

Effect of the Variation of the Mixing Coefficient on a Turbulent Confined Flame (CH₄/Air).

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Abstract. In combustion computational analysis, reduced mechanisms are often used in place of detailed kinetic chemistry. In this study we employed ANSYS Fluent Computational Fluid Dynamics (CFD) package, to analyze methane oxidation mechanism in a coaxial burner. The $k-\varepsilon$ scheme was used to model the effects of turbulence. The reaction kinetics employed in this study is that based on the work of Jones and Lindstedt [14]. This simplified model consists of 4 chemical reactions and 7 species, namely, CH₄, CO₂, CO, H₂O, O₂, H₂ and N₂. The focus is on assessing the performance of the Eddy Dissipation Model (EDM) in combination with two-equation turbulence models ($k-\varepsilon$) and chemical kinetics schemes by comparing predictions with experimental measurements.

Keywords : Combustion, Simulation, Fluent software, EDM mode, Co-flow

1. Introduction

Computational models can help predicting flame composition, regions of high and low temperature inside the burner, and detailed composition of exit byproducts. Detailed computational results can also help better predict the chemical structure of flames and understand flame stabilization processes. These capabilities make Computational Fluid Dynamics (CFD) an excellent tool to complement experimental methods for understanding combustion and thus help in designing and choosing better fuel composition according to the specific needs of a burner. With the advent of more and more powerful computing resources, better algorithms, and the numerous other computational tools in the last couple of decades, CFD has evolved as a powerful tool to study and analyze combustion. However, numerous challenges are involved in making CFD a reliable and robust tool for design and engineering purposes.

The numerical simulation is a useful tool because it can easily apply various conditions by simply changing the parameters. Methane is the simplest hydrocarbon fuel available; several studies have focused on methane-air flames.

The oxidation of methane is quite well understood and various detailed reaction mechanisms are reported in literature [1]. They can be divided into full mechanisms, skeletal mechanisms, and reduced mechanisms. The various mechanisms differ with respect to the considered species and reactions. However, considering the uncertainties and simplifications included in a turbulent flame calculation, the various mechanisms agree reasonably well [2]. In literature, several mechanisms of methane combustion are available.

We can cite: for detailed mechanisms: Westbrook [3], Glarborg *et al.* [4], Miller and Bowman [5], and recently, Konnov v.0.5 [6], Huges *et al.* [7], LCSR [8], Leeds v.1.5 [9], CERMECH [10] and the standard GRI-Mech v.3.0 [11], GRI-Mech v.1.2 [12] for reduced mechanisms: Westbrook and Dryer [13], and Jones and Lindstedt [14] (more than 2 global reaction). For skeletal mechanisms: Kazakov and Frenklach [15], Yungster and Rabinowitz [16], Petersen and Hanson [17], Hyer *et al.* [18] and Li and Williams [19].

The present investigation focuses on the simulation of turbulent confined diffusion jet flame (Natural-gas) with a fuel inlet velocity of 21.3 m/s. The reduced chemical kinetics scheme of Jones and Lindstedt [14] was used to describe the combustion process in terms of 7 species (CH₄, H₂, CO, CO₂, H₂O, O₂, and N₂ as inert) using the commercial code ANSYS FLUENT v12. Some modifications of the usually adopted models for the representation of the turbulence-kinetics interaction are introduced.

2. Problem Description

Experimental results of the turbulent jet flame are reported by Lewis and Smoot [20]. The geometrical configuration of the burner for predicted (Natural-gas/Air) turbulent combustion is that reported in Figure 1. The combustor is oriented vertically to minimize three-dimensional effects. The geometry for this test is a cylindrical combustor with coaxial injectors, where the natural gas is injected by the primary tube and the air through the secondary annulus, as shown in figure 1. The total pressure of the combustor is 94 KPa. In the fuel stream, the uniform inlet gas velocity is 21.3 m/s and the flow rate is 2.982 g/s, with a temperature of 300K. In the air stream, the uniform inlet air velocity is 29.9 m/s and the flow rate is 36.3 g/s, with a preheated temperature of 589 K.

