Journal of Engineering Physics and Thermophysics, Vol. 75, No. 5, 2002

NUMERICAL INVESTIGATION OF UNSTEADY HEAT EXCHANGE IN IGNITION FOR REACTIVE CHANNEL WALLS BY THE FLOW OF A HIGH-TEMPERATURE VISCOUS GAS

V. M. Ushakov[a] **and O. V. Matvienko**[b]

UDC 536.533

A study is made of the process of ignition of reactive channel walls by a laminar flow of hot gases, including the stages of heating of a substance and of reacting in the surface layer with self-acceleration of the chemical reaction. The process is determined by the heat exchange between the gas and the wall, the strength of the heat source in the chemical-reaction zone, and the sink of heat due to conduction in the radial and axial directions. In the stage of self-heating, we can have heat sink not only deep into the wall and/or through its external boundary but into the gas flow as well. The problem has been solved in a conjugate formulation. The influence of the temperature, the velocity of the gas at the entrance to the channel, and the wall thickness on ignition characteristics has been studied.

In the case of flow of a high-temperature gas in different technological devices, the problem of its interaction with the walls arises. For inert walls this problem is reduced to calculation of thermal stresses developing in the walls of the technological devices and to calculation of strength characteristics. Where the channel walls are made of reactive material an additional problem arises, which is associated with the possibility of igniting the channel walls by a high-temperature gas flow.

It is well known [1] that the course of a chemical reaction in channel walls is largely determined by the conditions of heat exchange of these walls with the gas flow and the ambient medium. If the intensity of heat removal through the external boundary is sufficiently high and the flow temperature does not exceed a certain critical value, the reaction in the channel walls occurs in a low-temperature regime characterized by a small depth of decomposition of the wall material. When these conditions are not fulfilled, ignition of the channel walls occurs.

In most cases, a theoretical investigation of the local process of ignition of reactive channel walls by the convective heat flux is modeled with the use of a heat-conduction equation with conditions of the third kind for a specified (constant, as a rule) coefficient of heat exchange between the gas and the channel walls [1–5].

However, the use of the steady-state coefficient of heat exchange in solving ignition problems leads, in many cases, to inadequate results [6], since the process of ignition is known to be substantially unsteady. To overcome this problem one must use information on an unsteady variation in the heat-transfer coefficient in specifying the boundary conditions. Unfortunately, this information, both experimental and theoretical, is absent at present for a wide range of variation of basic parameters. Therefore, in a more rigorous formulation, one should consider the equations describing the process of ignition in the wall in conjugation, i.e., in combination with the two-dimensional equations of hydrodynamics and heat exchange in a heated gas, and write the boundary conditions at the gas–wall boundary in the form of conservation laws [6].

Physical Formulation of the Problem. Below we consider the process of ignition of reactive channel walls by the laminar flow of hot gases, including the stages of heating of a substance and of reacting in the surface layer with the self-acceleration of the chemical reaction. The process is determined by the heat exchange between the gas and the wall, the strength of the heat source in the chemical-reaction zone, and the sink of heat by conduction in the radial and axial directions. In the stage of self-heating, we can have heat sink not only deep in the wall and/or through its external boundary but into the gas flow as well.

---

[a] Tomsk State Pedagogical University, Tomsk, Russia; email: VMU@mail2000.ru; [b] Tomsk State University of Architecture and Civil Engineering, Tomsk, Russia. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 75, No. 5, pp. 81–85, September–October, 2002. Original article submitted September 25, 2001; revision submitted April 4, 2002.

1062-0125/02/7505-1107$27.00

In actual technological devices, ignition of channel walls by a high-temperature gas flow is a rather difficult problem since one must take into account the turbulence of the gas flow, thermal stresses in the channel walls which can lead to a variation in the properties of the wall material and even to its destruction, phase transitions at the gas–wall boundary, and the course of reactions in the gas phase.

Nonetheless, a study of the ignition of channel walls by the flow of a laminar high-temperature gas within the framework of the solid-phase ignition model is a rather important problem, since in addition to being of independent scientific interest it enables one to better understand the mechanism of ignition of the channel walls and can be the starting point for further investigations with the use of more complex models.

