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## CFD SIMULATION OF PARTIALLY PREMIXED PILOTED CH4/AIR SANDIA FLAME (D) COMBUSTION AND EMISSINOS

***ABSTRACT*** *In this study, a numerical simulation of a piloted CH4/air (Sandia flame D) model, for partially-premixed combustion, with varying levels of O2/N2 by volume, is presented. The turbulence and combustion are modeled by the standard k–ε and burning velocity model(BVM) which also called turbulent flame closure (TFC) model which is used with laminar flamelet to give detailed chemistry. The main purpose this study is to predict the effect of the O2 and N2 volume percentage, on the turbulent flame characteristics and formation of harmful substances and emissions. Computations were achieved by the ANSYS CFX.*

***Key words:*** *Sandia flame-flamelet-emission-burning velocity model-partially premixed combustion.*

***МАСУД ХАДЖИВАНД***

## CFD МОДЕЛИРОВАНИЕ ГОРЕНИЯ SANDIA FLAME (D) МЕТАНО-ВОЗДУШНЫХ СМЕСЕЙ С ЧАСТИЧНЫМ ПРЕДВАРИТЕЛЬНЫМ ПЕРЕМЕШИВАНИЕМ

***АННОТАЦИЯ*** *В данном исследовании представлено численное моделирование горения предварительно частично перемешанной метано-воздушной смеси с различными объемными долями $O_2$ и $N_2$. Турбулентность и горение смоделированы с помощью стандартной k–ε модели турбулентности и модели скорости распространения пламени, которая известна также как модель смыкания турбулентного пламени и используется для ламинарного пламени с подробным описанием химических реакций. Основной целью данного исследования является прогнозирование влияния различного процентного соотношения $O_2$ и $N_2$ на характеристики турбулентного пламени и образование вредных веществ и эмиссию. Расчеты проведены с помощью ANSYS CFX.*

***Ключевые слова:*** *Sandia пламени-емиссия- скорость распространения пламени, горение предварительно частично перемешанной смеси.*

### Introduction

Modeling turbulent reacting flow fields in combustion science has gained significant interest in both academia and industry with the development of high powered computers. Validation of combustion models in a turbulent flow field is necessary, and experimental data in combustion such as gas turbine engines are limited [1].

The accurate prediction of combustion in practical systems has attracted the attention of many researchers over the last few decades because of its potential impact on the development of improved combustion equipments. Better thermal efficiency and lower pollution emission are two of the benefits that can be obtained from the development of advanced combustion models. Over the years, several combustion models that account for the interaction between turbulence and chemistry have been developed and applied to a number of flames ranging from simple jet flames to complex combustion chambers.

The numerical simulation is a beneficial tool in computational fluid dynamics (CFD) because it can easily employ various conditions by simply changing the parameters [2]. Description of complex interactions between turbulence and chemistry is a great challenge for the computational models of turbulent combustion. In the past two decades, several modelling approaches have been developed to treat such interactions, among which the eddy dissipation model (EDM) [3], transported probability density function (PDF) equation methods [4], conditional moment closure (CMC) [5] and flamelet models [6] are most exercisable and successful ones.

Beside that Reduction of pollutant emissions is important task of interest in combustion technology. The accurate prediction of pollutants of interest such as carbon monoxide, CO, nitric oxide, NO. Control of NOx emissions in the combustion process has become an important criterion that is achieved by changing air conditions in a combustor. NOx (NO and NO2) is produced in a combustor through four established mechanisms: the thermal NO, the prompt NO, the nitrous oxide mechanism and fuel NO. The latter two are of less importance for this study since they are little influenced by flame temperature or flame structure. The thermal NO mechanism is described by the oxidation of atmospheric nitrogen (N2) in high-temperature regions of the flame and post flame gases through the Zeldovich reaction scheme [7]. The prompt NO mechanism describes the formation of NO under fuel rich conditions, involving reactions between hydrocarbons radicals (CH) and N2. Prompt NO is usually found early in the flame region, near the burner, where the CH free radicals were just released from the main hydrocarbon chain.

In this study the (Sandia flame *D*) was chosen as the test case, in a partially premixed type of combustion with 3 type of boundary condition of cold flow (air), pilot flame and the main jet with premixed methane and air.

In premixed combustion the fuel and oxidant are mixed before the reaction takes place. To initiate the combustion the air to fuel ratio of the mixture has to be within the flammability limits and the local mixture temperature has to be higher than the self-ignition temperature (energy barrier). The premixed combustion will be explained by combustion of methane in air which is a model fuel of gas turbines (main component of natural gas). The actual oxidation of CH4 to CO2 and H2O consists of large number of basics reactions taking place at the molecular level [8].

In present study an attempt has been made through CFD approach to analyze the combustion characteristics of partially premixed methane-air (Sandia flame *D*) combustion, such as flame structure, maximum total temperature, species mass fraction of H2O-H2-CH4-O2-CO-CO2-NO, turbulent and laminar burning velocity and mixture fraction, in different percentage of O2 and N2 take parting in combustion process, for 4 various flames.

The first simulation is for the same Sandia flame *D* with the same parameters and characteristics. In this work the results of simulation were compared with the experiment data in Third international workshop on measurement and computation of turbulent none premixed flames in Boulder Colorado in July and August 1998 year (TNF3 workshop). The experimental results of Sandia/Darmstadt Piloted CH4/Air Flame *D* in this workshop were reported by Robert Barlow in Sandia National Laboratories.

All the simulation in this study were carried out by CFD code, ANSYS CFX including laminar flame model of combustion with burning velocity model (BVM) for simulating of partially premixed flames [9].

### The purpose of this study

The purpose of this study is to simulate combustion process of partially premixed combustion of methane-air in Sandia flame *D* by varying levels of O2 and N2 take part in combustion process and to predict of level of harmful substances (CO, CO2, NO), mass fraction of species, flame structure and shapes, along the axial distance of our domain of simulation (Sandia flame *D*) and to compare them with the experiments.

### Governing equations and turbulence model

The mathematical equations describing the fuel combustion are based on the equations of conservation of mass, momentum, and energy together with other supplementary equations for the turbulence and combustion. In this investigation the standard k-ε turbulence model is used. The equations for the turbulent kinetic energy k and the dissipation rate of the turbulent kinetic energy ε are solved Several models of turbulence have been put forward by different authors. These models differ in complexity and range of applicability; they also involve the solution of different numbers of differential equations. The turbulence model incorporated in this work is the high Reynolds number *k*–ε two equation model. This model requires the solution of two differential equations, for the two turbulence properties: the kinetic energy of turbulence *k*, and its dissipation rate ε. The model is moderate in complexity. It has been extensively used by many investigations and has proved to be adequate over a wide range of flow situation. Here the governing differential equations are presented below in details (Launder, and Spalding, 1974). Differential equations for turbulence-energy *k* and dissipation rate ε used in combustion are respectively as follows:

$$\frac{\partial(\rho k)}{\partial t}+\nabla.(\rho U k)=\nabla.\left[\left(\mu+\frac{\mu_t}{\sigma_g}\right)\nabla k\right]+P_k-\rho\varepsilon\,, \quad (1)$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\nabla.(\rho U\varepsilon)=\nabla.\left[\left(\mu+\frac{\mu_t}{\sigma_g}\right)\nabla\varepsilon\right]+ +\frac{\varepsilon}{k}\left(C_{\varepsilon 1}P_k-C_{\varepsilon 2}\rho\varepsilon\right). \quad (2)$$

### Laminar Flamelet and burning velocity Models

The model for premixed or partially premixed combustion can be split into two independent parts: 1-Model for the progress of the global reaction: Burning Velocity Model (BVM), also called Turbulent Flame Closure (TFC) 2-Model for the composition of the reacted and non-reacted fractions of the fluid.In PDF laminar flamelet model The mass fractions in the the non-reacted fraction of the fluid $\widetilde{Y}_{ifresh}$ are obtained by linear blending of fuel and oxidizer compositions. The species mass fractions in the burned fraction of the fluid, $\widetilde{Y}_{iburned}$ are computed by applying the Flamelet model [9]. For the reaction progress in the combustion simulation a single progress variable $\widetilde{c}$ is used to describe the progress of the global reaction. The composition of the fluid is determined by blending the compositions of the non-reacted state (fresh gases) and the reacted state (burned gases), where $c = 0$ corresponds to fresh materials and $c = 1$ corresponds to fully reacted materials.

