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Modeling of Unsteady Filtration Gas Combustion

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Unsteady filtration gas combustion with various gas flow parameters is studied by mathematical modeling. Transition processes due to a sudden change in the calorific value of the gas mixture, gas flow velocity, and flow direction are considered. Trends and mechanisms of change in the structure of the filtration gas combustion wave and its propagation velocity are analyzed for various types of transition processes. It is found that with a sudden change in gas flow parameters, the flame can abruptly move large distances in the porous medium. Subsequently, at the new flame localization, a wave of filtration gas combustion forms which corresponds to the changed parameters of the gas flow. If in the porous medium, the amount of heat is insufficient, the transition process ends with quenching. As the gas flow direction changes, the combustion wave continues to propagate in the former direction for some time, which can lead to the spread of the high-temperature zone in devices based on the reverse process with a homogeneous gas-phase reaction.

Key words: filtration gas combustion, porous medium, unsteady combustion.

INTRODUCTION

Extensive theoretical and experimental studies of steady-state traveling waves of filtration gas combustion (FGC) have revealed a number of properties of interest for practical applications [1–5]. However, in the design of practical burner devices based on f FGC, traveling combustion waves come in conflict with the requirement of long operation with limited burner sizes. In the well-known reverse process [6], this conflict, in particular, is resolved by a periodic change in the gas flow direction, which is followed by a change in the direction of combustion wave propagation. As a result, on the one hand, the useful properties of traveling waves, such as the superadiabatic effect, are utilized, and, on the other hand, the heated zone is localized in a limited region of the burner due to a periodic change in the direction of FGC wave propagation.

A FGC wave is a complex consisting of a thermal wave in the porous medium and a conjugated gas combustion wave. A change in the direction of gas filtration leads to a change in the structure of the FGC wave, which will be called the transition process. Due to the high thermal inertia of the porous medium, the transition process can lasts a few minutes or even tens of minutes. Such transition processes provide important information for designing real burner devices. Transition processes due to a change in gas-mixture flow parameters (gas velocity, mixture composition) can also occur during routine switching in devices based on FGC or in emergencies. Some of such transition processes have been studied experimentally [7].

The aim of the present work was to study transition processes due to a change in gas flow characteristics. The most convenient method for this purpose is numerical modeling, which allows online monitoring of any changes in the characteristics of the combustion wave.

METHOD OF SOLUTION

The modeled system is a tube of radius R_w which is completely or partly filled with a porous medium. A combustible mixture flows into the tube from one

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end and combustion products escape from the other end. The combustion wave is assumed to be plane and one-dimensional, and the possible effects of the front curvature are not considered.

The system of equations describing the propagation of a one-dimensional unsteady combustion wave in a chemically inert porous medium consists of the heat-transfer equations for the gas (1) and porous medium (2), the mass-transfer equation for the deficient component of the gas mixture (3), the mass conservation equation for the flow (4), and the equation of state (5):

$$\varepsilon_g \rho c_p \left(\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left(\varepsilon_g \lambda \frac{\partial T}{\partial x} \right) + \alpha S_c (T_s - T) + Q \varepsilon_g \rho Y W, \quad (1)$$

$$\rho_s (1 - \varepsilon_g) c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x} \left((1 - \varepsilon_g) \lambda_s \frac{\partial T_s}{\partial x} \right) + \alpha S_c (T - T_s) + 2 \frac{\alpha_w}{R_w} (T_0 - T_s), \quad (2)$$

$$\varepsilon_g \rho \left(\frac{\partial Y}{\partial t} + v \frac{\partial Y}{\partial x} \right) = \frac{\partial}{\partial x} \left(\varepsilon_g \rho D \frac{\partial Y}{\partial x} \right) - \varepsilon_g \rho Y W, \quad (3)$$

$$\frac{\partial \varepsilon_g \rho}{\partial t} + \frac{\partial \varepsilon_g \rho v}{\partial x} = 0, \quad (4)$$