In the present work, the process of ignition is modeled with allowance for the following assumptions:

1. When $t > 0$, constant values of the velocity, pressure, and density of the gas are maintained at the entrance to the channel, which holds in the case where the time of ignition of the condensed medium is much shorter than the period of action of the ignition device.

2. Consideration is given to a nonreactive igniting gas; the gas flow is axisymmetric.

3. In modeling the process of ignition, use is made of the solid-phase model within the framework of which it is assumed that it is the totally exothermal processes in the condensed phase of the process of ignition that are responsible for the ignition [1]. Possible phase transitions (evaporation, melting, ablation) are disregarded. Chemical reaction in the gas phase is also not taken into account.

Mathematical Model. The processes of heat exchange in the gas phase $0 \le r < r_{\text{in}}$ are condensed on the basis of the unsteady equations of motion and heat transfer of a viscous fluid in the approximation of a narrow channel [5]:

$$\rho_{\text{g}} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial r} \right) = - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial u}{\partial r} \right), \quad \frac{\partial p}{\partial r} = 0 \, ; \tag{1}$$

$$\frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (rv) = 0 \, ; \tag{2}$$

$$\rho_{\text{g}} c_{p,\text{g}} \left(\frac{\partial T_{\text{g}}}{\partial t} + u \frac{\partial T_{\text{g}}}{\partial x} + v \frac{\partial T_{\text{g}}}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_{\text{g}} \frac{\partial T_{\text{g}}}{\partial r} \right) + \mu \left(\frac{\partial u}{\partial r} \right)^2 . \tag{3}$$

Heat transfer in the solid phase $r_{\text{in}} < r \le r_{\text{ex}}$ is described by the heat-conduction equations with allowance for the exothermal reaction proceeding by the Arrhenius law [4]:

$$\rho_{\text{c}} c_{\text{c}} \frac{\partial T_{\text{c}}}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_{\text{c}} \frac{\partial T_{\text{c}}}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_{\text{c}} \frac{\partial T_{\text{c}}}{\partial r} \right) + Q k_0 (1 - \eta)^n \exp \left(- \frac{E}{RT_{\text{c}}} \right); \tag{4}$$

$$\frac{\partial \eta}{\partial t} = k_0 (1 - \eta)^n \exp \left(- \frac{E}{RT_{\text{c}}} \right); \tag{5}$$

$$\mu = \mu (T) , \quad \lambda_{\text{g}} = \lambda_{\text{g}} (T) , \quad \lambda_{\text{c}} = \lambda_{\text{c}} (T) , \quad c_{p,\text{g}} = c_{p,\text{g}} (T) , \quad c_{\text{c}} = c_{\text{c}} (T) . \tag{6}$$

The initial and boundary conditions have the form

$$t = 0 : \quad u = u_{\text{ent}} (x, r) , \quad v = v_{\text{ent}} (x, r) , \quad T_{\text{g}} = T_{\text{c}} = T_{\text{ent}} \, ; \tag{7}$$

$$x = 0 : \quad u = u_{\text{ent}} (x, r) , \quad v = 0 , \quad T_{\text{g}} = T_{\text{g,ent}} (t) , \quad T_{\text{c}} = T_{\text{c,ent}} , \quad \text{or} \quad \frac{\partial T_{\text{c}}}{\partial x} = 0 \, ; \tag{8}$$

$$x = L: \ \frac{\partial^2 u}{\partial x^2} = 0 , \ \ v = 0 , \ \ \frac{\partial^2 T_c}{\partial x^2} = 0 ; \tag{9}$$

$$r = 0: \ \frac{\partial u}{\partial r} = 0 , \ \ v = 0 , \ \ \frac{\partial T_g}{\partial r} = 0 ; \tag{10}$$

$$r = r_{in}: \ u = 0 , \ \ v = 0 , \ \ T_g = T_c , \ \ \lambda_g \frac{\partial T_g}{\partial r} = \lambda_c \frac{\partial T_c}{\partial r} ; \tag{11}$$

$$r = r_{ex}: \ T_c = T_{c,ex} \ \text{ or } \ \frac{\partial T_c}{\partial r} = 0 . \tag{12}$$

In the basic calculations, we set $T_{c,ent} = T_{c,ex}$ and $T_{c,ent} = T_{g,ent}$.

