

Extension of the Combustion Limits for a Porous Burner by External Heating

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In this work, a new method for extending the concentration limits of combustion of gases in a porous burner by enhancing the preflame processes by external heating is theoretically justified.

The principle of fuel combustion under “excess enthalpy” conditions and also some designs of practical burners with external heat exchangers were first proposed by Weinberg [1, 2]. Combustion of a reactive gas mixture within a porous solid matrix is a striking example of controlling combustion by an “internal” heat exchanger. Owing to a high thermal conductivity of the matrix, the preflame zone forms under the action of additional heat fluxes from the heated matrix [3–5]. The additional heat action on the preflame zone increases the burning velocity and extends the concentration limits of combustion. As a consequence, the porous matrix allows one to burn mixtures that are incombustible under normal conditions and also mixtures that are highly lean or rich in fuel. Along with the heat action on the preflame zone, it is also proposed to use a chemical action by applying a catalyst layer to the inner surface of pores. Combustion of lean mixtures within catalytic and noncatalytic porous matrices is a promising method for reducing emissions of harmful substances (first of all, nitrogen oxides) in stationary gas turbine power plants. Another important application is disposal of hazardous waste and toxic agents.

In this work, to further extend the concentration limits of combustion in comparison with those reached previously [3–5], it is proposed to use local external heating of the porous matrix. Some qualitative estimates of the fundamental possibility of this approach were made earlier [6]. To theoretically justify the new method, let us consider a mathematical problem of

combustion of a reactive gas mixture within a porous solid matrix with external heating.

Let a long tube of diameter d with two open ends be filled with a homogeneous porous matrix of porosity $\varepsilon \leq 1$ (at $\varepsilon = 1$, there is no matrix) and a gas mixture with fuel–air ratio Φ and temperature $T = T_0$. On the outer surface of the tube, a heater (e.g., electric) of length l and specific heat power q may be mounted. After ignition of the mixture, a heat wave involving chemical transformations, i.e., a flame, emerges in the gas and the matrix. To retain the flame within the tube, it is necessary to feed a fresh mixture at a certain rate u , which is equal to the normal burning velocity u_n . The problem is to determine u_n , the spatial structure of the heater–flame stationary complex, and also the conditions for the existence of this complex.

The problem was solved under the following simplifying assumptions: (1) the flow is one-dimensional (all the quantities depend on time t and the longitudinal coordinate x), (2) the gas pressure is constant ($p = p_0$), (3) the gas is ideal, (4) the flame is laminar, (5) the diffusion of species of the gas mixture is independent, (6) the thermophysical properties of the porous matrix are constant, (7) the heat loss to the environment by radiation is negligible, (8) the chemical interaction between the gas and the matrix is insignificant, and (9) the heat propagation in the matrix is a quasi-stationary process. The last assumption means that the temperature profile is instantaneously adjusted to the heat wave in the gas.

The following notation is used: M is the number of chemical species in the gas; Y_j is the mass fraction of the j th species ($j = 1, 2, \dots, M$); ρ is the density; c is the specific heat; λ is the thermal conductivity; D_j is the diffusion coefficient of the j th species; θ is the heat source (sink) power in chemical reactions; α is the heat-transfer coefficient between the gas and the porous matrix; w_j is the change in the concentration of the j th species in chemical reactions; N is the number of elementary chemical reactions in the gas phase; H_k , A_k , E_k , and n_k are the heat, preexponential factor, activation energy,

and temperature exponent for the k th reaction, respectively; $v'_{j,k}$ is the stoichiometric coefficient of the j th species being a reagent of the k th reaction; $v''_{j,k}$ is the stoichiometric coefficient of the j th species being a product of the k th reaction; R^0 is the gas constant; G_j is the molecular weight of the j th species; $Re = \rho_g u_g d_p \mu^{-1}$ is the Reynolds number; d_p is the effective diameter of pores in the porous matrix; u_g is the gas velocity ($\rho_0 u_n = \rho_g u_g$); μ is the viscosity; Z is the number of pores per unit matrix length; the subscripts g, s, and 0 refer to the gas phase, the matrix, and the initial mixture, respectively; j is the chemical species number; and k is the reaction number.