$$\widetilde{Y}_i=(1-\widetilde{c})\widetilde{Y}_{ifresh}+\widetilde{c}\,\widetilde{Y}_{iburned}\,. \quad (3)$$

The reaction progress variable is completed by solving a transport equation:

$$\frac{\partial\overline{\rho}\widetilde{c}}{\partial t}+\frac{\partial(\overline{\rho}\widetilde{u}\widetilde{c})}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\left(\widetilde{\rho}D+\frac{\mu_t}{\sigma_c}\right)\frac{\partial\widetilde{c}}{\partial x_j}\right]+\overline{\omega}_c\,. \quad (4)$$

The burning velocity model (BVM), also known as tubule flam closure (TFC), is used to close the combustion source term for reaction progress.

$$\overline{\omega}_c = \overline{\rho}_u S_T \left|\nabla \widetilde{c}\right| - \frac{\partial}{\partial x_j}\left[\overline{\rho} D \frac{\partial \widetilde{c}}{\partial x_j}\right]. \quad (5)$$

Where $S_T$ is the closure developed by Zimont et al is used for turbulent burning velocity:

$$S_T = AGu`^{3/4} S_L^{1/2} \lambda_u^{-1/4} l_t^{1/4}. \quad (6)$$

Where The leading factor, *A*, is a modeling coefficient that has the universal value $P = 0.5$ and the stretching factor *G* is:

$$G = \frac{1}{2} erfc\left[-\frac{1}{\sqrt{2\sigma}}\left(\ln\left(\frac{\varepsilon_{cr}}{\varepsilon}\right) + \frac{\sigma}{2}\right)\right]. \quad (7)$$

where *erfc* denotes the complimentary error function and σ is the standard deviation of the distribution of ε, with $\mu_{str}$ being an empirical model coefficient (default – 0.28). $\lambda_u$ is the thermal diffusivity of the unburned mixture. The turbulent flame speed closure model is completed with the following models for integral velocity fluctuations level. The integral turbulent and Kolmogorov length scales are given by:

$$l_t = \frac{k^{3/2}}{\varepsilon} \text{ and } \eta = \frac{V^{3/4}}{\varepsilon^{1/4}}.$$

The critical dissipation rate, $\varepsilon_{cr}$, is computed from a specified critical velocity gradient, $g_{cr}$ and the kinematic viscosity of the fluid, $\nu$, according to: $\varepsilon_{cr} = 15\nu g_{cr}^2$.

For the laminar flame let model, under flamelet regime hypothesis, the spices transport equations are simplified to:

$$\rho \frac{\rho Y_k}{\partial t} - \frac{\rho \chi 1}{2Le_k} \frac{\partial^2 Y_k}{\partial Z^2} = \omega_k. \quad (8)$$

The simplified energy equation is:

$$\rho \frac{\rho Y_k}{\partial t} - \frac{\rho \chi 1}{2Le_k} \frac{\partial^2 Y_k}{\partial Z^2} = \frac{1}{C_P} \sum_{K=1}^{N} h_k \omega_k. \quad (9)$$

With the laminar scalar dissipation:

$$\chi 1 = 2D.(\nabla Z)^2. \quad (10)$$

An external program CFXRIF solves these equations to obtain a laminar flamelet table, which is integrated using beta PDF to have the turbulent flamelet library. This library provides the mean species mass fraction as functions of mean mixture fraction $\widetilde{Z}$, variance of mixture fraction $\widetilde{Z}``^2$ and turbulent scalar dissipation rate $\widetilde{\chi}$:

$$\widetilde{Y}_i = \widetilde{Y}_i\left(\widetilde{Z}, \widetilde{Z}``^2, \widetilde{\chi}_{st}\right). \quad (11)$$

On the other hand, 2 transport equations are solved in the CFD code, the first gives mixture fraction:

$$\frac{\partial \overline{\rho} \widetilde{Z}}{\partial t} + \frac{\partial\left(\overline{\rho} \widetilde{u}_j \widetilde{Z}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_z}\right)\frac{\partial \widetilde{z}}{\partial x_j}\right]. \quad (12)$$

And the second equation gives the mixture fraction variance:

$$\frac{\partial \overline{\rho} \widetilde{Z}}{\partial t} + \frac{\partial\left(\overline{\rho} \widetilde{u}_j \widetilde{Z}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_{\widetilde{Z}``^2}}\right)\frac{\partial_{\widetilde{Z}``^2}}{\partial x_j}\right] + 2\frac{\mu_t}{\sigma_z}\left(\frac{\partial_{\widetilde{z}}}{\partial_{xj}}\right) - \overline{\rho}\widetilde{\chi}. \quad (13)$$

The turbulent dissipation scalar is modeled by:

$$\widetilde{\chi} = C_\chi \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z}``^2. \quad (14)$$

To interpolate species mass fraction from turbulent flamelet table, the CFD program use the mixture fraction, mixture fraction variance and the turbulent scalar dissipation.

### NOx modeling

The formation of NO is a slow process which kinetically rate limited. Unlike other spices the mean value of NO cannot be obtain from flamelet library equation.

When modeling NO*x* formation in methane-air combustion, the thermal NO and prompt NO are taken into account. In the simulation process, we solve the mass transport equation for the NO species, taking into account convection, diffusion, production and consumption of NO and related species. This approach is completely general, being derived from the fundamental principle of mass conservation. For thermal and prompt NO*x* mechanisms, only the following NO species transport equation is needed [10].

$$\rho \frac{\partial Y_{\mathrm{NO}}}{\partial t} + \rho u_i \frac{\partial Y_{\mathrm{NO}}}{\partial x_i} = = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Y_{\mathrm{NO}}}{\partial x_i}\right) + S_{\mathrm{NO}}. \quad (15)$$

The source term $S_{\mathrm{NO}}$ is to be determined for different NOx mechanism. $Y_{\mathrm{NO}}$ is mass fraction of NO species in the gas phase and *D* is effective diffusion coefficient.

### Model description and the Geometry of Sandia flame *D*, meshing and boundary condition

The Flame *D* from the Sandia TNF workshop is a piloted methane-air diffusion flame [11]. The central main jet consists of a 25/75 % (by volume) methane-air mixture. The fuel has been premixed with air in order to minimize the formation of polycyclic aromatic hydrocarbons and soot. The central main jet is surrounded by a pilot jet and a slow coflow of air outside.

The hot mixture from the pilot jet besides stabilizing the main jet is also responsible for igniting the fuel which is injected from the main jet. The pilot jet is further surrounded by an air co-flow after the burner exit. The bulk velocities of the main jet, pilot and air co-flow are $U\infty = 49.6$ m/s, $Up = 11.4$ m/s and $Uc = 0.9$ m/s, respectively. The Reynolds number for

the main jet is Re = 224000 based on the nozzle diameter $d$ = 7.2 mm and the bulk jet velocity 49.6 m/s. The pilot flame was burning a mixture of C2H2, H2, air, CO2, and N2 with an enthalpy and equilibrium composition that is equivalent to a mixture of methane and air at an equivalence ratio of φ = 0.77. The fuel jet, pilot and co-flow compositions are specified in terms of the species mass fractions calculated from the experimental data documented in detail by Barlow and Frank [11].

The main jet inner diameter, $d$ = 7.2 mm Pilot flame annulus inner diameter = 7.7 mm (wall thickness = 0.25 mm) Pilot flame annulus outer diameter = 18.2 mm. Burner outer wall diameter = 18.9 mm (wall thickness = 0.35 mm) Wind tunnel exit = 30×30 cm. In this investigation the length of the burner is 700 mm. The schematic of the burner are shown in Fig. 1*a*, *b*.