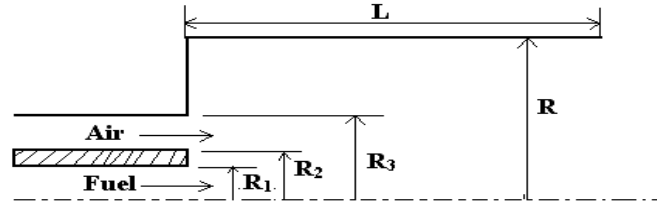


Fig. 1. Sketch of the computational domain [20].
 ($R_1=0.8\text{cm}$, $R_2=1.11\text{cm}$, $R_3=2.86\text{cm}$, $R= 10.16\text{cm}$, $L=1.525\text{m}$)

3. Turbulence model

The $k-\varepsilon$ model is one of the most widely-used turbulence models. This model also employs the Boussinesq approximation and includes two additional partial differential transport equations : one for the turbulent kinetic energy, k , and one for the dissipation, ε . In this paper we opt for the choice of the standard $k-\varepsilon$ model for its robustness, economy, and reasonable accuracy for a wide range of turbulent flows. In the $k-\varepsilon$ model, the Reynolds stress is closed using mean velocity gradient employing Boussinesq hypothesis as follows:

$$-\overline{\rho u_i u_j} = \mu_t \left(\frac{\partial \tilde{U}_i}{\partial x_j} + \frac{\partial \tilde{U}_j}{\partial x_i} \right) - \frac{2}{3} \left(\overline{\rho k} + \mu_t \frac{\partial \tilde{U}_k}{\partial x_k} \right) \quad (1)$$

Where the turbulent eddy viscosity is calculated by combining k and ε as follows :

$$\mu_t = \overline{\rho} C_\mu \frac{\tilde{k}^2}{\tilde{\varepsilon}} \quad (2)$$

In the case of a jet flame, a correction is necessary to accurately predict the spreading rate of the jet. This is performed by using the Pope correction, P_{pc} , as an additional term in the equation of turbulence dissipation rate (ε):

$$P_{PC} = \overline{\rho} C_{\varepsilon 3} \frac{\varepsilon^2}{k} S_\varepsilon \quad (3)$$

The term S_ε can be written as $S_\varepsilon = \omega_{ij} \omega_{jk} S_{ij}$ (Pope [21]), Where:

$$S_{ij} = \frac{1}{2} \frac{k}{\varepsilon} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (4)$$

$$\omega_{ij} = \frac{1}{2} \frac{k}{\varepsilon} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \quad (5)$$

As an option in the formulation of the $k-\varepsilon$ model, enhanced wall functions are selected in accordance with the grid design. This option ensures that appropriate modeling occurred to resolve the viscous sub-layer. Further definition of the $k-\varepsilon$ model utilizes the default ANSYS Fluent model constants:

$C_{\varepsilon 1} = 1.44$; $C_{\varepsilon 2} = 1.92$, $C_{\varepsilon 3} = 0.79$, $\sigma_k = 1$; $\sigma_\varepsilon = 1.3$ and $C_\mu = 0.09$

4. Chemical model

The reaction mechanism adopted in this work contains 7 chemical species and 4 reactions of Jones and Lindstedt (Table 1). The formation of NO_x is not taken into account. This mechanism was successfully utilized, in previous work [1].

Table 1: Jones and Lindstedt Reduced Multi-Step Chemical Kinetics Mechanism for CH₄/Air combustion and reaction rate coefficients [14].

No.	reaction	A_k (cgs units)	β_k	E_k (cal/mol)	Reaction orders
JL1	CH ₄ +0.5O ₂ → CO+2H ₂	7.82e+13	0	30.0e+03	[CH ₄] ^{0.5} [O ₂] ^{1.25}
JL2	CH ₄ +H ₂ O → CO+3H ₂	3.0e+11	0	30.0e+03	[CH ₄][H ₂ O]
JL3	H ₂ +0.5O ₂ → H ₂ O	1.21e+18	-1	40.0e+03	[H ₂] ^{0.25} [O ₂] ^{1.5}
JL4	CO+H ₂ O → CO ₂ +H ₂	2.75e+12	0	20.0e+03	[CO][H ₂ O]