Under the assumptions made, the problem of finding the velocity u_n and the distributions of temperature and reactant concentrations is reduced to a set of nonlinear ordinary differential equations:

the equation of heat propagation in the gas (stationary wave),

$$\frac{d}{dx} \left(\lambda_g \frac{dT_g}{dx} \right) - c_g \rho_0 u_n \frac{dT_g}{dx} + \theta(T_g, Y_j) - \frac{\alpha}{\varepsilon} (T_g - T_s) = 0, \quad (1)$$

the continuity equations for chemical species of the gas mixture (stationary wave),

$$\frac{d}{dx} \left(\rho_g D_j \frac{dY_j}{dx} \right) - \rho_0 u_n \frac{dY_j}{dx} + w_j = 0, \quad (2)$$

$j = 1, 2, \dots, M,$

and the equation of heat conduction in the porous matrix,

$$(1 - \varepsilon) \lambda_s \frac{d^2 T_s}{dx^2} + \alpha (T_g - T_s) + q = 0. \quad (3)$$

Unknowns in problem (1)–(3) are not only the functions $T_g(x)$, $Y_j(x)$, and $T_s(x)$ but also the velocity u_n .

The chemical sources were found from the relations [7]

$$\theta = \sum_{k=1}^N H_k A_k T_g^{n_k} \exp\left(\frac{-E_k}{R^0 T_g}\right) \prod_{i=1}^M \left(\frac{Y_i \rho_g}{G_i}\right)^{v'_{i,k}}, \quad (4)$$

$$w_j = G_j \sum_{k=1}^N (v''_{j,k} - v'_{j,k}) A_k T_g^{n_k} \exp\left(\frac{-E_k}{R^0 T_g}\right) \times \prod_{i=1}^M \left(\frac{Y_i \rho_g}{G_i}\right)^{v'_{i,k}}. \quad (5)$$

The gas density and the temperature were related by the equation of state of an ideal gas:

$$p = \rho_g R^0 T_g \sum_{j=1}^M \frac{Y_j}{G_j}. \quad (6)$$

The heat-transfer coefficient was expressed as [5]

$$\alpha = \begin{cases} \frac{\lambda_g}{d_p^2} \left(0.0426 + \frac{1.236}{\frac{L}{d_p}} \right) Re, & \varepsilon < 1 \\ \frac{0.1464 \lambda_g}{d_p^2}, & \varepsilon = 1, \end{cases} \quad (7)$$

$$d_p = \frac{1}{Z} \left(\frac{4\varepsilon}{\pi} \right)^{0.5}. \quad (8)$$

Here, L is the characteristic size of the heat wave (which is several times larger than the flame front thickness).

The velocity u_n can be found only when Eqs. (1)–(3) are shift-invariant. This means that, if $F(x)$ is a solution of the problem, then $F(x + \text{const})$ is also a solution of the problem. Equations (1) and (2) have this property since they do not explicitly contain the variable x . Equation (3) and, consequently, the function q characterizing the external heating should also have this property.

Let us assume that the heater has a fixed length l and its left end is at the point x_1 . The specific power of the heater is defined as

$$q = \begin{cases} q_0, & x \in (x_1, x_1 + l) \\ 0, & x \notin (x_1, x_1 + l), \end{cases} \quad (9)$$

where q_0 is a constant. For the function q to have the required property, it is necessary to somehow relate the position x_1 of the left end of the heater to the gas temperature T_g . This can be done as follows. A certain distance r_g and an auxiliary temperature T_g^0 are specified.