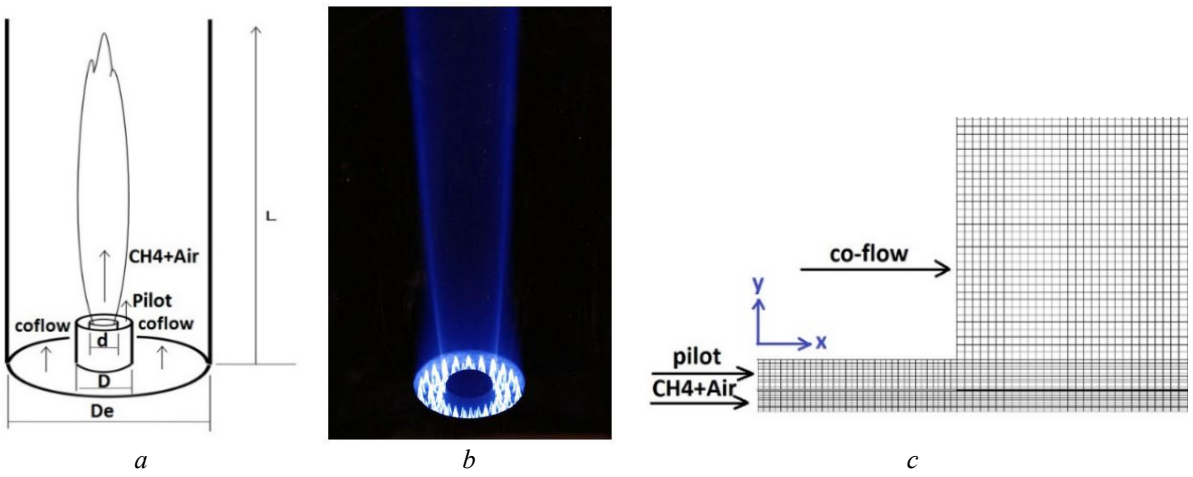
The problem is 2*d*-axisymmetric which has solved assuming symmetry about the center line. The computational domain was designed as a sector of 3 degrees with imposed periodic boundary conditions to reduce the computational cost. Domain structured mesh is made in ICEM CFD with 770000 number of elements, shown in Fig. 1*c*.

In this investigation 4 different flames were simulated with different level and varying of O2 and N2.

The first simulation of this study is the combustion simulation of Sandia flame *D* with its real boundary conditions and characteristics. For the other 3 cases of his study (flames 1, 2, 3) all the boundary condition are the same as in Sandia flame *D* except the levels and percentage of O2 and N2 which has shown in Table 1.

Table1 – Percentage of O2 and N2 by mass

| Cases | Flame-1 | Flame-2 | Flame-3 |
|---|---|---|---|
| O2 % | 25.32 | 29.53 | 33.75 |
| N2 % | 59 | 54.85 | 50.63 |
| CH4 % | 15.61 | 15.61 | 15.61 |




*a* *b* *c*

*Fig. 1 – Geometry and meshing: a – The schematic and geometric form of Sandia flame D; b – real schematic of Sandia flame D surrounding with pilot flame; c – 2d-conctracted mesh of simulation domain*

**Experimental results**

In this work the results of simulation were compared with the experiment data in Third international workshop on measurement and computation of turbulent none premixed flames in Boulder Colorado in July and August 1998 year (TNF3 workshop).

The experimental results of Sandia/Darmstadt Piloted CH4/Air Flame D in this workshop were reported by Robert Barlow in Sandia National Laboratories.

In Fig. 2. All the experimental data of temperature and species mass fraction (CH4, O2, CO, CO2, H2O, H2, OH, NO) are shown in Fig. 2, along the axial distance of the burner (Axial profile).

**Results and discussion of present simulation**

In this study all of 4 cases of simulation was performed in ANSYS CFX in a 2*D*-axisymmetric domain, including laminar flamelet modeling of combustion and burning velocity model (BVM). The convergence criteria in this simulation was at the MAX residual type with the $10^{-4}$ residual target and automatic time scale control and time scale factor of 1. All the simulation in 4 cases were converged successfully with different number of iteration, with solving the mass and momentum, heat transfer (energy), turbulence ($k$–ε), mass fraction of NO, species mixture fraction including mean and variance, temperature variance for predicting mass fraction of NO.

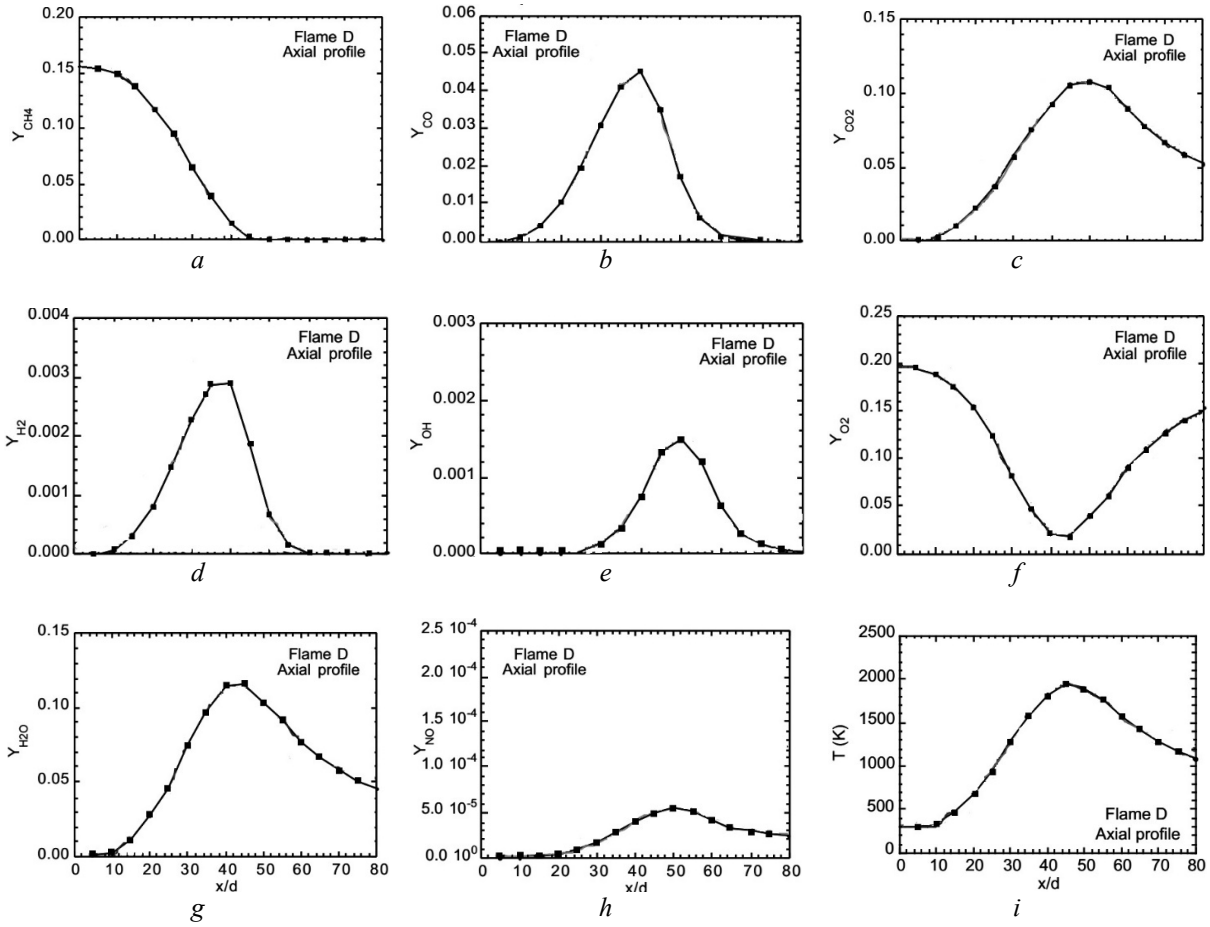
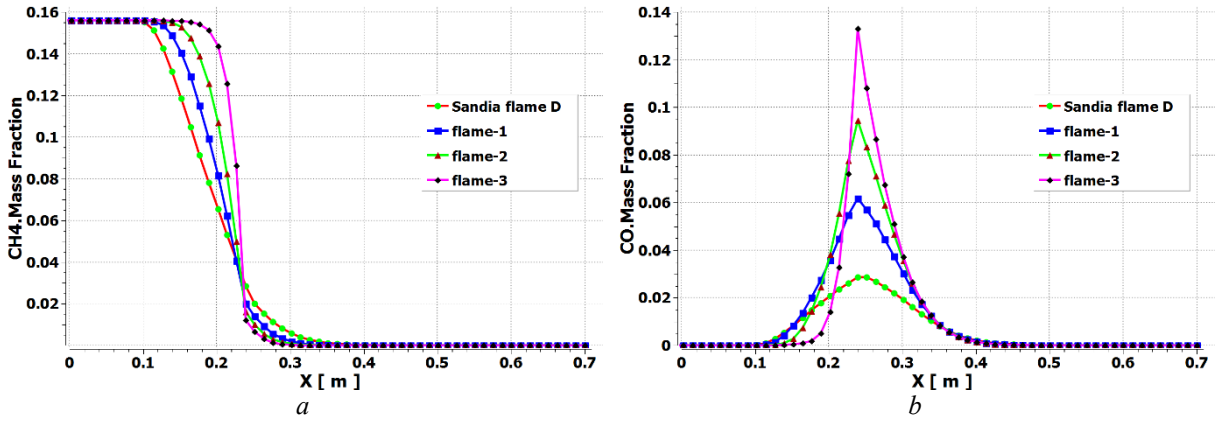