5. Eddy Dissipation Model

Most fuels are fast burning, and the overall rate of reaction is controlled by turbulent mixing. In non-premixed flames, turbulence slowly convects/mixes fuel and oxidizer into the reaction zones where they burn quickly. In premixed flames, the turbulence slowly convects/mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly. In such cases, the combustion is said to be mixing-limited, and the complex and often unknown, chemical kinetic rates can be safely neglected. Fluent provides a turbulence-chemistry interaction model, based on the work of Magnussen and Hjertager [22], called the eddy-dissipation model. The net rate of production of species *i* due to reaction *r*, $R_{i,r}$, is given by the smaller (i.e., limiting value) of the two equations below:

$$R_i = \nu'_{i,k} M_i A \rho \frac{\varepsilon}{k} \left(\frac{Y_R}{\nu'_{R,k} M_R} \right) \quad (6)$$

$$R_i = \nu'_{i,k} M_i A B \rho \frac{\varepsilon}{k} \left(\frac{\sum_P Y_P}{\sum'_j \nu''_{j,k} M_j} \right) \quad (7)$$

Where

A is an empirical constant equal to 4.0;

B is an empirical constant equal to 0.5;

M is a molecular weight

Y_P is the mass fraction of any product species, *P*;

Y_R is the mass fraction of a particular reactant, *R*;

ε is the turbulent dissipation rate (m²s⁻³);

K is the turbulent kinetic energy per unit mass (J/kg).

ν'_i, ν''_j is the stoichiometric coefficient for reactant *i* and product *j* in reaction

6. Simulation approach

The governing equations are solved using the Fluent CFD package modified with User Defined Functions in order to integrate the reaction rate formula proposed by Jones and Lindstedt [14]. Fluent was utilized because of its ability to couple chemical kinetics and fluid dynamics. In CFD, the differential equations governing the problem are discretized into finite volume and then solved using algebraic approximations of differential equations. These numerical approximations of the solution are then iterated until adequate flow convergence is reached. The SIPMLE algorithm [23] was chosen for the coupling between the velocity and the pressure. For all simulations presented in this paper, a First Order Upwind scheme was used for the conservation equation of momentum, turbulent kinetic energy, turbulent dissipation rate, mean mixture fraction. The Standard scheme [23] is used for interpolation methods for pressure. This means that the solution approximation in each finite volume was assumed to be linear. This saved on computational expense. In order to properly justify using a first order scheme, it was necessary to show that the grid used in this work had adequate resolution to accurately capture the physics occurring within the domain. In other words, the results needed to be independent of the grid resolution. This was verified by running simulations with higher resolution grids. In a reacting flow such as that studied in this work, there are significant time scale differences between the general flow characteristics and the chemical reactions. The criterion of convergence is the summation of residual mass sources less than 10⁻³ for the other terms of the transport equations and is 10⁻⁶ for energy equation. The computational space seen in Fig. 1 given a finite volume mesh is divided by a staggered non-uniform quadrilateral cell (Fig. 2). A total number of 5600

quadrilateral cells were generated using non-uniform grid spacing to provide an adequate resolution near the jet axis and close to the burner where gradients were large. The grid spacing increased in the radial and axial directions since gradients were small in the far-field. The combustion will be modeled using reduced 4-step reaction mechanism scheme and the radiative heat transfer of the diffusion flame is calculated with the P1 model [23]. The density is obtained from the ideal gas law. The interaction between turbulence and chemistry is often handled through the Eddy-Dissipation Model EDM. The controlling rate is assumed the slower between the kinetic values and turbulent mixing rate. The specific heat values for the species are defined as piecewise-polynomial function of temperature. The options used in this work are presented in tables 2 and 3.

Tab.2. Under-relaxation factors.

Pressure	0.3
Density	0.5
Body forces	1
Momentum	0.7
Turbulent viscosity	1
Y_i	0.9
Energy	0.4
Turbulent kinetic energy 'k'	0.8
Turbulent dissipation rate 'ε'	0.8
Radiation model 'P1'	0.8

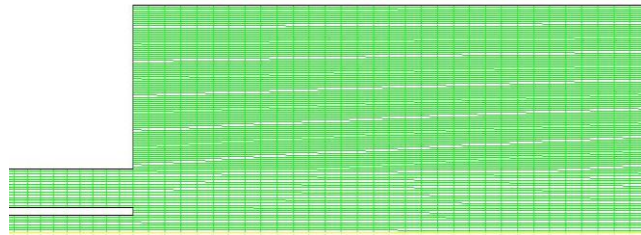


Fig.2. Mesh of combustion chamber.