$$\rho T = \text{const}. \quad (5)$$

Here T and T_s are the temperatures of the gas and the inert porous medium, Y is the relative mass concentration of the deficient component of the gas mixture, v is the velocity of the carrier gas, ρ and ρ_s are the density of gas and the porous medium, c_p and c_s are their specific heat capacities, λ and λ_s are the thermal conductivities, ε_g is the porosity, α is the interfacial heat-exchange coefficient, α_w is the external heat-transfer coefficient, S_c is the specific surface of the porous medium, D is the diffusion coefficient of the deficient component of the gas mixture, $Q = c_p(T_b - T_0)$ is the thermal effect of the reaction, T_b is the adiabatic combustion temperature of the gas mixture, $W = k_0 \exp(-E/(RT))$ is the rate of the effective one-phase chemical reaction, where k_0 is the preexponential factor, E is the activation energy, and R is the universal gas constant.

The boundary conditions for system (1)–(5) are specified as follows. At the tube inlet boundary: $v = v_{\text{inl}}(t)$, $T = T_{\text{inl}}$, and $Y = Y_{\text{inl}}$, where the superscript *inl* denotes the inlet values of the gas velocity, temperature, and concentration of the deficient reacting component in the gas mixture. At the output boundary, soft boundary conditions are specified: $\dfrac{\partial T}{\partial x} = \dfrac{\partial Y}{\partial x} = 0$.

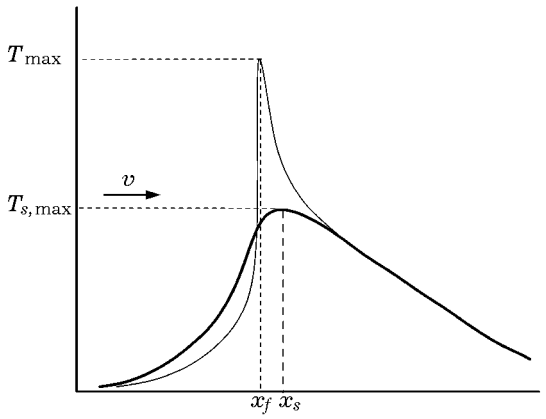

Fig. 1. Structure of the wave of filtration gas combustion: the thin curve is gas temperature profile and the thick curve is the porous medium.

The initial conditions ($t = 0$) are as follows: $v = v_0(x)$, $T = T_0(x)$, $T_s = T_{s0}(x)$, and $Y = Y_0$. Ignition is performed by naked flame or by the heated region of the porous medium. The type of ignition is specified by the initial profiles $T_0(x)$ and $T_{s0}(x)$. In the case of ignition by an naked flame, on the right or on the left in the tube there is a region which is not filled with a porous medium.

The method of numerical solution of the system is described in detail in [8]. Because the length of the combustion zone is very small, to perform an accurate calculation of flow parameters in this zone, we used a nonuniform adaptive difference mesh with the maximum refinement in the vicinity of the maximum of the heat-release function in Eq. (1). The difference mesh was modified as this maximum moved. The flow parameters were reinterpolated by means of local B-splines. The program was tested on several problems with *a priori* known solutions [8].

The program calculates temperature profiles of the gas and the porous medium, the fuel concentration profile, and the gas velocity at each time and determines the coordinate of the chemical reaction zone. The program allows a change in the gas flow parameters (gas mixture composition, specified by adiabatic combustion temperature, and the velocity and direction of the gas mixture flow) at a specified time or with a specified period, making it possible to study various transition processes.

RESULTS AND DISCUSSION

We shall treat the transition process as a process of change in combustion-wave characteristics. The FGC wave is a complex consisting of a thermal wave in the

porous medium and a gas combustion wave, which will be identified with the flame (Fig. 1). As the dynamic characteristics of the filtration combustion wave it is possible to use the maximum temperatures of the gas ($T_{\max}$) and the porous medium ($T_{s,\max}$), the coordinates corresponding to the maximum temperatures of the gas (x_f) and porous medium (x_s), their relative position, and the propagation velocities of the flame (u) and thermal wave in the porous medium (u_s). The latter are determined as dx_f/dt and dx_s/dt, respectively.

Transition Processes Due to Changes in the Calorific Value of the Mixture and Filtration Velocity

Experiments have shown that transition processes due to small changes in the gas flow parameters that do not change the direction of FGC wave propagation are trivial and predictable [7]. Calculations have confirmed the experimental trends of such transition processes. Therefore, here we shall consider only transition processes accompanied by changes in the direction of motion of the wave.