*Fig. 2 – The experimental data and results of species mass fractions along the axial profile of Sandia flame D, reported by Robert Barlow August 1998 year (TNF3 workshop): a – CH4; b – CO; c – CO2; d – H2; e – OH; f – O2; g – H2O; h – NO; i – total temperature*

For the first and second cases of the present simulation we reached the convergence in 1656$^{th}$ iteration, for the third and fourth cases of simulation we reached the convergence in 2010$^{th}$ and 3249$^{th}$ iteration. This means that the convergence has become more difficult by decreasing the level and percentage of O2.

The boundary condition and characteristics of the first simulation is the same of Sandia flame *D*. In this investigation we compared the experimental data with the first simulation to confirm the accuracy of the simulation, implementing by PDF Laminar Flamelet Model (LFM) including Burning Velocity Model (BVM).

The plots of simulation results are presented in Fig. 3.



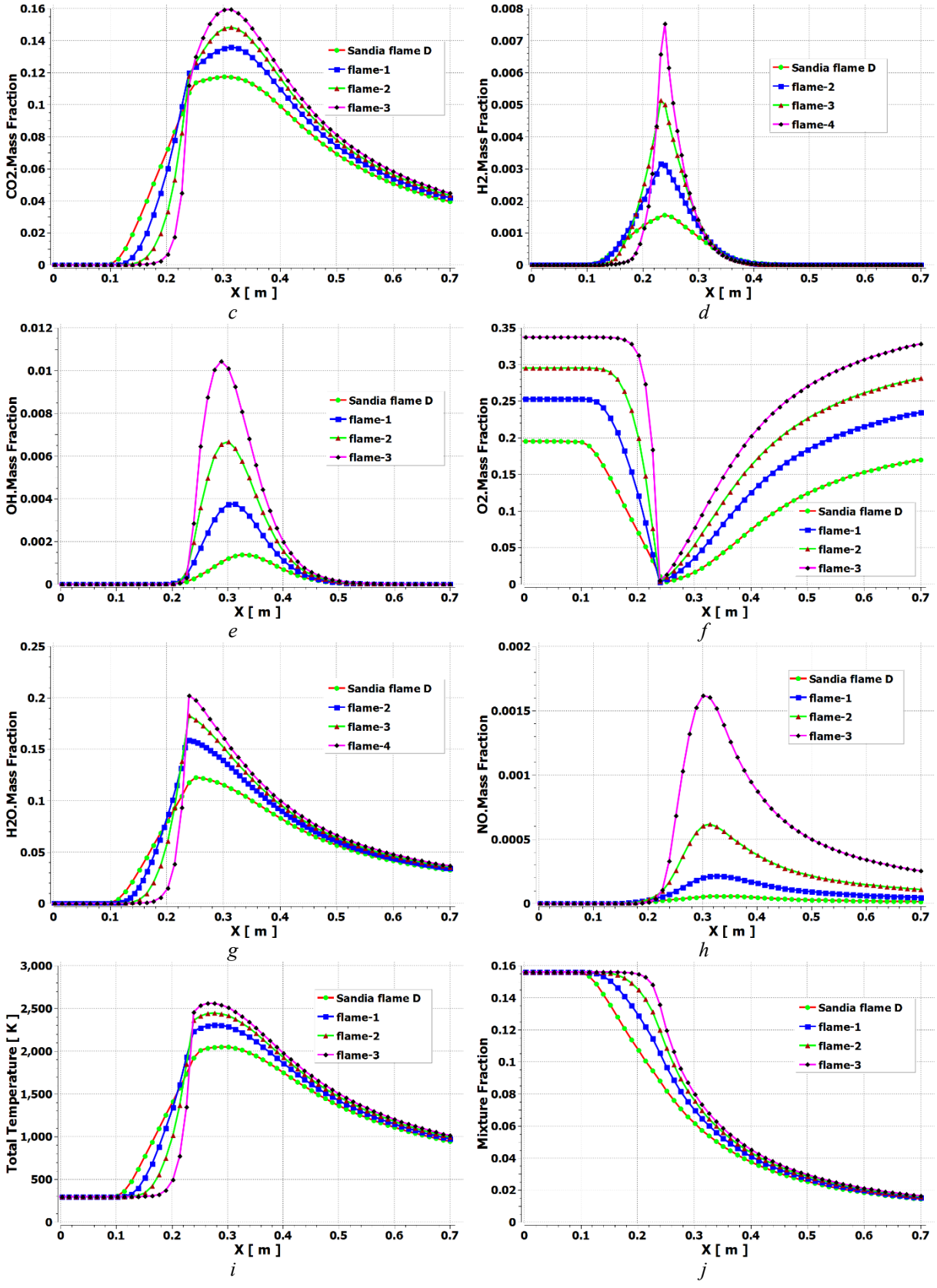
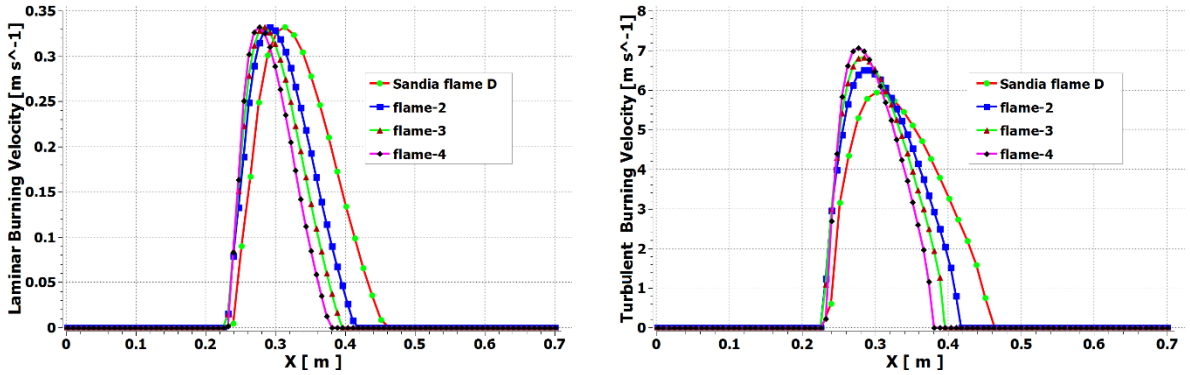
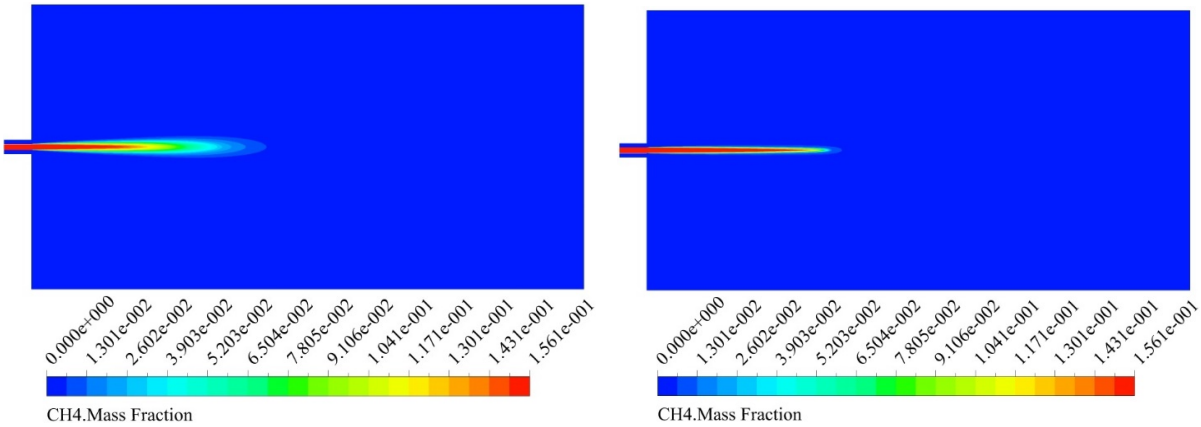