Tab.3. Discretization and computational model step.

Solver Type	Pressure Based
Viscous Model	Turbulent (k-ε model)
Gravitational Effect	On
2D-Space	Axisymmetric
Pressure-Velocity Coupling	SIMPLE
Pressure	Standard
Momentum Equations Discretization	First Order Upwind
Species Equations Discretization	First Order Upwind
Energy Equations Discretization	First Order Upwind
Turbulent kinetic Energy	First Order Upwind
Turbulent Dissipation Rate	First Order Upwind

7. Results

7.1. Validation model

In this section, we present simulations results and compare with the experimental data. The simulations are done using standard k-ε model and Eddy Dissipation Model (EDM) with Jones and Lindstedt chemical oxidation mechanism of methane. The Reduced mechanism of Hyer was previously validated on the base of Non-Premixed flames. Then, the mechanism implemented into the CFD code ANSYS-Fluent, using the method of directed relation graph and Quasi Steady State Assumption [21]. The mechanism was incorporated into the Fluent by the means of a user defined function that uses the subroutine (Define-Net-Reaction-Rates) to compute the species reaction rates which are fed into the turbulence-combustion model [21]. The FORTRAN subroutine is linked to Fluent through the (DNRR) argument macro. This macro is called by the EDM model and is used to compute the closed turbulent species reaction rates. The EDM uses the FORTRAN reaction rates as an input to the turbulent reaction rates. In this manner, the UDF is a complement to the EDM model and does not bypass the EDM model. Once the reduced mechanism is constructed and executed, the subroutine that computes the chemical source terms is automatically generated. A coupled set of nonlinear Quasi Steady State species equations are numerically solved within the subroutine to provide the necessary elementary reaction rates for the reduced mechanism. This subroutine which is compatible with FLUENT is specified in the user defined function and returns the molar production rates of the species given the pressure, temperature, and mass fractions [21]. The under-relaxation factors are

different for different variables varying from 0.45 to 0.8. The energy equation is very difficult to converge, so the factor is taken as 0.45. The inlet turbulent specification method is ‘intensity and length scale’. Turbulence intensity is 10% and turbulence length scales are 0.008m for fuel and 0.0175 m for air. Radial composition profiles for CH₄, CO₂ and Temperature (K) at several axial locations (x = 10, 25 and 50 cm) are shown in Figures 3 to 5 and the test results of Lewis and Smoot [22] are also shown. Those figures show that the calculated results are in good agreement with experimental data.

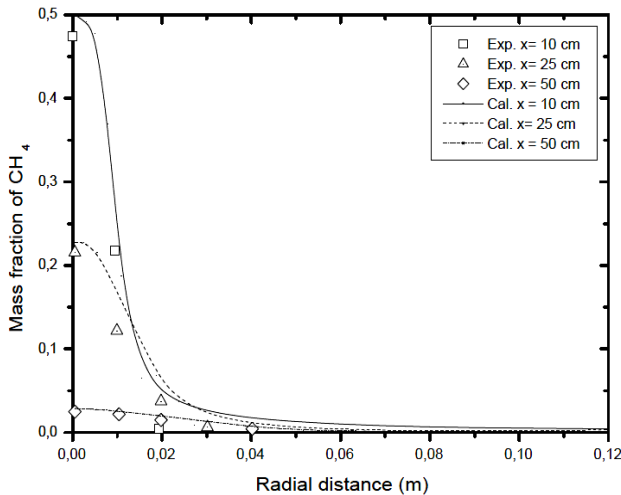


Fig.3. Radial CH₄ mole fraction profiles at several axial locations.

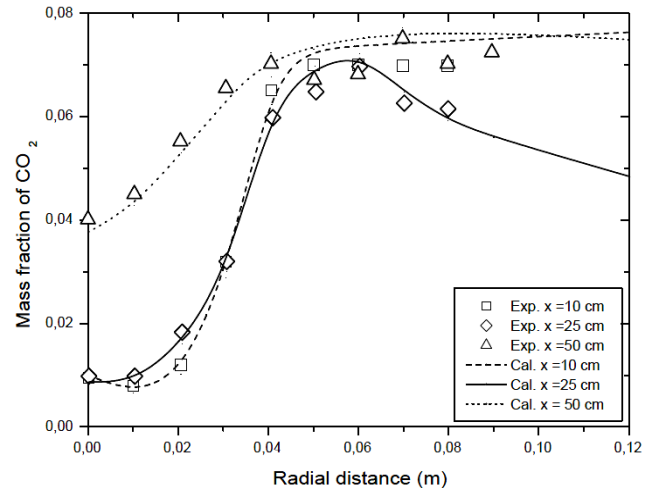


Fig.4. Radial CO₂ mole fraction profiles at several axial locations.

