MATHEMATICAL MODEL OF THE GAS COMBUSTION RATE IN A VORTEX CHAMBER

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A mathematical model of the combustion rate of a gaseous fuel in a turbulent flow, which enters into a numerical procedure for calculation of a combustion chamber, is presented. Results of calculations according to the model are compared with experimental results.

1. THEORY

We considered three models of the combustion rate based on the EDC vortex concept and the k-ε turbulence model. They were incorporated into a comprehensive numerical model of a vortex combustion chamber which includes the following models: a model of vortex turbulent gas flow, a model of convective heat and mass transfer, and a model of turbulent diffusion combustion with consideration for the chemical kinetics and radiation heat transfer. Results obtained with the use of the proposed calculation of the combustion chamber and including the above-mentioned models of the combustion rate were compared with our experimental data obtained on a laboratory gas burner with a vortex combustion chamber. Experimental results include profiles of temperature and concentrations of combustion products along the chamber axis.

The main feature of the model based on the EDC concept is the neglect of oscillations of concentrations of components and temperatures, as in the majority of models of turbulent gas combustion, and instead, the intensity of diffusion of reactants is calculated before their mutual contact on the molecular level.

The assumption that the chemical reaction starts when reactants (heated to a certain temperature) are mixed on the molecular level is important in models of the type [1, 2]. Conditions for this mixing in a turbulent flow of a gas mixture exist only in fine structures whose scales correspond to the Kolmogorov's microscale, and they actually constitute the final stage of a stepwise process of vortex dissipation.

This concept assumes that the chemical reaction takes place only in isolated regions filled with fine structures whose volume takes a small fraction of the total turbulence space. It is also assumed that the fine structures exist in the form of vortex pipes, surfaces, or bands and are characterized by one or two scales.

In order to model the chemical reaction rate within the framework of this concept, one should know the fraction of fine structures in the total turbulent flow, as well as the intensity of the mass transfer between fine structures and the surrounding flow.

1.1. Mass Fraction and Mass Flow in Fine Structures. The mass flow between fine structures and the surrounding flow (expressed in mass fractions) is proportional, according to [1], to the ratio of the mass fraction of fine sructures and the time scale of their lifetime, i.e.

$$\dot{m} \propto \frac{\gamma^*}{\tau^*} = \frac{u^*}{L^*}\gamma^*,$$ (1)

where L^*, u^*, and τ^* are the characteristic length, velocity, and time scale of the fine structures, and γ^* is the mass fraction of the flow that fills the fine structures in the total turbulence space.

If one assumes that L^*, u^*, and τ^* correspond to the parameters of Kolmogorov's microscale, then

$$L^* = (\nu^3/\varepsilon)^{1/4}, \quad u^* = (\nu\varepsilon)^{1/4}, \quad \tau^* = (\nu/\varepsilon)^{1/2}. \tag{2}$$

Let us transform Eq. (1) using relationships (2):

$$\dot{m} = a_1 \sqrt{\varepsilon/\nu}\, \gamma^*. \tag{3}$$

The expression for the mass fraction of fine structures (γ^*) can be obtained in an analysis of the ratio of the energy transfer in fine structures and large vortexes [1]. Finally, we have

$$\gamma^* = (u^*/u')^3 \propto (u'L'/\nu)^{-3/4} = R_t^{-3/4} \tag{4}$$

or

$$\gamma^* = a_2 R_t^{-3/4}, \tag{5}$$

where $R_t = k^2/\nu\varepsilon$ is the turbulent Reynolds number.

1.2. Combustion Rate Under the Assumption of an Infinitely Fast Chemical Kinetics. According to the concept assumed, the gas combustion rate depends on the intensity of the mass transfer between the surrounding flow and fine structures under conditions of dynamic equilibrium with the chemical kinetics. The rate of conversion of the i-th component participating in the chemical reaction can be expressed by the equation

$$r_i = \dot{m}\rho\,(y_i^0 - y_i^*), \tag{6}$$

where $y_i^0 = c_i^0/\rho^0$ and $y_i^* = c_i^*/\rho^*$ are the mass fractions of the i-th component in the surrounding flow and fine structures, respectively.

The ratio of the average mass fraction of the i-th component and the mass fraction of the same component in fine structures is determined by the following expression:

$$y_i = y_i^*\gamma^* + y_i^0\,(1 - \gamma^*). \tag{7}$$

By substituting Eq. (7) into (6) we obtain

$$r_i = \frac{\dot{m}\rho}{1 - \gamma^*}\,(y_i^0 - y_i^*). \tag{8}$$

When one takes into account the relationships for $\dot{m}$ and γ^*, it becomes evident that y_i^* is the only unknown quantity in the right-hand side of Eq. (8).