*Fig. 3 – The species mass fraction results of present simulation:*
*a – CH4; b – CO2; c – CO2; d – H2; e – OH; f – O2; g – H2O; h – NO;*
*i – total temperature; j – mixture fraction*



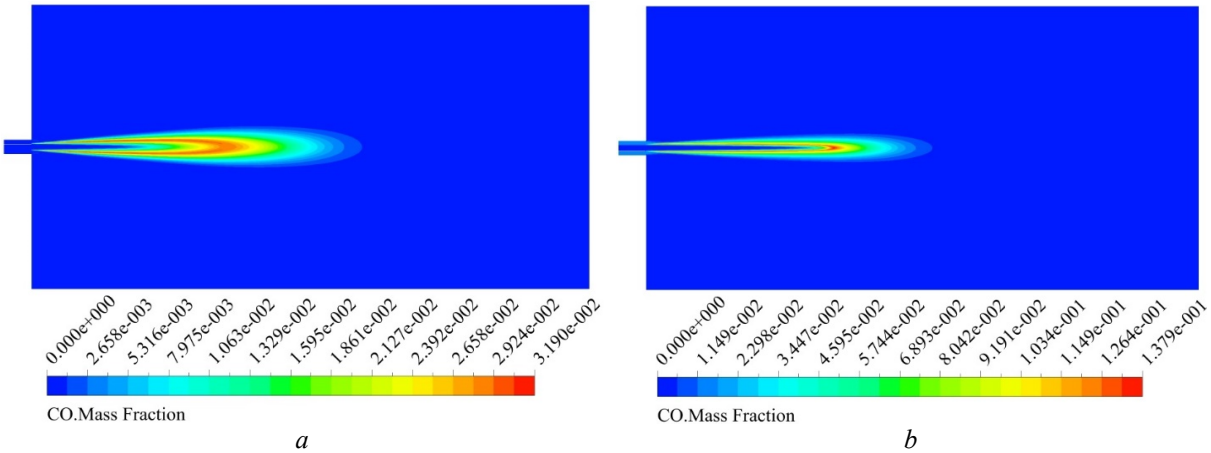

*a* *b*

*Fig. 4 – Laminar and turbulent burning velocity: a – laminar burning velocity of the simulation; b – turbulent burning velocity of simulation*




*a* *b*

*Fig. 5 – Contour plots of CH4 mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*




*a* *b*

*Fig. 6 – Contour plots of CO mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*

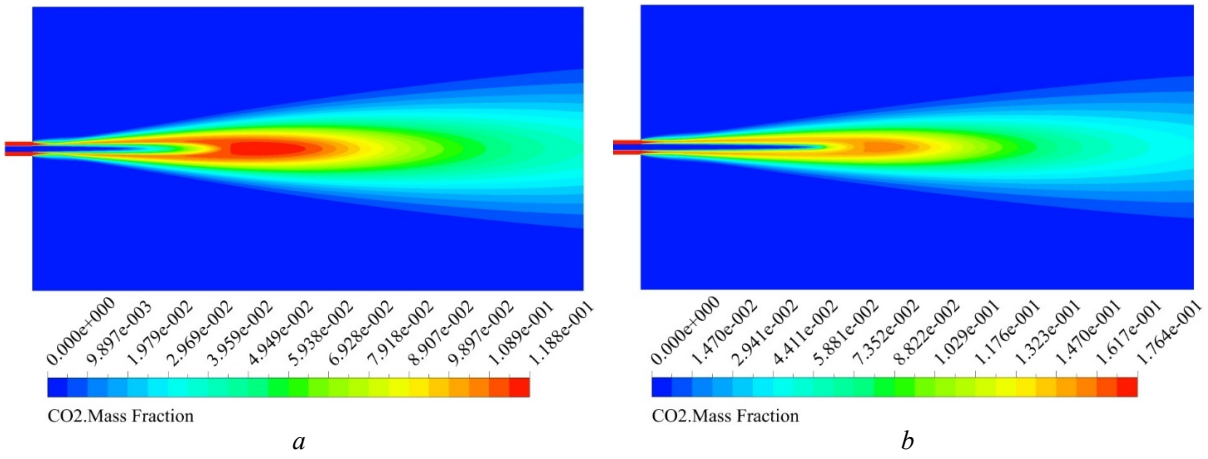



*Fig. 7 – Contour plots of CO2 mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*

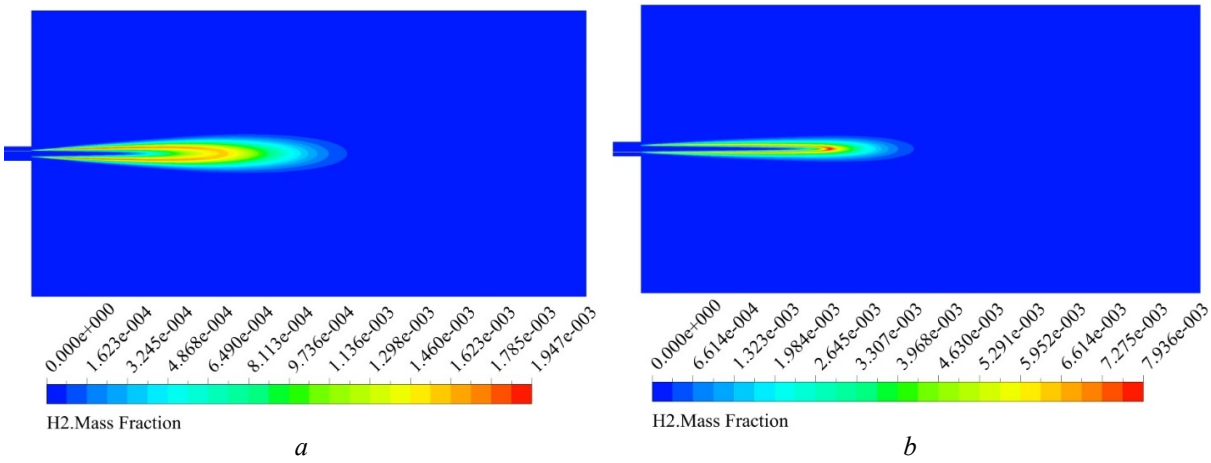



*Fig. 8 – Contour plots of H2 mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*

