MODELING OF TURBULENT COMBUSTION OF NONPREMIXED GASES


Conditions for carbon-monoxide-emission modeling by combustion chambers of gas turbine engines powered by fuel gas are analyzed. Mechanisms of CO formation based on the front combustion model are examined. They influence CO emission by the only chemical parameter, i.e., by the critical value of scalar dissipation at flame breaking. Combustion chamber tests are carried out. They show that the introduced parameter allows us to generalize test results at different pressures.

The possibility of nonpremixed-gas turbulent-combustion modeling in the case of a finite reaction rate is analyzed. Here modeling is defined as a procedure of a complex-geometry combustion-chamber testing that involves identical determining criteria under both modeling and operating conditions in spite of a difference in the absolute values of individual parameters. The problem has assumed great importance because of the necessity to create ecologically clean gas-turbine engines and plants and the considerable increase in the cost of their testing. The latter is due to the high pressures under operating conditions. Taking into account that each facility is equivalent in power to an average electric power station, it is obvious that considerable amounts of money could be saved with low-pressure testing. Only one aspect of the problem is discussed in this article; namely, carbon-monoxide emission by fuel gas chambers.

Generally speaking, the problem stated has no solution, i.e., a change in any parameter or group of parameters is significant. There are actually many reactions in the system and thus many Damkohler criteria (relation between hydrodynamic and chemical reaction times). They depend differently on temperature T and pressure p. Thus, p and T must be the same under modeling and operating conditions. Then, only scale modeling is possible, which is not sufficient to solve practical problems. Only an approximate solution of the problem can be found through analysis of its essential features.

Among the features are separate air and fuel supply and turbulent flow, which result in composition fluctuations at each point. They will be described by the reduced fuel concentration z, which is the mass concentration of all the fuel atoms contained in all chemical compounds. While the quantity z characterizes the composition at every point at every time moment, the air–fuel ratio α is understood traditionally.

The main peculiarity of the system is a sharp dependence of reaction rates on temperature. For this reason the main chemical conversions take place in the most-heated zones. In our case, these zones are localized near the stoichiometric surface, z = z_s, which is curved and moves at random because of hydrodynamic pulsations. It is shown [1] that the unaveraged heat and mass transfer equations

\[ \rho \frac{\partial e_\alpha}{\partial t} + \rho u_k \frac{\partial e_\alpha}{\partial x_k} = \nabla D \nabla e_\alpha + \rho W_\alpha \]

reduce to simple expressions in the reaction zone

\[ N \frac{d^2 e_\alpha}{dz^2} + W_\alpha = 0, \quad N = D \nabla z^2, \]

(1)
They have asymptotic precision if the reaction zone thickness tends to zero. Here \( \rho \) is the density, \( c_a \) is the enthalpy or mass concentration, \( u_k \) is the velocity, \( t \) is the time, \( x_k \) is the coordinate, \( D \) is the molecular diffusion coefficient, and \( N \) is the scalar dissipation. The last value is the only turbulence characteristic which influences the proceeding of reactions. It describes the rate of mixing up to molecular level.

A boundary-value problem for system (1) is stated for \( z = 0 \) (pure air) and \( z = 1 \) (pure fuel). It is shown \([2]\) that the boundary conditions have little effect on the solution within the reaction zone. The applicability of system (1) to describe turbulent diffusion combustion for a finite reaction rate is demonstrated in \([2]\) by analyzing numerous experiments with laboratory flames (including the ones where CO concentration is measured). The peculiarity of industrial combustion chambers is that the Damkohler number \( Da \), calculated for the time of any reaction, is considerably smaller than in laboratory flames. As shown in \([2]\), the formation of CO under these conditions is influenced by factors which cannot be described with the help of system (1). The first one is essential to the early stages of mixing and combustion, when the scalar dissipation is on the average high. The boundary-value problem for system (1) actually has two solutions. One solution corresponds to combustion; the other, to slow-reaction mixing. The first solution exists only if \( N < N_{cr} \). In other words, combustion is possible only if the mixing velocity does not exceed a certain value.

The quantity \( N_{cr} \) is a purely chemical parameter. It can be interpreted with the help of a theory \([3]\), which shows that combustion in a diffusion flame halts if the fuel flow to the front becomes greater than the flow in a normal flame spreading in a stoichiometric mixture. This reasoning leads to the equation \([2]\)

\[ N_{cr} = b \frac{u_n^2 z_1^2 \rho_0^2}{D_s p_0^2} \]

where \( u_n \) is the propagation velocity of a normal flame in a stoichiometric mixture, subscripts 0 and s refer to a fresh mixture and to stoichiometric-mixture combustion products, and \( b \) is a numerical coefficient which equals 1 in the context of the theory \([3]\). Numerical calculations \([2]\) for different types of fuel show that the value of \( b \) is really on the order of 1 (0.88-1.60) in spite of considerable \( N \) variation (by more than a factor of 10).

Notice that the scalar dissipation fluctuates on the reaction-zone surface. For this reason, when it has high average values, the stable combustion condition \( N < N_{cr} \) is satisfied only in some of its parts. In other words, "holes" appear in the flame, through which incomplete-combustion products find their way into lean low-temperature tongue parts where reactions are frozen. Since in gas turbine combustion chambers \( \alpha >> 1 \), these zones are generally observed at the outlet. Thus, in the process under consideration part of the CO cannot burn out in principle.

System (1) does not describe this phenomenon, since it is not valid outside the reaction zone. If there are "holes" in the flame it is not valid either, as concentration gradients start playing a considerable role along the reaction zone in this case. But they were not taken into consideration in the derivation of (1). Nevertheless, it turns out to be useful when analyzing the form of criteria describing the analyzed process. Indeed, CO flow into the lean tongue parts is determined by the turbulence characteristics, the area of the "holes," and the specific CO concentration in the rich part of the flame \( z > z_1 \). The latter value is weakly dependent on the chemical kinetics, as calculations show (see \([2, Fig. 13]\)). The area of the "holes" can only be influenced by the value of \( N_{cr} \). Thus, it can be assumed that the influence of the first mechanism on CO formation is described only by the parameter \( N_{cr} \).

The second mechanism of CO formation operates in the regime of developed combustion. Analysis of solutions of system (1) shows that there exists a fairly narrow zone of compositions where reactions are abruptly frozen. Calculations \([2]\) show that this zone is situated near the surface \( z = z_1 < z_4 \) and the value of \( z \) has weak dependence on the hydrodynamics, initial temperature, and pressure. In particular, \( z = 0.042-0.038 \) for methane was obtained with \( N \) changed by three orders of magnitude, with the initial temperature changed by a factor of 2 and the pressure by a factor of 15. This result is directly connected with the sharp reaction rate dependence on temperature and thus, on composition.

It is obvious from what has been said that a zone with \( z < z_1 \) can be recognized where reactions can be neglected. The CO concentration in this zone is described by a diffusion equation without source terms. In this case, the boundary conditions are specified on the surface \( z = z_1 \). Evidently, they can be found from the solution of system (1). It leads to carbon monoxide diffusion from the surface \( z = z_1 \) into lean zones where it is frozen, i.e., the same process as in the formation of "holes" takes place.

It is important that CO concentration on the surface \( z = z_1 \) is a universal function of the criterion \( N/N_{cr} \) (see \([2, Fig. 9]\)). This conclusion does not follow from model (1) and points only to a certain universality of typical fuel oxidation kinetics. Thus, the influence of the second mechanism on CO formation is described by the single chemical parameter \( N_{cr} \) as well.