Under conditions of intense chemical kinetics, the quantity y_i^* has a very small value and therefore can be neglected. Therefore, under the assumption that $y_i^* = 0$, Eq. (8) transforms into the expression for the combustion reaction rate

$$r_d = \frac{\dot{m}\rho}{1 - \gamma^*}\, y_{min}, \quad y_{min} = \min\left\{ y_{fu}, \frac{y_{O_2}}{s_{fu}} \right\}, \tag{9}$$

where $\xi_{fu} = nM_{O_2}/M_{fu}$ is the stoichiometric ratio for oxygen and fuel.

In [3], Eq. (9) is used also in cases of lower intensity of the chemical reaction compared to that given by the expression for the chemical kinetics of the combustion reaction

$$r_{ch} = k_0 \exp\left(- E_a/RT\right) \rho^{(a+b)}\, y_{fu}^a\, y_{O_2}^b. \tag{10}$$

In this case the smallest value of the rate of diffusion under conditions of the "lack of reagents" towards fine structures and the chemical reaction rate is taken for the combustion rate, i.e.

$$r_{fu} = \min \left\{ r_d, r_{ch} \right\}. \tag{11}$$

As has been already noted, the above-mentioned models of the combustion rate involve certain approximations. Expression (9) is valid only for portions of the flow in which the chemical reaction rate is infinitely high. When the combination of Eqs. (9) and (10) (i.e., relationship (11)) is used, then the use of expression (9) is admissible also in the case when r_{ch} is not infinitely high, since in this case Eq. (9) is valid when $r_d < r_{ch}$ instead of $r_d \ll r_{ch}$. In the above-mentioned models the assumption $y_i^* = 0$ is not always substantiated. Therefore, we have made an attempt to develop our own model based on the concept of a vortex, but involving a smaller number of approximations regarding the value of y_i^*.

1.3. Model of the Combustion Rate Under the Assumption of a Finite-Rate Checmical Reaction ($y_i^* \neq 0$). When developing this model, basic assumptions of the EDC modeling, according to which the chemical reaction takes place solely within fine structures where reagents are mixed on the molecular level, are taken into account. Then the fine structures comprise in practice a miniature continuous perfect-mixing reactor. The conversion rate of the i-th component in the fine structures corresponds to the difference in mass flow rates of a given component at the entry and in the finest structures (before their decay) under conditions of dynamic equilibrium of the mass transfer and chemical reaction. These mass flow rates depend on concentrations of the i-th component in the fine structures and in the surrounding flow and on the time scale of the fine structures. In accordance with the aforesaid, one can write the expression for the conversion rate of the i-th component:

$$r_i^* = \left(c_i^0 \frac{\rho^*}{\rho^0} - c_i^* \right) / \tau^*. \tag{12}$$

If one assumes that the time scale τ^* can be defined by Eqs. (1) and (3), then the only unknowns that enter into formula (12) are quantities in the numerator of the right-hand side of the equation (c_i^0 and c_i^*, i.e., y_i^0 and y_i^*). In order to evaluate them, one can use the equation of mass balance of the i-th component in the fine structures

$$\frac{\rho^* y_i^0}{\tau^*} - \frac{\rho^* y_i^*}{\tau^*} = r_{ch}^*, \tag{13}$$

where r_{ch}^* is the chemical reaction rate at reagent concentrations relevant to the fine structures.

The mass fractions y_i^0 and y_j^0 can be expressed from Eq. (7) in terms of the quantities y_i, y_i^*, and y_j, y_j^*, where y_j^* is the concentration of the excess reagent and can be determined from the theory of a perfect-mixing flow reactor using the relationship

$$\frac{\rho^0}{\rho^*} c_j^* = c_j^0 - s_{fui} \left(c_i^0 - c_i^* \frac{\rho^0}{\rho^*} \right) \tag{14}$$

or

$$y_i^* = y_j - s_{fui} \left(y_i - y_i^* \right). \tag{15}$$

In the general case, densities are not equal in fine structures and the surrounding flow, i.e., $\rho^* \neq \rho^0 \neq \rho$, and therefore one should determine one more unknown $\rho^* = \gamma^* m / \psi^* V = \gamma^* \rho / \psi^*$ where $\psi^* = V^* / V$. If one assumes that the volume fraction of fine structures is proportional to the ratio of the turbulent length of the smallest and largest vortices, then the following relationships hold:

TABLE 1. Source Terms in Equation of Conservation of Components of Combustion of C_xH_{2x+2} Gaseous Fuel from Methane Homolog Series

Components	Source term S_{Φ_i} in chemical reactions of combustion	
	one-stage reaction	two-stage reaction
CO	0	$r_{fu} - x(M_{CO}/M_{fu})r_{CO}$
O_2	$((3x + 1)/2)(M_{O_2}/M_{fu})r_{fu}$	$((2x + 1)/2)(M_{O_2}/M_{fu})r_{fu} + 1/2(M_{O_2}/M_{CO})r_{CO}$
CO_2	$x(M_{CO_2}/M_{fu})r_{fu}$	$(1 + 1/2M_{O_2}/M_{CO})r_{CO}$
H_2O	$(x + 1)(M_{CO_2}/M_{fu})r_{fu}$	$(x + 1)(M_{CO_2}/M_{fu})r_{fu}$

$$\psi^* \approx \gamma^* \Rightarrow \rho^* \approx \rho . \tag{16}$$

In accordance with the aforesaid, we can assume that the density in the fine structures is approximately equal to that in the surrounding flow, i.e., to the average density of the space under consideration.

By introducing expressions (10), (15), (7), and (16) into balance equation (13), we obtain the nonlinear equation with one unknown (y_i^*):

$$\frac{\rho (y_i - y_i^*)}{\tau^* (1 - \gamma^*)} = k_{ch} \rho^{(a+b)} y_i^{*a} [y_i - s_{fui} (y_i - y_i^*)]^b ,$$

$$k_{ch} = k_0 \exp (- E_a/RT) . \tag{17}$$

When solving Eq. (17) and evaluating the quantity y_i^*, expression (12) can be used for calculation of the conversion rate of the i-th component. With allowance for Eqs. (7) and (16), it takes the form

$$r_i^* = \frac{\rho (y_i - y_i^*)}{\tau^* (1 - \gamma^*)} . \tag{18}$$

Inasmuch as r_i^* corresponds to the mass of fine structures, and i is the limiting reactant, the equation for evaluation of the combustion rate at a finite rate of the chemical reaction can be presented in the following form:

$$r_{fu} = \begin{cases} r_i^* \gamma^* , & \dfrac{y_{O_2}}{s_{fu}} \geq y_{fu} , \\[2ex] \dfrac{r_i^* \gamma^*}{s_{fu}} , & \dfrac{y_{O_2}}{s_{fu}} < y_{fu} . \end{cases} \tag{19}$$

An analysis of Eq. (17) shows that at very large values of the reaction rate constant, y_i^* takes small values, which corresponds to the assumption of the previous model that the quantity y_i^* cannot be neglected in the case of intense chemical kinetics. In this case expression (19) is virtually identical to relationship (4). This means that the given model is reduced to the preceding one in the case of intense chemical kinetics but has wider applications, since it is valid also for turbulent flow regions where the chemical reaction is not very fast.

2. APPLICATION OF THE COMBUSTION RATE MODEL IN CALCULATIONS OF TURBULENT FLOWS WITH CHEMICAL REACTIONS

The above-enumerated models are rather convenient for their incorporation into complex numerical calculations of a turbulent space with chemical reactions, since they do not require solution of additional differential equations, and the constants are determined based on known regularities of the turbulence structure or are available
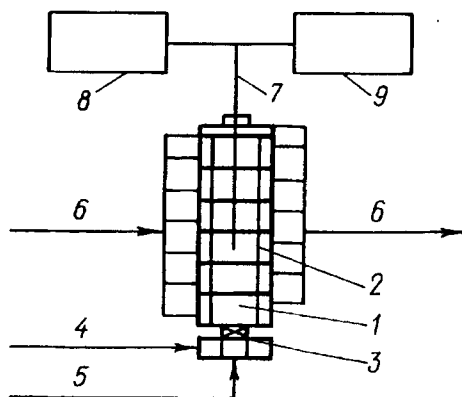
Fig. 1. Diagram of experimental installation.

from the literature (chemical kinetics constants). Application of the proposed models is possible, e.g., in calculation of the turbulent gas flow in an axisymmetric space based on averaged Navier-Stokes equations and the k-ε turbulence model with the numerical solution of equations by the method of control volumes according to the SIMPLE algorithm [4].