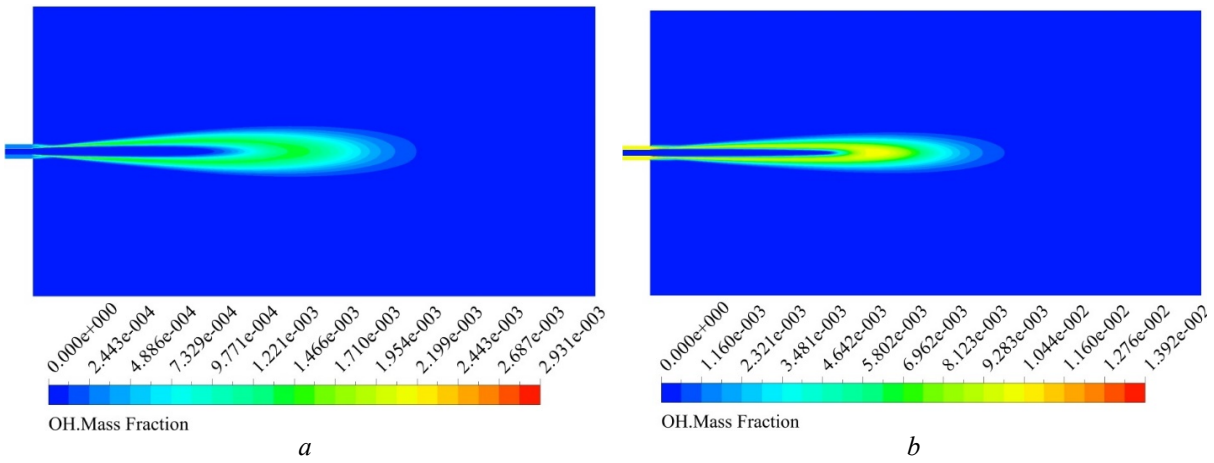
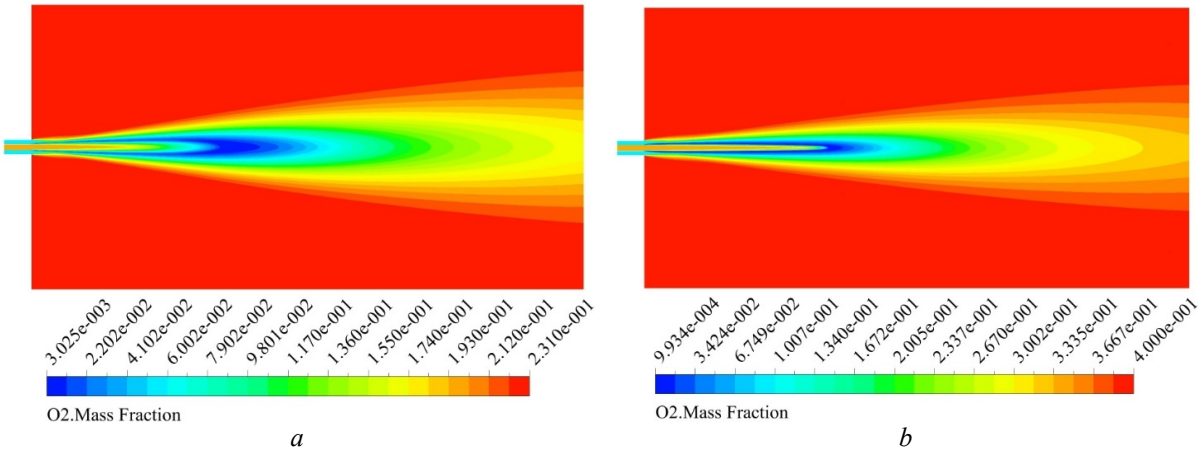
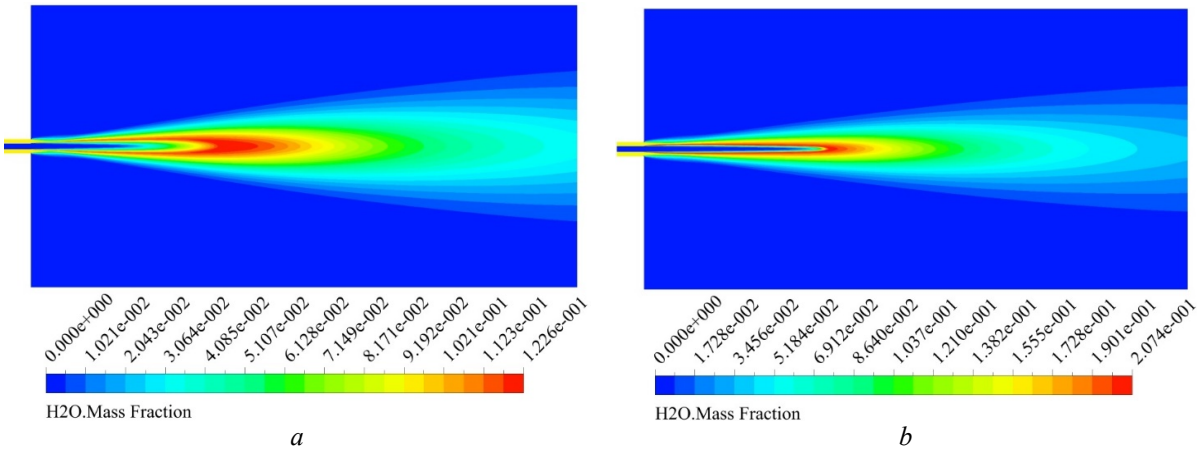



*Fig. 9 – Contour plots of OH mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*



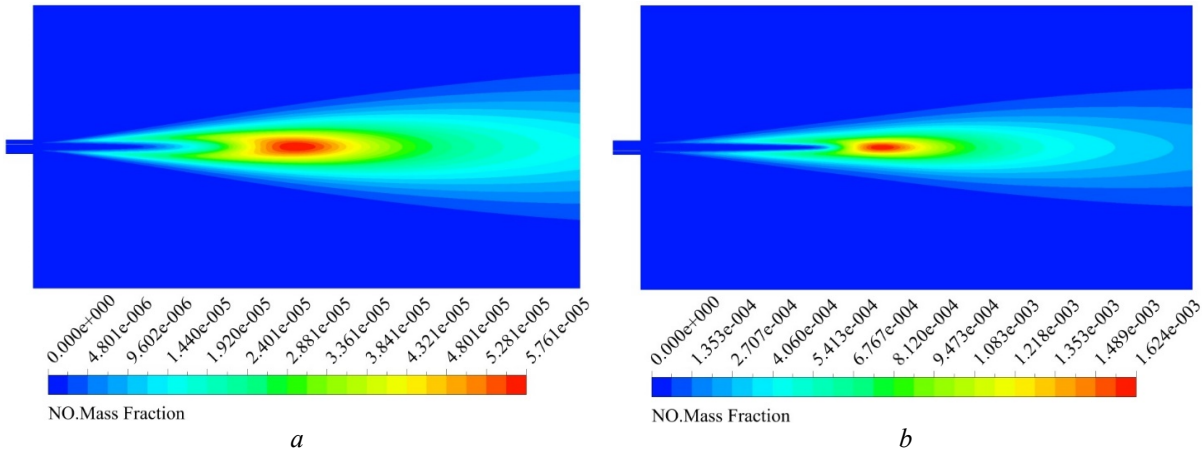

*a* *b*

*Fig. 10 – Contour plot of O2 mass fraction: a – Sandia flame D simulation; b – flame 3 simulation*