Figure 2 shows transition process due to an instantaneous change in the methane content in a methane–air mixture from 9 to 4%. In this example, the porous medium consists of granular carborundum with a mean grains size of 2.5 mm and porosity of 0.45. The length of the tube with the porous medium is 25 cm. A feature of this transition process is that the steady-state filtration combustion wave of the 9% mixture is countercurrent to the gas flow, and that of the 4% mixture is concurrent to the gas flow. Accordingly, in the transition process, the direction of wave propagation should change. The filtration combustion wave of the 9% methane–air mixture was initiated by the region of the porous medium between coordinates of 20 and 24 cm and heated to 1500 K. In a few minutes after initiation, a steady-state FGC wave formed and propagated at a velocity of −0.010 cm/sec (Fig. 2c). The propagation of the FGC wave from left to right is taken to be the positive direction. The minus sign of the velocity means that the wave propagates against the gas flow. The steadiness of the filtration combustion wave of a 9% mixture is indicated not only by the constancy of the propagation velocity but also by the constant distance between the coordinates x_f and x_s (Fig. 2a) and the constancy of the maximum temperatures of the gas and the porous medium (Fig. 2b) up to the time of change in the mixture composition.

At the time $t = 600$ sec, supply of the 9% mixture is replaced by supply of the 4% mixture. In the structure of the FGC wave, this leads to a sharp decrease in the height of the gas peak against the thermal wave in the porous medium (see Fig. 1) and, hence, a decrease in the flame temperature (see Fig. 2b). In addition, the gas peak becomes wide, i.e., the chemical reaction becomes distributed. Whereas for the 9% mixture, the width of the reaction zone is tenth of millimeter, after the replacement by the 4% mixture, it increases to 1–2 cm. In the above example, the value of $T_{\max}$ decreases by more than 600 K, and the height of the gas peak immediately after the replacement of the mixture is less than 100 K. In this case, the flame moves abruptly in the gas flow to the region of the maximum temperature of the porous medium, as is evident from the merging of the coordinates x_f and x_s after the change in the mixture composition. This change in the structure of the FGC wave, on the one hand, makes it possible to minimize the heat loss from the reacting gas, and on the other hand, it provides additional heating of the gas from the porous medium to the moment of ignition, i.e., increases the enthalpy of the gas.

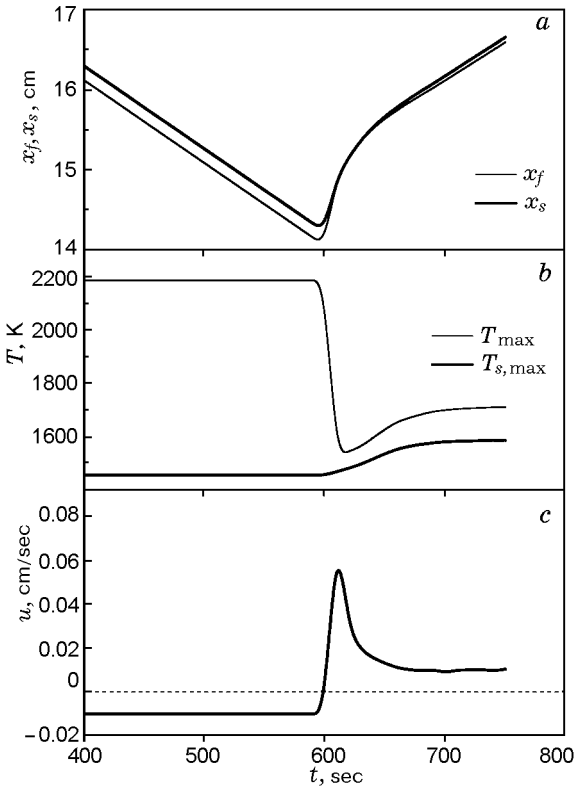

Fig. 2. Time dependences of the coordinates of the flame and the maximum temperature point of the porous medium (a), the maximum temperatures of the gas and porous medium (b), and the velocity of propagation of the FGC wave (c) with a change in the parameters of the gas mixture: gas flow parameters are 9% CH_4 + air, $v = 0.2$ m/sec ($t < 600$ sec), 4% CH_4 + air, and $v = 0.2$ m/sec ($t > 600$ sec).