The problem has been solved by the finite-difference method using economical implicit schemes. The pressure gradient has been determined using the condition of constancy of the flow rate. The method of splitting is used to solve the equation of heat conduction in the wall [5]. By virtue of the nonlinearity of the problem, iterations are performed at each time step.

To determine the time and temperature of ignition by a high-temperature supersonic jet we used the Averson–Barzykin–Merzhanov method of critical conditions [1], which records the moment of ignition of the channel wall from the coincidence of the heat fluxes from the hot cases and due to the chemical reactions occurring in decomposition of the wall material.

The thermophysical and kinetic characteristics have been borrowed from [1]. The initial data for the wall material were as follows: $E = 1.46 \cdot 10^2$ kJ/mole, $Q = 1.13 \cdot 10^6$ J/kg, $k_0 = 0.9 \cdot 10^{14}$ 1/sec, $c_c = 1.46$ kJ/(kg·K), $\lambda_c = 2.34 \cdot 10^{-2}$ J/(m·sec·K), and $\rho_c = 1.6 \cdot 10^3$ kg/m^3. The nitrogen flow was considered as the igniting medium. We varied boundary conditions (8) and (11), the wall thickness, the temperature, and the initial temperature.

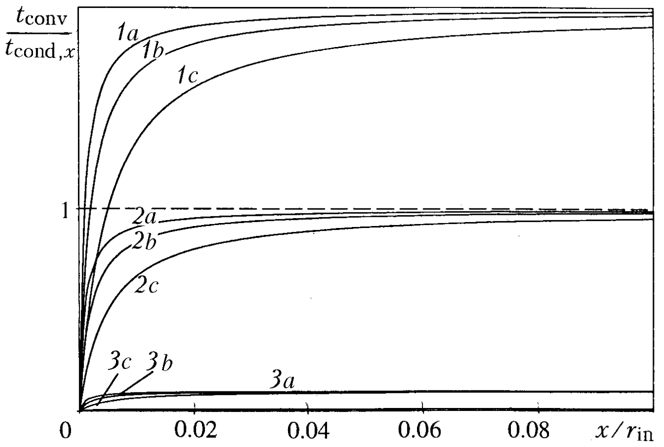
Analysis of Results. The total time of ignition in a certain cross section can be represented as the sum of the heating time and the chemical-reaction time:

$$t_* = t_h + t_{ch} . \tag{13}$$

Under the conditions of conjugate heat exchange, the channel wall is heated as a result of both the conductive heat transfer in the wall with a characteristic time of $t_{cond,x} = x^2/a_c$ and the convective-conductive heat exchange associated with propagation of a thermal wave in the gas and conduction of heat from the gas to the wall in the radial direction. Evaluating the longitudinal transfer of heat in the gas, we obtain that for Péclet numbers of $\text{Pe}_{x,g} = \rho_g c_{p,g} u_{ent} x \lambda_g^{-1} \geq 10^2$ the convective transfer is much larger than the conductive one and to calculate the characteristic hydrodynamic time we can use the estimate $t_d = x/u_{ent}$. The time of conductive heating of the wall in the radial direction is $t_{cond,r} \approx H^2/a_c$ in order of magnitude. The characteristic time of convective-conductive heat exchange can be taken to be $t_{conv} = t_d + t_{cond,r}$.