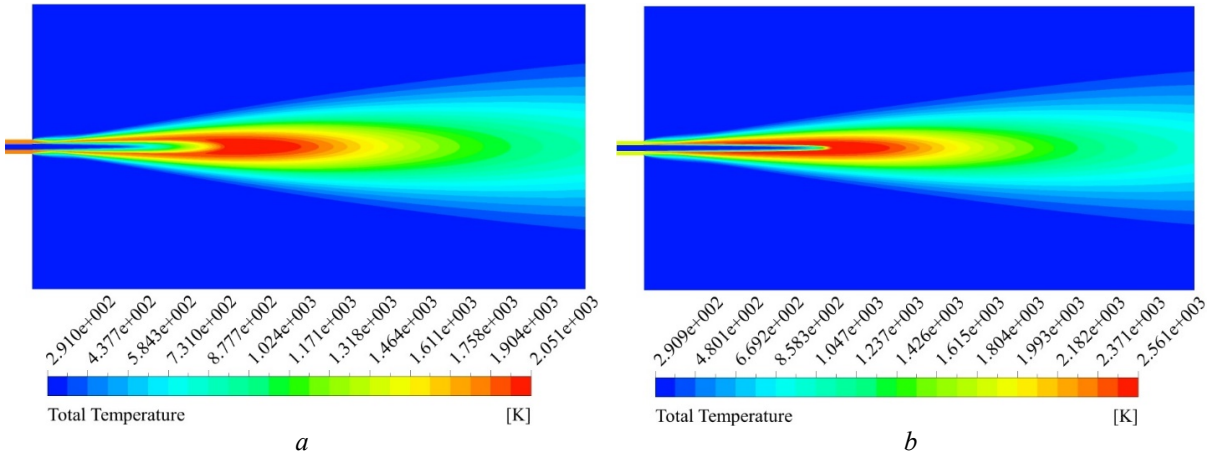

*a* *b*

*Fig. 11 – Contour plot of H2O mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*



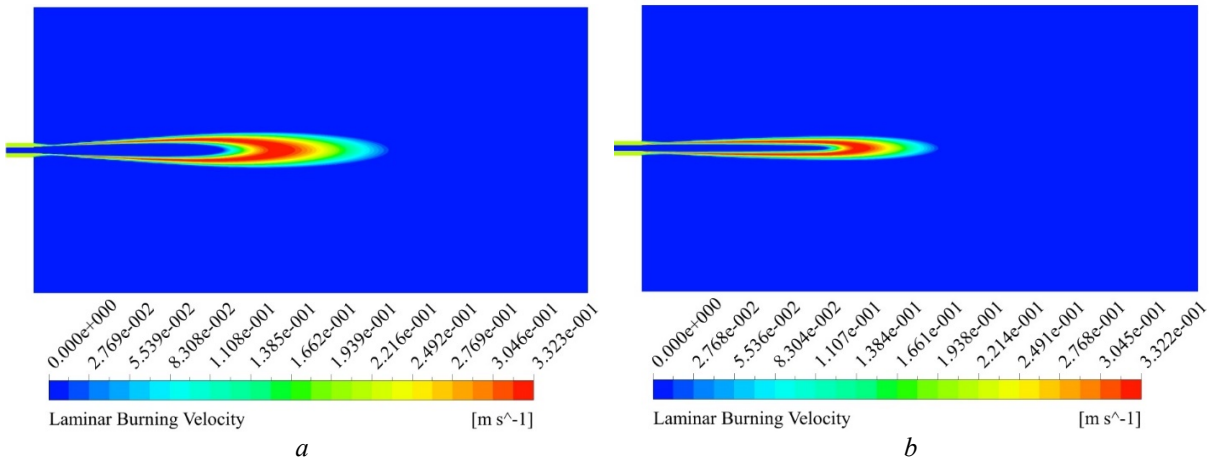

*a* *b*

*Fig. 12 – Contour plot of NO mass fraction: a – Sandia flame D simulation; b – flame-3 simulation*



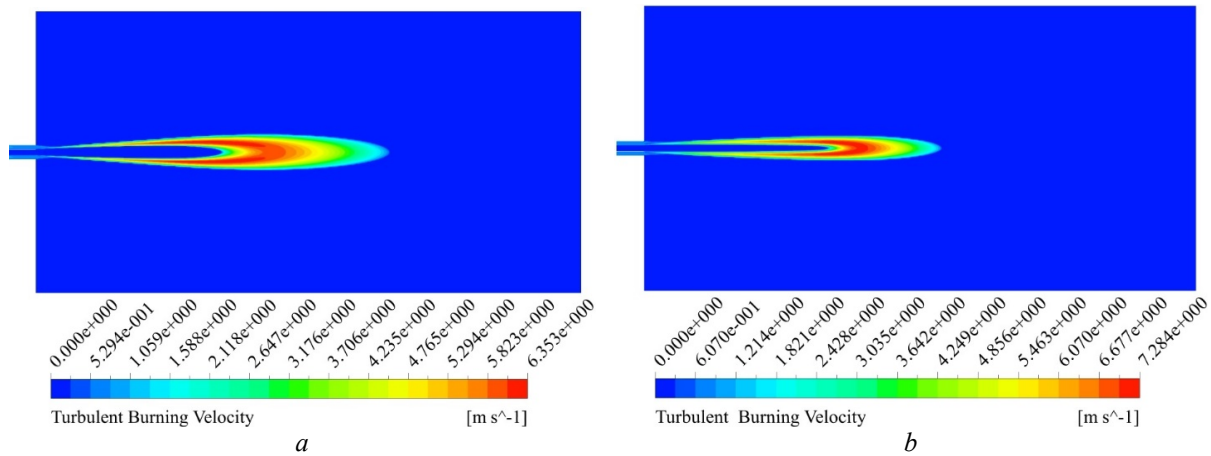

*a* *b*

*Fig. 13 – Contour plot of total temperature: a – Sandia flame D simulation; b – flame-3 simulation*




*a* *b*

*Fig. 14 – Contour plot of laminar burning velocity: a – Sandia flame D simulation; b – flame-3 simulation*




*a* *b*

*Fig. 15 – Contour plot turbulent burning velocity: a – Sandia flame D simulation; b – flame-3 simulation*

The Methane is partially-premixed with an O2+N2 mixture, which has varying volume fractions of oxygen in nitrogen. For the first case of this study (Sandia flame *D*) the volume fraction of O2 and N2 is about 21 % and 79 % and in other cases (flames) the volume fraction of O2 increase and the volume fraction of N2 decrease.

We will discuss about the maximum value of species mass fraction and temperature during the simulation of combustion process. All the discussion about the results are along the axial distance (*X* coordinate).

To compare the experimental data with the present simulation, the initial mass fraction of CH4 is 0.1561 which has the minimum value during the combustion on ($X = 0.4$ m) shown in Fig. 2*a*. While in our investigation the minimum value of CH4 for the first case (Sandia flame *D*), can be seen in ($X = 0.35$ m) shown in Fig. 3*a*. So the minimum value of CH4 mass fraction for flame 1, 2, 3 are not significant.

The experimental date for the mass fraction of CO is present in Fig. 2*b* which has the maximum value of 0.045 while the maximum mass fraction of CO in present modeling is 0.035 for the first case of Sandia flame *D* along the *X* coordinate, shown in Fig. 3*b*. With increasing the volume percentage of O2 for the flames 1, 2, 3 the mass fraction of formation of O2 will decrease too. For the flame 1, 2, 3 the maxim mass fraction of CO is 0.06, 0.092, 0.135 along the axial distance of the burner shown in Fig. 3*b*.

The maximum mass fraction of CO2 in experiments is 0.11 shown in Fig. 2*c* while for the Sandia flame *D* case in present simulation results is 0.116. For the flames 1, 2, 3 the maximum mass fraction is 0.135, 0.147, 0.16, shown in Fig. 3*c*.

The mass maximum mass fraction of H2 in experiments done by Barlow, is 0.0028 shown in Fig. 2*d*, but the maximum value of mass fraction for Sandia flame *D* simulation in this study is 0.0017 and beside that for the flames 1, 2, 3 the maximum value of them is 0.0031, 0.0051, 0.0075 shown in Fig. 3*d*.

The experimental data for the mass fraction of OH showed the maximum value of 0.0015 that we can see it Fig. 2*e* and beside that the mass fraction for the Sandia flame *D* in this simulation is 0.0017 while these values in flames 1, 2, 3 is 0.0039, 0.0065, 0.012 which has been shown in Fig. 3*e*.