In these calculations, the parameters of the combustion rate model (τ^*, y_i^*, γ^*, etc.) are found separately for each control volume, and the quantity r_{fu} is evaluated on their basis, i.e., the source term (S_{Φ_i}) in the equation of conservation of the i-th component participating in the combustion reaction

$$\frac{\partial\,(\rho U y_i)}{\partial x} + \frac{1}{r}\frac{\partial}{\partial r}\,(r\rho V y_i) = \frac{\partial}{\partial x}\left(\frac{\mu_{\mathrm{eff}}}{\sigma_m}\frac{\partial y_i}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{\mathrm{eff}}}{\sigma_m}\frac{\partial y_i}{\partial r}\right) + S_{\Phi_i}, \tag{20}$$

where $\mu_{\mathrm{eff}} = \mu + C_{\mu}\rho k^2/\varepsilon$, and σ_m and C_{μ} are constants of the k-ε model.

The form of the source term in expression (20) is affected, along with the combustion rate, by the stoichiometry of the reaction, and it is important whether the combustion process is considered as a one- or multistage chemical reaction.

Source terms from Eq. (20) in the case of a one-stage combustion reaction of a gaseous fuel from the methane homolog series (C_xH_{2x+2}) are presented in Table 1 separately for each of the components.

When the combustion reaction is considered as a two-stage chemical reaction with CO as an intermediate product, then two processes are monitored: incomplete fuel combustion and oxidation of carbon monoxide, and the rates of the two reactions r_{fu} and r_{CO} are determined using the proposed model. Table 1 presents sources (i.e., sinks) of components in the two-stage reaction of combustion of a gaseous fuel from the methane homolog series.

3. EXPERIMENTAL

Experiments for checking the described modes were carried out on a laboratory model of a high-rate gas burner with a vortex combustion chamber and included measurements of the profiles of the temperatures and concentrations of combustion products of the propane-butane mixture (O_2, CO_2, and CO) along the chamber axis. In order to determine the temperature boundary conditions we measured the heat flux on the walls.

Figure 1 presents a diagram of the setup for the experimental investigation of the burner. The burner is situated vertically with its flame directed upwards to provide more convenient manipulation with the measuring probe 7. Gas 4 and air 5 are supplied via the burner's inlet. Here a vortexer 3, which creates a tangential component of the air feeding velocity, is also situated. The combustion chamber consists of ring segments 1 with double walls 2 between which water 6 flows.

The measuring probe consists of sensors 8 for determination of temperature (type K thermocoax 1 mm in diameter) and a steel pipe 9 (with an outer diameter of 2 mm) for gas sampling. The tightly bound thermocouple and sampling probe can easily be mounted at any point along the axis of the combustion chamber, and, due to their small thickness, they do not introduce substantial perturbations into the gas flow pattern.

TABLE 2. Empirical Constants of Combustion Rate Model

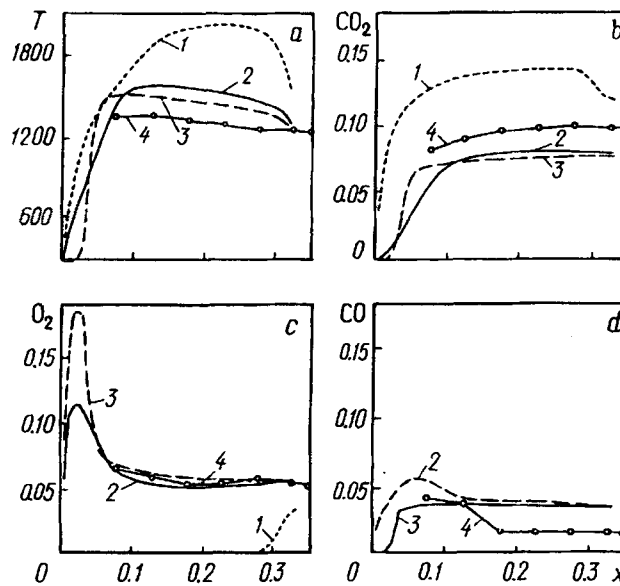| Components	Constants					
	a_1	a_2	k_0	E_a/R	a	b
Fuel	1	2.5	$4.2 \cdot 10^{11}$	7396	0.5	0.5
CO	1	2.5	$1.4 \cdot 10^{12}$	11,583	0.5	0.5

Fig. 2. Comparison of numerical results with experimental data: a) temperature profiles; b) concentration profiles of CO_2, c) O_2; and d) CO (1, model 1; 2, 2; 3, 3; 4, experiment).

The heat flux via the walls of the combustion chamber is measured by the calorimetric method. As has already been pointed out, all six cylindrical segments, as well as the plates on the top and bottom of the chamber, have double walls, between which cooling water flows. By measuring the temperature at the inlet and outlet and the water flow for each of the segments separately, one can obtain data on the distribution of the heat flux over the walls of the combustion chamber.