To evaluate the characteristic time of heating we must take into account that the ratio of the convective heat flux in the gas to the conductive axial transfer of heat in the wall is substantial in conjugate problems of heat exchange, since in some cases heat-exchange zones can form in the cross sections still to be reached by the hot gas from the entrance because of the effect of anticipating transfer of heat by conduction from the gas to the wall and along the channel [5]. This ratio is characterized by the parameter $K_\lambda^{-1}\text{Pe}_x = \rho_g c_{p,g} u_{ent} x \lambda_c$. For moderate $K_\lambda = \lambda_2/\lambda_1 < 1$ the influence of axial transfer in the wall manifests itself only for relatively low velocities of motion of the medium and in the cross sections adjacent to the beginning of the tube (Fig. 1). Thus, the estimate $t_h = \min \{t_{cond,x}, t_{conv}\}$ holds for t_h.

The quantity t_h is usually substantially higher than the time of chemical reaction t_{ch} (self-heating stage) that agrees in order of magnitude with the time of adiabatic heating



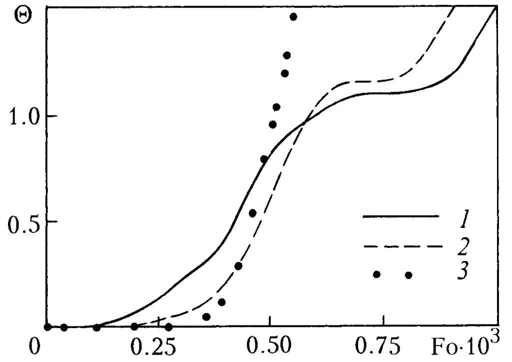


Fig. 1. Ratio of the characteristic time of heating of the wall because of convective heat transfer to the characteristic time of heating of the wall because of axial conductive heat transfer: 1) K_λ = 0.5, 2) 1, and 3) 10; a) Pe = 200, b) 500, and c) 1000.

Fig. 2. Wall temperature vs. time (Pe = 200, x/H = 1, $T_{g,ent}$ = 593 K, H = 0.5 cm): 1) y = 0, 2) 0.5, and 3) 1.

TABLE 1. Dimensionless Times of the Processes of Ignition and Establishment of Heat Equilibrium

Parameters	Pe = 200			Pe = 1000		
$T_{g,ent}$, K	503	553	593	503	553	593
Fo_1	$0.65{\cdot}10^{-1}$	$0.37{\cdot}10^{-2}$	$0.55{\cdot}10^{-3}$	$0.63{\cdot}10^{-1}$	$0.36{\cdot}10^{-2}$	$0.53{\cdot}10^{-3}$
Fo_2	$0.94{\cdot}10^{-1}$	$0.51{\cdot}10^{-2}$	$0.69{\cdot}10^{-3}$	$0.91{\cdot}10^{-1}$	$0.49{\cdot}10^{-2}$	$0.67{\cdot}10^{-3}$

$$t_{ch} \approx t_a = \rho_c c_c \frac{RT_a^2}{EQk_0} \exp\left(\frac{E}{RT_a}\right), \tag{14}$$

where $T_a = Q/(c_c\rho_c)$ is the adiabatic combustion temperature.

Table 1 gives the dimensionless times of the processes of ignition and establishment of heat equilibrium for different $T_{g,ent}$; these times are characterized by the Fourier parameter Fo = $a_c t/H^2$. Here Fo_1 is the time in which the temperature $T_{g,ent}$ is reached in the wall and Fo_2 is the ignition time according to criterion (13). The dynamics of decrease in Fo_1 and Fo_2 with increase in the temperature difference is clearly seen. For the process of ignition the time of heating of the entire wall over the thickness is much shorter than the ignition time. A thin surface layer of the channel wall is heated; thereafter the chemical reaction is strongly accelerated and the channel is ignited.

The temperature and the ignition time depend on both the thermophysical properties of a substance and kinetic reaction constants and the condition of heat exchange with the external source. For low velocities of flow which determine heat transfer the times characterized by the parameters Fo_1 and Fo_2 virtually coincide. With increase in the flow velocity the ignition times decrease (see Table 1, Pe = $2{\cdot}10^2$ and 10^3, Pe = $u_{ent}r_{in}/a_g$).