Initially, from the equation $T_g(x_0) = T_g^0$, x_0 is found, and then, from the equality $x_1 = x_0 + r_g$, the coordinate x_1 is determined. Actually, in this case, we have

$$q(x - x_0) = \begin{cases} q_0 & \text{at } r_g \leq x - x_0 \leq r_g + l \\ 0 & \text{at } x - x_0 < r_g, \quad x - x_0 > r_g + l. \end{cases} \quad (9')$$

Formula (9') implies that the function q depends not simply on x but on the difference $x - x_0$ and, owing to this, is shift-independent. Generally speaking, the unknown velocity u_n will be a function of r_g .

The thermophysical properties of the gas mixture (c_{gj} , D_j , and λ_g) were assumed to be functions of tem-

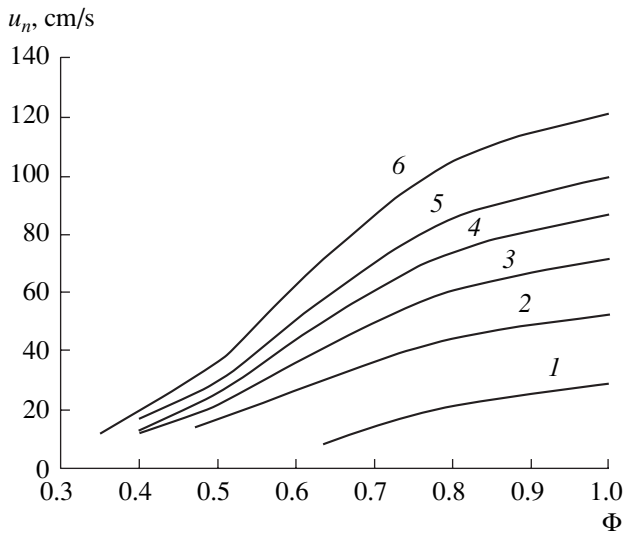


Fig. 1. Velocity u_n vs. fuel–air ratio Φ for flame propagation: (1) in the tube with a cold wall at $\varepsilon = 1$ and $T_s = T_0$ (critical conditions: $\Phi_* = 0.635$ and $u_{n*} = 7.85$ cm/s); (2) in the tube with the porous matrix without heating; and in the tube with the porous matrix with heating at (3) $0.01\theta_{\max}$, (4) $0.02\theta_{\max}$, (5) $0.03\theta_{\max}$, and (6) $0.05\theta_{\max}$.

perature and pressure and were calculated from known formulas [8] using literature data [8, 9]. In the calculations, a detailed kinetic mechanism of methane oxidation [10] was used. The mechanism contains 260 elementary reactions (130 forward reactions and 130 reverse reactions) involving 31 species (CH_4 , O_2 , H_2 , H_2O , CO , CO_2 , N_2 , NO , O , H , N , OH , HO_2 , H_2O_2 , CH , CH_2 , CH_3 , HCO , H_2CO , CH_3O , NO_2 , NO_3 , NH , NH_2 , NH_3 , N_2H_3 , N_2H_4 , HNO , CN , HCN , and NCO).

The boundary conditions for Eqs. (1)–(3) have the form

$$x \rightarrow -\infty, \quad T_g = T_s = T_0, \quad Y_j = Y_{j0}, \quad (10)$$

$$x \rightarrow +\infty, \quad \frac{dT_g}{dx} = \frac{dT_s}{dx} = \frac{dY_j}{dx} = 0. \quad (11)$$

The set of Eqs. (1)–(3) together with relations (4)–(9) under boundary conditions (10) and (11) was solved numerically by the relaxation method [11] using a modification of a computation program [12]. A most important advantage of the relaxation method is a good convergence of iterations at different initial distributions of problem parameters. The calculations were performed for methane–air mixtures with $\Phi \leq 1$ at $T_0 = 293$ K and $p_0 = 0.1$ MPa. The parameters of the porous matrix were the following: $\varepsilon = 0.9$, $\lambda_s = 0.597$ W/(m K), and $Z = 8$ cm⁻¹. The parameters of the external source were the following: $l = 0.4$ cm, $x_1 = 1.2$ cm, $T_g^0 = T_0 + \Delta T$ ($\Delta T \ll T_0$), and $q_0 = (0 - 0.05)\theta_{\max}$, where θ_{\max} is the maximal energy release power in the flame in the chemical reactions at a given Φ without external heating (for lean mixtures, for which the flame cannot propagate