4. COMPARATIVE ANALYSIS OF EXPERIMENTAL AND NUMERICAL RESULTS

We analyzed three variants of the proposed method of calculation of the combustion rate: model 1 that assumes that the chemical reaction is one-stage and takes place at an infinite rate (i.e., $y_i^* \neq 0$); model 2 is the same as model 1 except for a two-stage combustion reaction; and model 3 corresponds to chemical reactions with finite (small) rates under the assumption of a two-stage chemical reaction. The assumed constants of the proposed models related to turbulent diffusion in the fine structures and chemical kinetics are presented in Table 2.

Byggstoyl and Magnussen [1] propose somewhat different values of the constants related to the diffusion in fine structures: $a_1 = 2.43$ and $a_2 = 9.7$, and it should be noted that the value of a_1 was obtained using a model of a stepwise process of dissipation of turbulent vortex energy, whereas a_2 is an empirical constant. In the same work the constants were assumed to have other values (presented in Table 3 of [1]) were assigned to the constants, which provide a better agreement between the model and experiment. In this case the constant a_1 is determined under an assumption that the time scale of fine structures is equal to the characteristic time of Kolmogorov's microscale.

Constants from the Arrhenius expression (10) were taken from [5]. As is evident from Table 2, exponents over concentrations were $a = b = 0.5$, and therefore Eq. (17) can be solved analytically, which substantially reduces the computing time. We also carried out a test calculation with the constants proposed in [6]. However, these coefficients do not permit analytical solution of Eq. (17), but the final result differs insignificantly from results of calculations carried out with coefficients from Table 2.

As has been already noted, the above-mentioned combustion models were used in the comprehensive numerical calculation of a vortex combustion chamber. Inasmuch as the assumed combustion model is two-dimensional, we considered profiles of the temperature and concentrations of combustion products only along the chamber axis to provide a more straightforward comparison of results.

All the results presented correspond to conditions when air is fed into the combustion chamber via the ring notch of the vortexer at an angle of 45° with respect to the burner axis. This means that the axial and tangential components of the air velocity at the inlet and outlet of the combustion chamber were equal.

Figure 2 presents temperature profiles along the axis of the combustion chamber obtained from measurements and calculation using the three above-mentioned variants of combustion in a turbulent gas flow. As is evident from the figure, the agreement with the experimental results is better when the more complex combustion model is used. The best coincidence with the measured data is demonstrated by model 3, where, in addition to the use of a two-stage chemical reaction, the reagent concentrations in the fine structures are calculated. This model is also valid for conditions of finite chemical reaction rates.

The huge deviation of model 1 from the experimental results compared to models 2 and 3 can be explained by the use of a one-stage chemical reaction under the given conditions of the combustion process, since experiments were carried out with intense cooling of the combustion chamber, which is favorable for incomplete combustion, whereas model 1 assumes a complete combustion reaction with CO_2 and H_2O as the only products.

Temperature profiles obtained with models 2 and 3 deviate much less from the measured profile. The deviation between models 2 and 3 is more substantial in regions closer to the place where gases are fed into the chamber. This takes place most likely since model 2 uses the assumption that the chemical reaction rate is infinitely high in all regions of the turbulence space. In regions near the chamber's bottom the chemical reaction rate is small owing to lower temperatures and incomplete mixing of reagents, and therefore model 2 deviates more substantially in this region from the experiment and model 3.

Figure 2b-d presents concentration profiles for CO_2, O_2, and CO, respectively, along the axis of the combustion chamber. The analysis carried out for temperature profiles is valid also for concentrations of components participating in the combustion process: it can only be added that it is evident from the results presented that the maximum difference between models 2 and 3 is observed near the bottom of the combustion chamber, i.e., in regions of mixing of the fuel and air.

NOTATION

c, weight concentration of components of combustion process; E_a, chemical reaction activation energy; k, kinetic energy of turbulence; k_{ch}, chemical reaction rate constant; k_0, constant in the Arrhenius expression; L', characteristic length of turbulence; M, molar weight; n, number of moles of oxygen in stoichiometric equation of combustion reaction; R, gas constant; r, combustion process rate and radial coordinate; T, absolute temperature; U, flow velocity component along the axial direction; u', turbulence velocity; V, volume and flow velocity component along the radial direction; x, number of carbon atoms in fuel molecule and axial coordinate; ε, dissipation of kinetic energy of turbulence; μ, dynamic molecular viscosity; ν, kinematic viscosity; ρ, density; ψ^*, volume fraction of fine structures.

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