Figure 2 gives the dimensionless temperature of the wall as a function of the time ($\Theta = (T - T_{g,ent})/(T_{g,ent} - T_{ent})$ for different wall layers and $y = (r - r_{in})/(r_{ex} - r_{in})$ for the case of heat insulation of the external boundary). In the figure, one observes all the characteristic times of the process. In the initial period ($t < t_d$), until the flow of the hot gas reaches the specified cross section, the wall temperature remains constant and equal to T_{ent}. Then one observes heating of the wall to the flow temperature. If the intensity of heat removal is sufficiently high, the chemical reaction in the wall occurs in the low-temperature regime characterized by slight temperature changes. If the intensity of the heat release in the wall exceeds the value of the heat removal, the chemical reaction occurs in the high-temperature regime. In this case, the reaction rate has time to substantially increase by the instant of time t_{ch}, which leads to an increase in the rate of heat release in the narrow layer adjacent to the interior wall surface and hence to ignition.

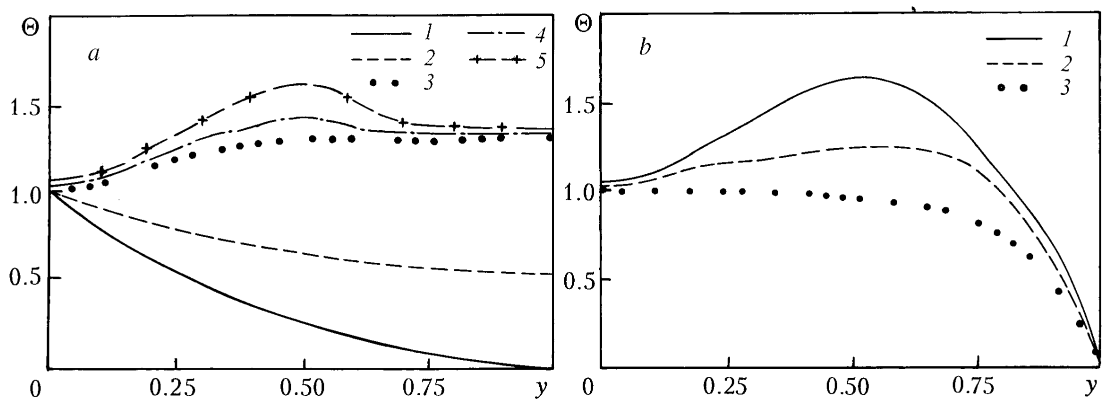


Fig. 3. Temperature distribution over the radial coordinate (Pe = 200, $x/H = 1$, $T_{g,ent} = 593$ K) for $H = 0.5$ cm (a) [1) Fo = $0.7 \cdot 10^{-4}$, 2) $0.14 \cdot 10^{-3}$, 3) $0.26 \cdot 10^{-3}$, 4) $0.32 \cdot 10^{-3}$, and 5) $0.66 \cdot 10^{-3}$] and Fo = $0.8 \cdot 10^{-3}$ (b) [1) $H = 0.5$, 2) 0.2, and 3) 0.1 cm].

The distribution of the temperature inside the wall is analogous to its distribution at the internal boundary. We note that the initial period characterized by the temperature T_{ent} is somewhat longer for $y > 0$ than for $y = 0$. The reason is that heating of the internal wall layers begins upon reaching the specified cross section by the flow of the hot gas and upon heating of the layers adjacent to the internal boundary of the tube. The heating time for the internal layers of the wall is shorter than for $y = 0$ since the internal layers are heated not only due to the transfer of heat from the gas flow but due to the chemical heat release in the wall as well. As a result, the time of adiabatic heating t_a becomes shorter for $y > 0$, which contributes to the appearance of an ignition source in the bulk of the wall.

The temperature distribution over the dimensionless thickness of the wall (and in the boundary layer) at different instants of time is shown in Fig. 3a. Once the thermal wave reaches the channel wall (in the time t_d), the step of heating begins and the wall temperature increases to the gas-flow temperature. As the temperature in the channel wall increases, the chemical reaction leading to an increase in the temperature is intensified. As a result, a nonmonotonic temperature profile with a maximum T_{max} is formed in the channel wall. The value of the maximum increases with time, and at t_a the temperature in the channel wall attains the adiabatic combustion temperature T_a, which indicates ignition.

