

# NUMERICAL SIMULATION OF TURBULENT FLAMES

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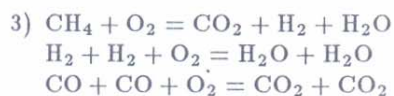
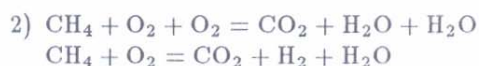
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The joint velocity — species concentration probability density function method (Joint PDF Method) has been applied for modeling two-dimensional transient variable-density turbulent flows with detailed simulation of combustion chemistry. The numerical algorithm is based on the Lagrangian Monte Carlo method [1], Eulerian Finite Volume method [2], and the method of Local Linearization for Equations of Chemical Kinetics [3]. Systematically reduced detailed reaction mechanisms as well as overall reaction mechanisms for hydrocarbon fuel oxidation and pollutant formation have been developed and implemented for the numerical analysis of a number of applied problems.

## 1 Reduced Reaction Mechanisms for Fuel Oxidation and Pollutant Formation

Chemical processes of oxidation and combustion of a specified fuel-oxidizer system are essentially dependent of physical conditions. In the absence of turbulence, there are two possibilities for a combustion process: to proceed with 1) no mixing between unburned gas and reaction products (e.g., constant volume ignition, ignition behind a shock wave), and 2) superposition of reaction and diffusion processes (e.g. laminar flame propagation). Depending on the assumption used in this concern, the systematic reduction of a detailed reaction mechanism can result in different reduced mechanisms.

Two systematically reduced reaction mechanisms of methane oxidation have been developed. The first is based on the numerical integration of equations for 1-D laminar flame propagation with due regard for the detailed chemistry (130 elementary reactions with 17 species). The second is based on solving the problem of methane-air mixture auto-ignition. For modeling  $\text{NO}_x$  formation the reaction mechanism of fuel oxidation has been supplemented with an additional block of reactions: 1) reactions of air nitrogen with oxygen, 2) reactions of air nitrogen with intermediate combustion products (prompt  $\text{NO}_x$ ), and 3) reactions of fuel nitrogen (ammonium additive) with intermediate combustion products. The calculations of laminar flame propagation and auto-ignition delay were coupled with the reduction procedure which made it possible to select governing elementary reactions during solution of the problems. The reduced mechanisms thus obtained exhibit all specific features of the complete detailed reaction mechanism. However, the number of reactive species in the mechanisms appears to be too large for simulating multi-dimensional turbulent reactive flows. Therefore, further reduction is undertaken by using the approach of [4]. In addition, for the preliminary approximate calculations, three overall reaction mechanisms of methane oxidation have been developed. The overall reactions have been written in the form resembling realistic elementary reactions (no fraction exponents in the expression for the reaction rates) which is convenient for using standard kinetic codes when solving applied problems. The mechanisms are presented below:



The corresponding reaction constants have been chosen by fitting the predicted and measured laminar flame velocities for mixtures of different composition, at different initial temperature and pressure with

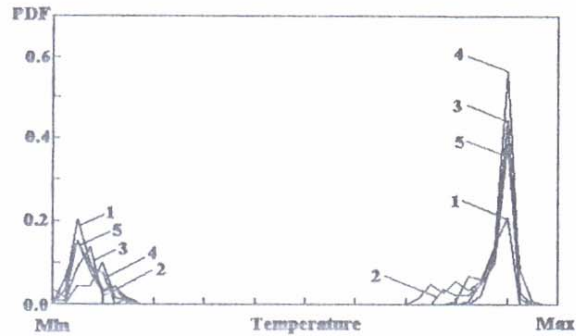


Figure 1: Premixed turbulent flame. PDF of temperature in a fixed location at the flame front at different time. 1 --  $t = 14$  ms, 2 -- 28 ms, 3 -- 42 ms, 4 -- 56 ms, 5 -- 70 ms after ignition.

further updating to cover available auto-ignition delay data under conditions of vigorous reaction in flame (1000 K).

The overall mechanism of  $\text{NO}_x$  formation has been also suggested. It is composed of two reactions which are added to one of the overall mechanisms of fuel oxidation:



The first reaction is applied for modeling prompt NO. The use of  $\text{CH}_4$  as a reaction participant ensures NO production only in the reaction zone (in a detailed reaction mechanism this role is played by the radicals like CH and  $\text{CH}_2$ ). The second reaction is applied for modeling thermal NO. Its reaction rate incorporates the equilibrium constant of the  $\text{O}_2 \rightleftharpoons 2\text{O}$  process.

## 2 Calculations of the Limit of Turbulent Flame Stabilization

The problem of hydrogen- and methane-air flame stabilization in a combustion chamber with different bluff bodies has been solved numerically by the Joint PDF Method. The predicted results are directly compared with the experimental data obtained in a chamber  $20 \times 60 \text{ mm}^2$  cross section, under conditions of ambient and lower pressure, initial temperature 20–250 °C, flow velocity up to 120 m/s, and initial 2–10% turbulence. Satisfactory agreement with measured results on the critical conditions of flame stabilization have been obtained.

The problem of a premixed methane-air turbulent flame stabilized at the sharp edge of the combustion chamber (simulating gas turbine combustor) has been also analyzed. Figure 1 shows the evolution of temperature PDF in a fixed point located nearby the developing flame front. Ignition has been initiated by hot combustion products placed into the core of the zone. Clearly, the PDF is bimodal, i.e. exhibits two distinct maxima. The first maximum corresponds with the initial reactive mixture, the second represents combustion products. No intermediate state is realized because of fast oxidation reactions. The comparison of predicted results with available experimental data on flame position and  $\text{NO}_x$  concentration has been made for the conditions relevant to gas turbine combustors. The method was shown to provide satisfactory predictions.

## 3 Turbulent Jet Diffusion Flame

The problem of turbulent diffusion flame arising in the mixing layer of two coaxial methane and oxygen high-velocity (100 m/s) jets in a combustion chamber with a strong recirculation zone has been also solved. The analysis of joint probability density functions has revealed a number of important features of turbulent diffusion flames. The spectra of species concentrations and temperature appeared to be continuous, however some dominating values were apparent in different flow portions.

## 4 Auto-ignition Behind a Shock Wave

A joint PDF method has been applied for modeling auto-ignition of methane-oxygen mixture behind a shock wave. It has been shown that turbulent transport processes play insignificant role in the development of a post-shock reaction zone.

## 5 Pollutant Formation in Turbulent Flames

The test section geometry and conditions of some available experimental investigations were simulated in calculations aimed to compare directly the predicted and measured level of  $\text{NO}_x$  formation in turbulent diffusion and premixed flames. The predicted results appeared to agree with the experimental findings within the factor of 2 to 4.

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