The experimental data from Fig. 2*f*, and present simulation data in Fig. 3*f* about the mass fraction of O2, showed that the minimum mass fraction of O2 is located where, there is the maximum flame temperature.

The value of H2O for the experiment result is 0.115 which is presented in Fig. 2*g* while the mass fraction of H2O of this simulation for Sandia flame *D* is 0.12 and beside that the H2O mass fraction value for the flame 1, 2, 3 is 0.16, 0.18, 0.2, shown in Fig. 3*g*.

One of the most parameters in all combustion simulation is the maximum temperature and formation of NOx. Despite the reduction in nitrogen and increasing of oxygen level, the level of NO increases, mainly due to the higher flame temperatures enhancing the thermal-NO mechanism. CO levels also show an increase while CO2 on the other hand, barely seems to change with only a very small increase as the oxygen levels increase.

The simulation in this study showed that the maximum mass fraction of NO in Sandia flame *D* simulation is $5.7 \cdot 10^{-5}$ along the axial profile shown in Fig. 3*h* with the maximum total temperature of 2050 K , shown in Fig. 3*i*. Beside that the mass fraction value for the NO in other flames (1, 2, 3) shown in Fig. 3*h* are $2 \cdot 10^{-4}$, $61 \cdot 10^{-4}$, $16 \cdot 10^{-2}$ with the maximum temperature of 2307 K, 2447 K, 2560 K, shown in Fig. 3*i*. The level of NO mass fraction and total temperature in experimental data is $5 \cdot 10^{-5}$ with the maximum temperature of 1950 K which are presented in Fig. 2*h* and 2*i*. To compare experiment with the present simulation it is clear that the level of NO and total temperature are not significant.

In ANSYS CFX, in burning velocity model of premixed and partially premixed the mixture fraction value is the same the value of fuel and the value of oxidizer is he $(1 - Z)$ where $Z$ is the mixture fraction [9].

So the value of mixture fraction and CH4 are the same as 0.156. The Fig. 3*j* show the plots of changing the mixture fraction along the axial profile of burner.

**Laminar and turbulent burning velocity**

The laminar burning velocity, is a property of the combustible mixture. It is defined as the speed of the flame front relative to the fluid on the unburnt side of the flame. The burning velocity relative to the burnt fluid will be higher by a factor equal to the expansion ratio. Physically, the laminar burning velocity depends on the fuel, the equivalence ratio, the temperature of the unburnt mixture (preheating) and on pressure. Depending on the configuration in the simulation, it may be possible sometimes to neglect preheat and pressure dependencies. However, for partially premixed combustion, it is very important to account for the dependency on equivalence ratio. Specifically, the flammability limits have to be obeyed [9].

For turbulent flow, the effective or turbulent burning velocity will differ from the laminar burning velocity. Typically, turbulence will increase the burning velocity, because wrinkling of the flame front results in an increased effective flame surface. At very high turbulence, the opposite effect may occur, leading to a decrease in the effective burning velocity because of local extinction. A model is required to describe the turbulent burning velocity as a function of laminar burning velocity and turbulence quantities.

The burning velocity is defined relative to the unburnt fluid. Relative to the burnt fluid, it will be higher by a factor equal to the fluid expansion ratio [9].

The result plots of laminar and turbulent burning velocity are shown in Fig. 4*a*, *b*. For the simulation of Sandia flame *D* and the other 3 cases.

The result of simulation shows that the Laminar and turbulent burning velocity will change by reduction of N2 and increasing the level of O2. The plots in Fig. 4*a* for the modeling of Sandia flame *D*, which has the minimum level O2 shows that, the laminar velocity is about 0.32 m/s like the other 3 flames, but it has the maximum propagation to ($X = 0.45$ m) while the minimum flame propagation ($X = 0.39$ m) is for the flame 3 which has the maximum level of O2 that is 33.75 %.

The plots for turbulent burning velocity in Fig. 4*b* show that the minimum burning velocity is for the Sandia flame *D* simulation (6 m/s), with the minimum level of O2 take parting in combustion process which is 21 % with the minimum propagation along the axial profile ($X = 0.39$ m) and the maximum burning velocity is 7 m/s for the flame-3 with the 33.75 % of O2 level with maximum propagation of ($X = 45$) along the axial profile.

The contour plots of species mass fractions (CH4, CO, CO2, H2, OH, NO, O2, H2O) and total temperature field (only for the case of Sandia flame *D* and the case-3) are presented in Fig. 5 to Fig. 15 including the contours of laminar and turbulent burning velocity.

The characteristics and flame structure are different from each other in this investigation.

It is clear that with increasing the level of O2 all of the characteristic of flame change with changing of flame structure and propagation.

From The counter plots from Fig. 5 to 15, it is clear that the flame with the minimum level of O2 has the maximum flame thickness and this is for the case of Sandia flame *D* and the flame with the maximum level of O2 has the minimum flame thickness.

The laminar flame velocity is a fuel property that depends only on the chemical composition. The turbulent flame velocity depends also on the flow conditions. It represents the interaction of the flame with the turbulence.

## Conclusion

In this study all of the combustion simulations were implemented in ASNSY CFX code including laminar flamelet model with the burning velocity model (BVM) or turbulent flame closure (TFC), to simulation the partially premixed combustion of piloted CH4/O2 Sandia flame D and all of the simulation results were compared with the experimental data done by Robert Barlow .

The domain of simulation was Sandia flame D in 2D-axisymmetric with the constructed grids implementing in ICEM CFD.

The stability limits of the range of piloted turbulent partially-premixed flames of CH4/Air investigated increase almost linearly with the amount of oxygen in the fuel–O2–N2 mixture

The results of present simulation show that there is not a significant error in simulation result comparing to the experimental data but a significant change observed in the maximum mass fraction of H2 which is 0.0028 for the experimental data and 0.0017 for the present simulation.

The value of the results of this simulation implementing by the selected combustion modeling (laminal flamelet model) with detailed chemistry mechanism of 100 reactions and 28 species with burning velocity model in ANSYS CFX, are acceptable comparing to the experimental data. This means that the results in this investigation are accurate.

Beside this, the investigation showed that, with varying the level of O2/N2 (maximum level of O2 and the minimum level of N2) the formation of NO will change because of maximum and minimum flame temperature.

The higher levels of oxygen also produce an increase in CO, CO2 and NO levels due to the higher flame temperature.

As the results show, beside the laminar flamelet and burning velocity model, 2 separate step reaction of NO formation (thermal and prompt), is an accurate way for modeling nitrogen oxide formation during the combustion process.

In laminar burning velocity model of combustion for premixed and partially premixed flames, a scalar (Reaction Progress) subdivides the flow field in two different areas, the burnt and the un-burnt mixture. Burnt regions are treated similar to a diffusion flame whereas the unburnt region is represented by the cold mixture. The mass fractions in the non-reacted fraction of the fluid, Yi,fresh , are obtained by linear blending of fuel and oxidizer compositions. The species mass fractions in the burned fraction of the fluid, Yi,burned , are computed by applying the flamelet model.

A lot of further analysis can be performed in the present study as a part of future work such as use different turbulence model and their effect on combustion process and species mass fraction or formation of NO and the characteristics of the flame such as flame thickness or propagation.

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***АНОТАЦІЯ*** *В даному дослідженні представлено чисельне моделювання горіння попередньо частково перемішаної метано-повітряної суміші з різними об'ємними частками $O_2$ і $N_2$. Турбулентність і горіння змодельовані за допомогою стандартної k–ε моделі турбулентності і моделі швидкості розповсюдження полум'я, яка відома також як модель змикання турбулентного полум'я і використовується для ламінарного полум'я з докладним описом хімічних реакцій. Основною метою даного дослідження є прогнозування впливу різного процентного співвідношення $O_2$ і $N_2$ на характеристики турбулентного полум'я та утворення шкідливих речовин і емісію. Розрахунки проведені за допомогою ANSYS CFX.*

***Ключові слова:*** *Sandia flame-ламінарне полум'я, емісія, швидкість поширення полум'я, горіння попередньо частково перемішаної суміші.*

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