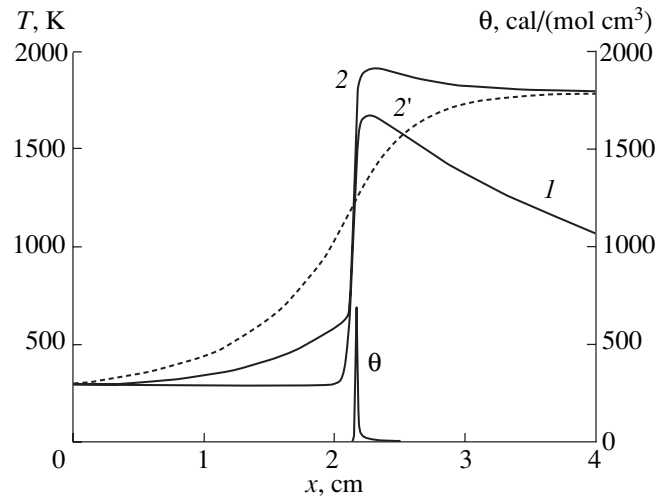


Fig. 2. Distributions of temperature T and the energy release function θ in the flame at $\Phi = 0.67$ and $q_0 = 0$ in the gas (solid lines) and the matrix (dashed lines) in the tube (1) without the porous matrix and (2) with the porous matrix without external heating.

without external heating, the θ_{\max} value at the limit of flame propagation was taken).

Figure 1 presents the calculated functions $u_n(\Phi)$ in lean methane–air mixtures. It is seen that external heating significantly extends the lower concentration limit of combustion of methane–air mixtures: from $\Phi = 0.47$ at $q_0 = 0$ (curve 2) to $\Phi \approx 0.35$ at $q_0 = 0.05\theta_{\max}$. Moreover, the laminar flame velocities in the tube with the porous matrix with heating (curves 3–6) considerably exceed the flame velocities in the gas (curve 1).

Figure 2 compares the calculated gas temperature profiles (solid curves) in the stationary laminar flame at $\Phi = 0.67$ in the tube without the porous matrix ($\varepsilon = 1$) and with the porous matrix ($\varepsilon = 0.9$) without external heating ($q_0 = 0$). The presence of the matrix leads to a significant increase in the preflame zone length in the gas flame and to an elevated combustion temperature. The calculated flame velocities in the tube without and with the porous matrix are 11.93 and 33.52 cm/s, respectively. Note that, on curve 1, the decrease in the temperature of the combustion products with distance from the flame front is caused by the heat loss to the tube wall.

Figure 3 compares the calculated temperature profiles of the gas and the porous matrix in the stationary laminar flame at $\Phi = 0.5$. At $\Phi = 0.5$ in the tube without the porous matrix, there is no stationary flame (see Fig. 1). Comparison of curves 1' and 2' shows that external heating increases the temperature in the preflame zone and favors faster flame propagation: the burning velocity without heating is 16.52 cm/s, whereas the burning velocity with heating is 21.20 cm/s.