In the given porous medium at the given filtration velocity, the steady-state filtration combustion wave of the 4% mixture is a concurrent wave. Because of the small calorific value of the gas, for this wave to exist, a more heated porous medium is required than for the 9% mixture. The transition to the concurrent direction occurs because, as the heat release decreases, the conductive heat flux against the gas flow at the first front of the thermal wave in the porous medium becomes much lower than the convective heat transfer due to the oncoming cold gas. As a result, the first front of the thermal wave in the porous medium and the entire FGC wave begin to propagate along the gas flow (concurrent wave) (see Fig. 2b and c at $t > 600$ sec). The concurrent wave mode is more economic since the combustion is sustained by effectively using the heat which was previously transferred to the porous medium by the hot products of gas combustion. The accelerated propagation of the FGC wave immediately after the change in the regime ($600 < t < 670$ sec in Fig. 2a and c) allows this heat to be used to heat the porous medium (Fig. 2b). The gas combustion temperature increases with increasing temperature of the porous medium. Furthermore, the chemical reaction zones is narrowed, and the released heat is less spread over the space and is more effectively expended for heating the gas, leading to an increase in the height of the gas peak (see Fig. 2b). The transition process is completed when thermal equilibrium is established between the gas combustion wave and the thermal wave in the porous medium, i.e., a steady-state FGC wave forms.

The critical moment of this transition process is the heating of the porous medium after the transition to the low-calorific mixture. Criticality manifests itself with increasing filtration velocity of the 4% mixture. Higher filtration velocities of the 4% mixture correspond to higher maximum temperatures of the porous medium in the steady-state wave. Therefore, the higher the gas filtration velocity after the transition to the 4% mixture, the larger the time of formation of the new steady-state FGC wave. Beginning at $v = 0.6$ m/sec, a steady-state wave does not form after the change in the mixture composition, and quenching occurs. This may be due to the fact that in the combustion wave formed before the transition to the 4% mixture, the amount of heat is not sufficient for the required heating of the porous medium.

Figure 3 shows the reverse transition process — from a low-calorific mixture (4% methane–air) to a high-calorific mixture (8%). In this case, the propagation direction also changes, but from a concurrent to countercurrent FGC wave. In this example, the porous medium consisted of ceramic spheres 6 mm in diameter. The filtration velocity of the 4% mixture was 0.3 m/sec, and that of the 8% mixture was 0.2 m/sec. The parameters were chosen so as to vividly demonstrate the features of this type of transition process. The combustion wave of the 4% mixture was initiated by the region of the porous medium located between coordinates of 20 and 60 mm and heated to 1700 K. In approximately 4 min, a quasisteady-state concurrent FGC wave formed, which propagated at a velocity of $1.65 \cdot 10^{-2}$ cm/sec. At the time $t = 300$ sec, the supply of the 4% methane–air mixture was replaced by supply of a 8% mixture. This led to a sharp increase in the flame temperature (Fig. 3b). Modeling shows that, at the first moment of supply, ignition of the 8% mixture occurred not by self-ignition in the heated porous medium but immediately from the flame of the 4% mixture, i.e., at the site where the flame velocity was counterbalanced by the gas flow velocity. Since the flame velocity of the 8% mixtures far exceeds the gas flow velocity at this site, the flame is transferred against the gas flow toward the less heated