When a temperature equal to the initial one is maintained on the exterior channel surface a significant role in the development of the ignition is played by the thickness of the channel wall H. When H is sufficiently high, the temperature of the gas flow and the internal layers of the channel wall change slightly because of the heat removal on the external wall. As the calculations show, for $H > 5\sqrt{a_c t_a}$ heat exchange on the external channel wall no longer influences the process of ignition. Conversely, if H is lower than a certain characteristic thickness H_*, the regime of ignition with a sharp temperature maximum near the phase interface is not realized (Fig. 3b). The reason is that the quantity of heat removed through the cold external wall exceeds the heat arrived from the hot gas and released as a result of the chemical reaction. The results of the numerical investigation have shown that the quantity H_* dividing the regime of ignition and the regime of steady-state heating is approximated with a high degree of accuracy (≈4%) by the expression

$$H_* = \sqrt{\left(\frac{E/R}{2T_{g,ent} + E/R} - T_{c,ex}\right)\frac{\lambda_c}{Qk_0}\,\exp\left[\frac{E}{RT_{g,ent}}\right]}. \tag{15}$$

If the adiabaticity condition is realized for the wall at the boundary $x = 0$, ignition initially occurs in cross sections which are the closest to the entrance. On condition that $T_{c,ent} = T_{g,ent}$ the downstream cross sections where the ignition conditions are attained earlier are the first to be ignited because of conduction in some cases.

NOTATION

a_c, thermal diffusivity of the wall, m^2/sec; c_c, specific heat of the wall, kJ/(kg·K); $c_{p,g}$, specific heat of the gas, kJ/(kg·K); E, activation energy, kJ/mole; H, wall thickness, m; k_0, preexponent, 1/sec; n, order of reaction; p, gas pressure, Pa; Q, thermal effect of the chemical reaction, kJ/kg; R, universal gas constant, J/(kmole·K); r, radial coordinate, m; T, temperature, K; t, time, sec; u, longitudinal-velocity component, m/sec; v, radial-velocity component, m/sec; x, axial coordinate, m; y, dimensionless radial coordinate; η, depth of decomposition of the wall material (dimensionless quantity); Θ, dimensionless temperature; λ, thermal conductivity, W/(m·K); μ, coefficient of dynamic viscosity, kg/(m·sec); ρ, density, kg/m^3; Fo, Fourier number; Pe, Péclet number. Subscripts: a, adiabatic; c, channel; ch, chemical; cond, conductive; conv, convective; d, dynamic; ent, entrance; ex, referring to the external wall; g, gas; h, heating; in, referring to the internal wall; max, maximum; *, ignition.

REFERENCES

1. V. N. Vilyunov, *Theory of Ignition of Condensed Substances* [in Russian], Novosibirsk (1984).
2. A. É. Averson, in: *Heat and Mass Transfer in Combustion Processes* [in Russian], Chernogolovka (1980), pp. 16–18.
3. I. G. Assovskii, Z. G. Zakirov, and O. I. Leipunskii, *Fiz. Goreniya Vzryva*, **19**, No. 1, 41–46 (1983).
4. V. N. Vilyunov, V. M. Ushakov, and É. R. Shrager, *Fiz. Goreniya Vzryva*, **6**, No. 3, 311–317 (1970).
5. S. G. Ivanushkin, L. V. Kim, V. I. Kondrashov, and V. E. Tomilov, *Internal Nonstationary Problems of Convective Heat Transfer* [in Russian], Tomsk (1980).
6. S. G. Ivanushkin, O. A. Kotikov, and V. M. Ushakov, in: *Ext. Abstr. of Papers presented at VIII Symp. on Combustion and Explosion* [in Russian], October 14–17, 1986, Chernogolovka (1986), pp. 46–49.