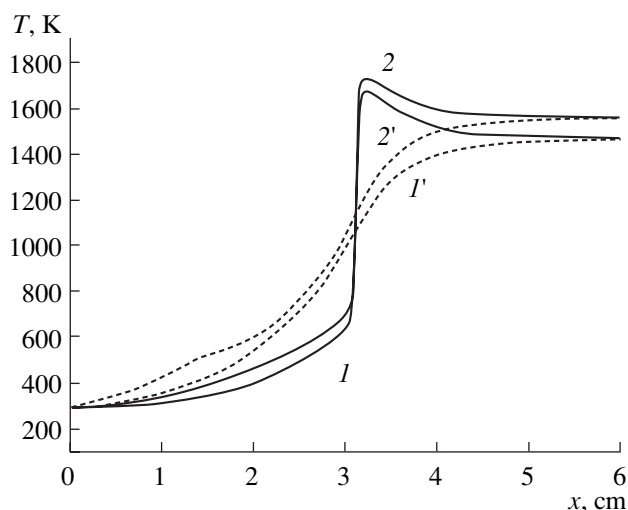


Fig. 3. Calculated temperature distributions in the flame at $\Phi = 0.5$ in the gas (solid lines) and the porous matrix (dashed lines) in the tube with the porous matrix (1) without heating ($q_0 = 0$) and (2) with heating ($q_0 = 0.01\theta_{\max}$).

Figure 4a compares the calculated temperature profiles of the gas and the porous matrix in the stationary laminar flame at $\Phi = 0.4$ and $q_0 = 0.01\theta_{\max}$ and $0.05\theta_{\max}$. The flame velocities in the two cases are 12.10 and 19.71 cm/s, respectively. Note that, without external heating, flame propagation at $\Phi = 0.4$ is impossible.

Figure 4b presents the limiting mode of stationary propagation of the heat wave. In this case, the chemical reactions in the gas are of extremely low intensity and the wave propagates solely owing to the external heating.

Of interest is the change in the concentration of nitrogen oxides in lean methane–air flames obtained in tubes with the porous matrix with and without external heating. The table presents the calculated concentrations of nitrogen oxides in the combustion products (prompt NO since thermal NO makes virtually no contribution) at various temperatures T_{gl} of the gaseous reaction products under different conditions. The table shows that, with enhancement of external heating, at the same temperature of the gaseous reaction products, the concentration of nitrogen oxides decreases and drops to very low values of about 2.72 ppm. The calculation showed that, e.g., at $\Phi = 0.4$ and 0.5, the NO concentrations in the thermodynamically equilibrium combustion products are 277 and 792 ppm, respectively. The respective equilibrium combustion temperatures are 1278 and 1478 K. Note that the formation of NO at such concentrations requires very long residence times of the combustion products at the above temperatures.

The table also presents the result of calculation at $\Phi = 0.4$ (no. 6) without external heating but at an elevated temperature of the initial mixture ($T_0 = 500$ K). It is seen that, in terms of the NO yield, local heating at