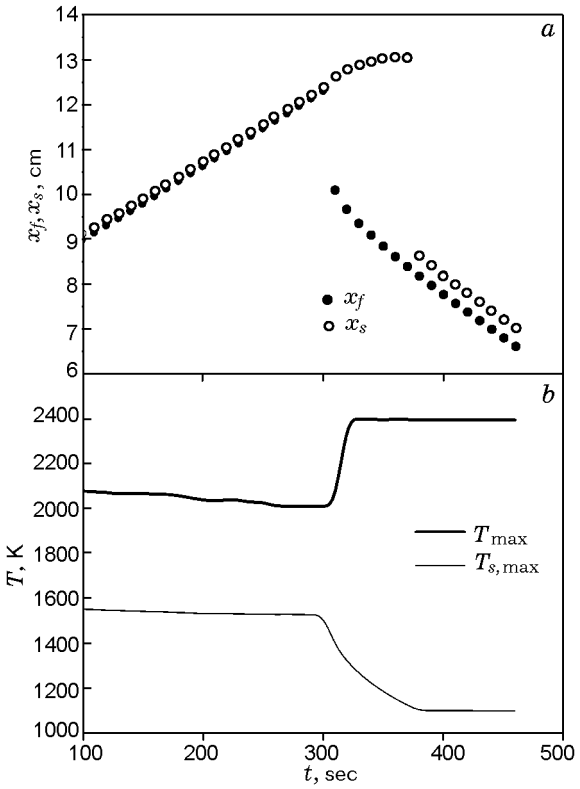

Fig. 3. Time dependences of the coordinates of the flame, the maximum temperature point of the porous medium (a), and the maximum temperatures of the gas and porous medium (b) with changes in the parameters of the gas mixture: gas flow parameters are 4% CH_4 + air, $v = 0.3$ m/sec ($t < 300$ sec), 8% CH_4 + air, and $v = 0.2$ m/sec ($t > 300$ sec).

porous medium (Fig. 3a). The distance of the flame transfer was about 2.5 cm, and the flame velocity during the transfer increased by two orders of magnitude and reached 1 cm/sec. After the transfer, the flame is stabilized at the site where the gas flow velocity counterbalances the flame velocity of the 8% mixtures. Here fast local heating of the porous medium due to heat exchange with the burning gas begins. At the former location of the flame, in contrast, the porous medium cools. As a result, a two-humped temperature distribution occurs: one maximum is located at the former location of the flame of the 4% mixture, and the second maximum is at the site of the new location of the flame of the 8% mixture. For some time, the temperature at the former maximum remains higher than that at the new maximum. In the case presented in Fig. 3a, it is about 70 sec. The jump of the coordinate of the maximum of T_s in Fig. 3a implies that at this time, the temperature of the porous medium at the new maximum became higher than that at the old maximum, and the distance between the old and new maxima is $\approx$5 cm.

As can be seen from Fig. 3a, the filtration combustion wave of the 8% mixture is countercurrent, i.e., after the transfer, the flame propagates against the gas flow. This regime is less economic, the porous medium is less heated and its maximum temperature in the steady-state filtration combustion wave of the 8% mixture is lower than that for the 4% mixture. Therefore, $T_{s,\max}$ decreases in the transition process. In approximately 1.5 min after the replacement of the mixture, the main dynamic characteristics of the FGC wave become quasisteady-state and the transition process is completed.

Transition Processes Due to a Change in the Direction of Gas Filtration

Figure 4 shows a transition process due to a change in the gas flow direction without changes in mixture composition and filtration velocity. This type of transition process is of interest in connection with attempts to design burners based on the reverse process with a homogeneous gas-phase reaction [6]. Calculations were performed for a 6% mixture with a gas flow velocity at the entrance to the porous medium of 0.4 m/sec. The porous medium was the same as in the first example. The FGC wave was initiated by the region of the porous medium between coordinates of 60 and 100 mm heated to 1700 K. The gas was initially supplied from the left. In approximately 3 min after the initiation, a quasisteady-state FGC wave formed, which propagated at a velocity of $2.3 \cdot 10^{-3}$ cm/sec (Fig. 4b and c).

At the time $t = 360$ sec, the gas flow direction was reversed. Figure 5 shows the change in the structure of the FGC wave after the change in filtration direction. Digit 1 denotes the structure of the wave at the last moment before the change in direction. This structure is typical of steady-state FGC waves. As can be seen from Fig. 4a, the flame is at the first front of the thermal wave in the porous medium at a distance $\approx$3 mm from the maximum temperature point of the porous medium. After that, the gas begins to be supplied from the right. Propagating in the heated porous medium, it is heated and ignited at a distance of $\approx$4 cm from the former location of the flame. In Fig. 4a, this is shown by the discontinuity of the coordinate of the flame. The temperature of the newly ignited flame is somewhat lower than earlier (Fig. 4b). This is due to the lower temperature of the porous medium at the flame location. In turn, the cause of the lower temperature of flame stabilization is the flat temperature profile of the porous medium on the right (profile 1 in Fig. 5), which provides more effective heating of the gas and, as a consequence, the attainment of the gas ignition temperature at a lower temperature of the porous medium.

