case *b* with a "slow" low-temperature portion of the solution. We note that the variant of Fig. 1c with two intersections of the distribution $u_{th}(T)$ and u_w, having as it is three characteristic temperatures T_1, T_2, and T_3, actually differs little from case *b*. We should take a larger quantity, i.e., T_3, as an asymptote in the traveling-wave model. In case *c*, the portion between T_0 and T_2 will have a finite size while the part of the profile between T_2 and T_3 will constantly be extended. We are unable to analytically describe the evolution of this part of the temperature profile, although it is clear that the velocity of extension will be lower than $u_w - u_{th}(T_2)$.

We note that in the given case the values of the asymptotes T_1 and T_2 were rather low for the chemical processes to be disregarded, and our consideration based on the single-temperature equation (11) is justified. With increase in these temperatures, chemical processes can begin and the simplified analysis given above will turn out to be inaccurate. The principle itself of the change in the height of the left-hand asymptote as a function of the relation $u_{th}(T)$ and u_w must be preserved.

We now return to the algorithm of solution of the problems of filtration combustion using the approximation of a steady-state wave. First of all we must analyze the profile of the thermal velocity and find its lowest value. For the profile $u_{th}(T)$ it will be $u_{th}^{\min} = u_{th}(T_0)$ in case *a* and $u_{th}^{\min} = u_{th}(T_3)$ in case *c*. If a tentative calculation for $u_w = u_{th}^{\min}$ shows that such a velocity is high for this set of parameters, targeting must be carried out for the left-hand asymptote T_0. If the algorithm of solution requires that u_w be increased, one should increase the left-hand asymptotic value from which the targeting must begin. The minimum temperature T_{as} at which the thermal velocity $u_{th}(T_{as})$ coincides with u_w ensuring solution of the problem is the asymptote sought. The solution obtained in the approximation of the steady-state filtration-combustion wave with such an asymptote yields the correct value of u_w and the correct form of the profiles for temperatures higher than the asymptotic one (see Fig. 2).

APPENDIX

Initial Parameters for the Above Three Variants of Calculations. In all the cases we consider the combustion of a methane/air gas mixture with a ratio of the volumes of 1/2.5 (the stoichiometric ratio is close to 4, i.e., corresponds to the reaction of incomplete oxidation of methane). To model the chemical kinetics we have employed the

TABLE 1. Initial Parameters and Results of Calculation According to the Model in Which the Traveling-Wave Approximation is Employed

Variant	G	T_0	T_{max}	$u_w \cdot 10^3$
a	0.126	300	1640	0.115613
b	0.592	425	1935	0.775074
c	0.174	710	1698	0.328973

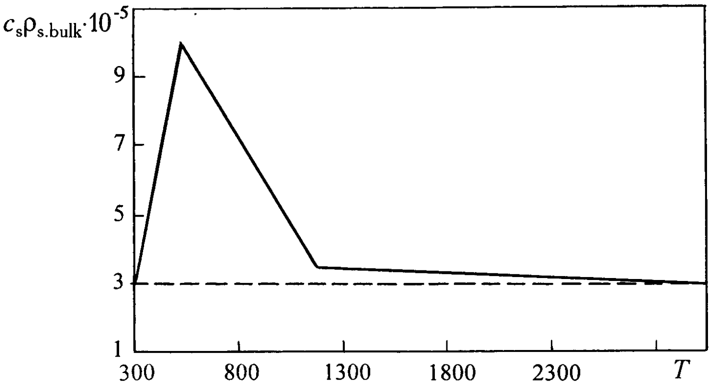

Fig. 3. Temperature dependences of the heat capacities employed in the calculations (dashed curve for variants *a* and *b*, solid curve for variant *c*).

scheme of [17]. The interphase heat exchange is described in accordance with [18]. The initial parameters employed to solve the problem in the traveling-wave approximation and the calculation results are given in Table 1. For variants *a* and *b* the calculations were carried out for a constant heat capacity of the porous charge, while in case *c* the quantity c_s changed piecewise-linearly, as is shown in Fig. 3.

NOTATION

c_g, specific heat capacity of the gas mixture, J/(kg·K); c_s, specific heat capacity of the charge material, J/(kg·K); E_g, specific enthalpy of the gas mixture, J/kg; G, specific mass flow rate of the gas mixture, kg/(m^2·sec); h_k, specific enthalpy of the kth component, J/kg; t, time, sec; T_g, gas temperature, K; ΔT_{ad}, adiabatic thermal effect of reaction, K; u_w, velocity of the filtration-combustion wave, m/sec; u_{th}, velocity of the thermal wave, m/sec; ε_p, intergranular porosity; W_k, molar mass of the kth component, kg/mole; x, space coordinate, m; Y_k, weight fractions of the components; Θ, skeleton temperature, K; T_{max}, maximum temperature in the porous charge, K; $\dot{\omega}_k$, rate of formation of the kth component, mole/(m^3·sec); α_{vol}, volumetric coefficient of interphase heat exchange, W/(m^3·K); λ_{ef}, effective coefficient of thermal conductivity of the charge, W/(m·K); $\rho_{s.bulk}$, bulk density of the charge, kg/m^3. Subscripts and superscripts: as, asymptotic value; ef, effective value; g, gas phase; k, index of the chemical element in question; p, porous medium; s, solid phase; th, thermal wave; w, filtration-combustion wave; ad, adiabatic conditions; s.bulk, value averaged over the volume; vol, volumetric; max, maximum.

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