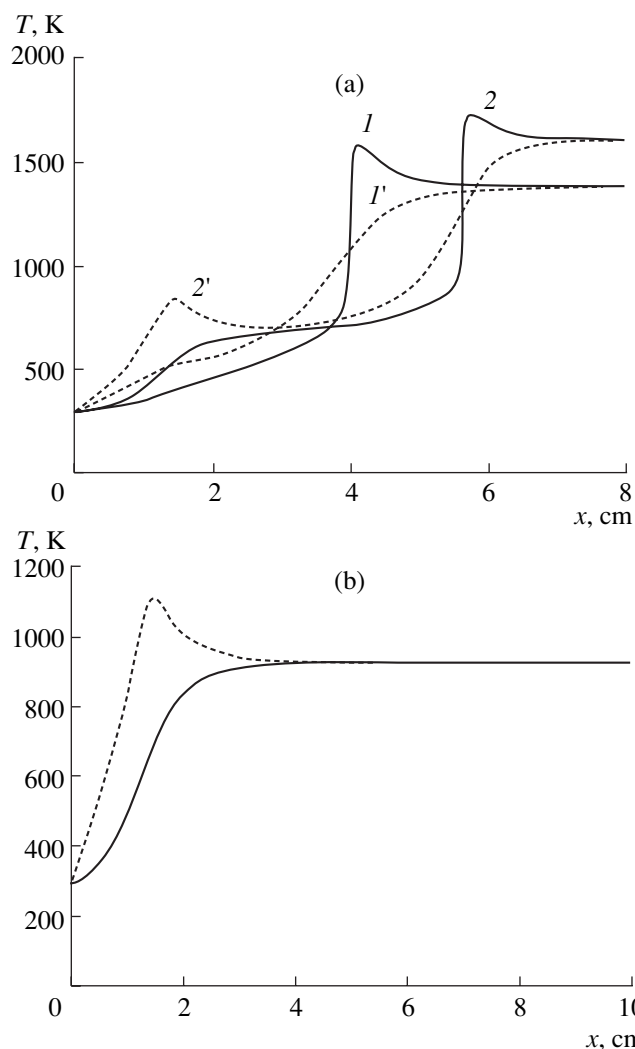


Fig. 4. Calculated temperature distributions in the flame in the tube with the porous matrix with heating in the gas (solid lines) and the porous matrix (dashed lines) at (a) $\Phi = 0.4$ and $q_0 = (1) 0.01\theta_{\max}$ and (2) $0.05\theta_{\max}$ and (b) $\Phi = 0.35$ and $q_0 = 0.05\theta_{\max}$.

constant specific power q_0 is equivalent to an increase in the initial temperature of the mixture to a value that ensures the same temperature of the combustion products (≈ 1468 K).

The last column of the table contains the values of the quantity J characterizing the ratio of the integral energy characteristic of the action of external heating to a similar characteristic of the chemical reaction in the gas phase.

Thus, local external heating leads to (1) extension of the lower concentration limit of combustion of methane–air mixtures, (2) an increase in the burning velocity, and (3) a significant decrease in the NO yield. To noticeably extend the lower concentration limit of combustion of methane–air mixtures, external heating whose power is much lower than the total energy release in the laminar flame at the propagation limit without heating is necessary. The physical mechanism

Calculated values of the gas temperature and the concentrations of nitrogen oxides in the combustion products

No.	T_{g1} , K	Φ	$[\text{CH}_4]_0$, %	$\frac{q_0}{\theta_{\max}}$	T_0 , K	[NO], ppm	J
1	1935 ± 35	0.75	7.30	0	293	47.6	0
		0.67	6.58	0.01	293	41.0	0.11
		0.6	5.93	0.02	293	30.2	0.18
		0.6	5.93	0.03	293	35.7	0.23
		0.55	5.46	0.05	293	28.3	0.28
2	1810 ± 25	0.67	6.58	0	293	29.2	0
		0.6	5.93	0.01	293	24.4	0.11
		0.55	5.46	0.02	293	19.0	0.16
		0.55	5.46	0.03	293	22.2	0.20
3	1680 ± 15	0.6	5.93	0	293	18.0	0
		0.55	5.46	0.01	293	15.5	0.09
		0.5	4.99	0.03	293	12.1	0.17
		0.45	4.51	0.05	293	9.61	0.30
4	1585 ± 20	0.55	5.46	0	293	11.3	0
		0.5	4.99	0.01	293	8.69	0.09
		0.45	4.51	0.03	293	7.32	0.22
		0.4	4.03	0.05	293	5.93	0.38
5	1534 ± 13	0.45	4.51	0.02	293	6.47	0.18
		0.4	4.03	0.03	293	7.32	0.30
6	1468 ± 8	0.45	4.51	0.01	293	5.09	0.11
		0.4	4.03	0.02	293	3.84	0.25
		0.4	4.03	0	500	3.21	0
7	1400 ± 2	0.5	4.99	0	293	6.44	0
		0.4	4.03	0.01	293	2.72	0.16

of extension of the flame propagation limits in the considered variant of the porous burner is related to the heat effect on the preflame zone. The calculations did not detect any significant effect of preflame chemical reactions caused by external heating on the combustion characteristics.

External heating can be used in combustion chambers with a porous filler in stationary gas turbine plants for attaining ultralow NO emissions. Because of short residence times of gas in such combustion chambers and further gas expansion in a turbine, the emission indices are mainly determined by prompt NO, rather than thermal NO. Although local heating was observed

to be equivalent to an increase in the temperature of the mixture entering the combustion chamber, local external heating seems to be more efficient to reduce heat loss and improve the explosion safety of the process. The possibility of optimizing the porous burner by varying the specific heat power q_0 along the length deserves additional investigation.

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