At the former location of the flame, the porous medium begins to cool since the heat source disappears, and at the new location of the flame, in contrast, it is rapidly heated. As a result, a transitional two-humped temperature profile occurs (profile 2 in Fig. 5). The temperature maximum of the porous medium is first at the cooling left hump; therefore, after the change in filtration direction, it decreases. Then, during heating of the porous medium at the new location of the flame, the maximum passes to the right, growing, hump. At this time, the coordinate x_s undergoes a jump and the temperature maximum of the porous medium begins to grow (see Fig. 4a and b). In this example, in even 10 sec after the change in filtration direction, the maximum appears at the new location of the flame, and in a minute, the temperature profile of the porous medium becomes monotonic (profiles 3 and 4 in Fig. 5). During heating of the porous medium, the flame temperature also increases at the second hump and in approximately 30 sec, it reaches the value which was before the change in filtration direction (see Fig. 4b).

It is not trivial that after the change in the direction of gas filtration, the FGC wave continues to propagate in the former direction (i.e., against the flow) for another 4 min (see Fig. 4a and c). Since only the gas flow direction is changed and the composition of the mixture and the velocity of its flow remain unchanged, it would be reasonable to expect that the newly ignited wave will also be concurrent, i.e., its propagation direction will be reversed together with the gas. This, however, does not

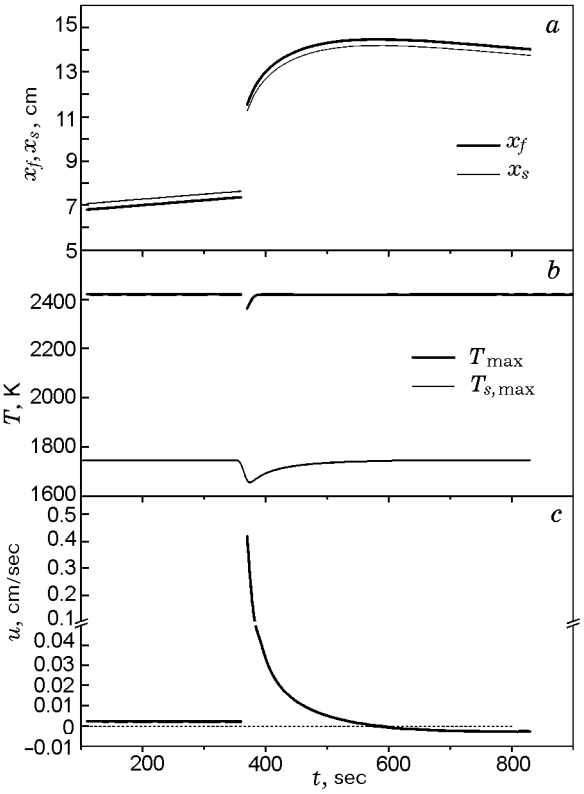

Fig. 4. Coordinates of the flame and the maximum temperature point of the porous medium (a), the maximum temperatures of the gas and the porous medium (b), and the velocity of propagation of the FGC wave (c) versus time during change in the filtration direction of the gas mixture: gas flow parameters are 6% CH_4 + air mixture, $v = 0.4$ m/sec ($t < 360$ sec), and $v = -0.4$ m/sec ($t > 360$ sec).

occur at once because the change in the structure of the FGC wave takes some time. The position of the flame on the temperature profile of the porous medium is determined by the balance of the mass of the gas, which reduces to the equality of the burning velocity and the flow velocity at the flame location. An increase in the temperature of the porous medium in the region of the new location of the flame leads to a gradual reduction in heat losses from the flame and, hence, to an increase in the combustion velocity, which becomes higher than the velocity of the countercurrent gas flow at the flame location. As a result, the flame is transferred against the flow toward lower temperatures of the porous medium (profiles 2–4 in Fig. 5). As can be seen from Fig. 4c, the velocity of this motion reaches 0.4 cm/sec, which is two orders of magnitude higher than the steady-state velocity of the wave for these parameters of the gas and the porous medium. The motion against the flow continues as long as the temperature of the porous medium increases. Simultaneously, in this stage of the transition

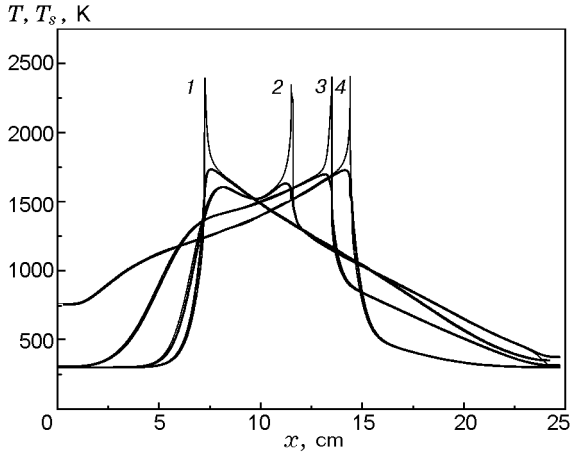

Fig. 5. Change in the temperature profiles of the gas (thin curves) and porous medium (thick curves) due to a change in the direction of gas filtration (parameters the same as in Fig. 4) for time from the moment of initiation 360 (1), 370 (2), 420 (3), and 540 sec (4).

process, the temperature profile of the porous medium becomes steeper on the right and flatter on the left, i.e., it tends to the mirror reflection of profile 1 in Fig. 5. This restructuring process is almost completed in 7 min after the change in filtration direction. The combustion wave becomes concurrent again, and its velocity is established at a level of $-2.3 \cdot 10^{-3}$ cm/sec, i.e., it coincides in absolute size with the velocity before the change in filtration direction (see Fig. 4c).

Thus, the total transition process due to a change in gas filtration direction is rather long — about 10 min. In devices based on the reverse process, the half-cycle is usually 1–2 min [6]. This implies that, in the reverse process, the parameters of the FGC wave are far from steady-state. Therefore, knowledge of the steady-state characteristics of FGC waves is not sufficient to predict the behavior of combustion waves in the reverse process. The second important result of the modeling performed is that, after the change in filtration direction, the combustion wave continues to move for some time in the same direction as before the change in filtration direction. If the period of the reverse process is small enough, this can lead to spreading of the combustion zone rather than to its localization. In addition, the FGC wave at this stage of the transition process is countercurrent to the gas flow. From the FGC theory, it is known that countercurrent FGC waves are energetically less favorable than concurrent wave and do not allow one to completely implement the idea of superadiabatic combustion, which underlies the reverse process [1]. The choice of optimal parameters of the reverse process requires detailed modeling with a wide variation of the parameters of the system.

CONCLUSIONS

• During a sharp decrease in the calorific value of the gas mixture, which requires a change in the direction of FGC wave propagation from countercurrent to concurrent, the following phenomena are observed: the flame is transferred toward the temperature maximum of the porous medium with subsequent fast motion in the concurrent direction. This motion is accompanied by heating of the porous medium with a gradual decrease in the propagation velocity to the steady-state value. This transition process can end with quenching if the amount of heat in the initial FGC wave is insufficient for the formation of a steady-state FGC wave at the new parameters of the system.

• In transitions from a concurrent to countercurrent wave due to a sharp increase in the energy of the gas flow, the flame abruptly moves large distances of about several centimeters against the flow at the moment of change in the parameters. This results in the formation of a transition structure of the FGC wave with a two-humped temperature distribution of the porous medium. In the experiment, this looks like disintegration of the single FGC wave into two separate hot spots, one of which soon quenches, and the second hot spot is heated to form a steady-state FGC wave corresponding to the new values of the system parameters.

• In the transition process due to a change in the direction of gas filtration, two-humped transitional temperature profiles of the porous medium are also formed. Another important property is that after the change in the filtration direction, the combustion wave continues for some time to propagate in the former direction, which in this case is countercurrent to the gas flow. This feature can reduce the efficiency of the homogeneous reverse process and lead to spreading of the combustion zone in devices based on this process.

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