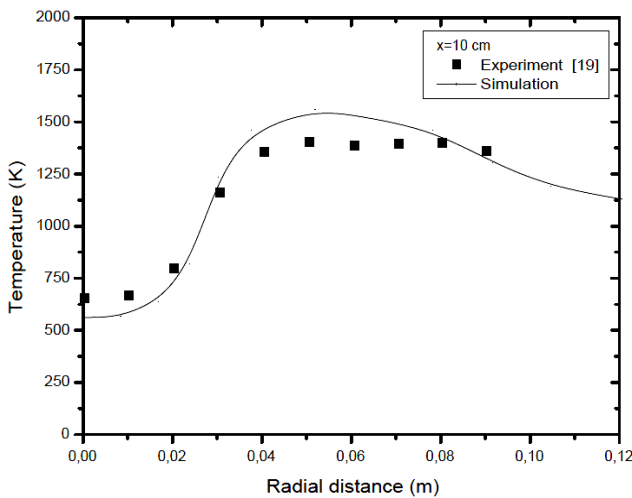


Fig.5. Temperature profile at x=10 cm.

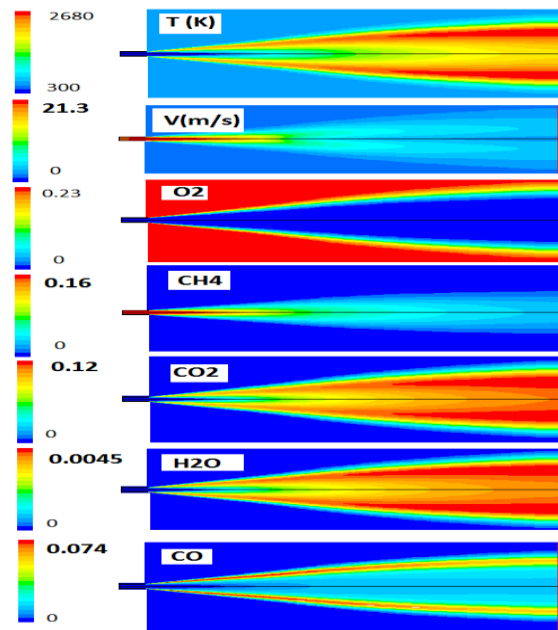


Fig. 6. Results of Non-Premixed CH₄-air flame using a Jones and Lindstedt reduced mechanism.

7.2. Effect the Mixing Coefficient (A and B)

In section 5, we introduced the standard scheme where eddy dissipation model (EDM) is used and the coefficients *A* and *B* were equal to 4 and 0.5 respectively that Magnussen and Hjertager [20]. In general, mixing plays a more important role than chemical reaction in turbulent flows. It is worth research in the effect on chemical species and temperature with different values of the coefficient, the use different *A* and *B*

values, double or half of normal value at different locations ($x=9.5, 24.6, 47.6$ and 78.5 cm). The detailed values are seen in Table 4.

Tab.4. The coefficients for different schemes.

Schs.	1	2	3	4	5	6	7	8	9
A	4	8	4	8	2	4	2	8	2
B	0.5	0.5	1	1	0.5	0.25	0.25	0.25	1

It is noticed that the largest flame is predicted by the 4-step scheme (Figure 6). It is observed that the predicted maximum temperature calculated for the turbulent diffusion flame using the J-L chemical kinetic mechanism 2680 K. In the 4-step mechanism, more reaction equations are computed, them more CPU time is spent and more difficult it is to convergence. The calculated results are shown in figures 7 to 9. It is seen that the distribution of CH_4 does not changed with the change of coefficients. The different schemes provide the satisfactory prediction for O_2 and CO_2 . For H_2O , increasing A and B is better than decreasing in general, the various effects of changing coefficient A and B must be considered, current values of A and B are acceptable.

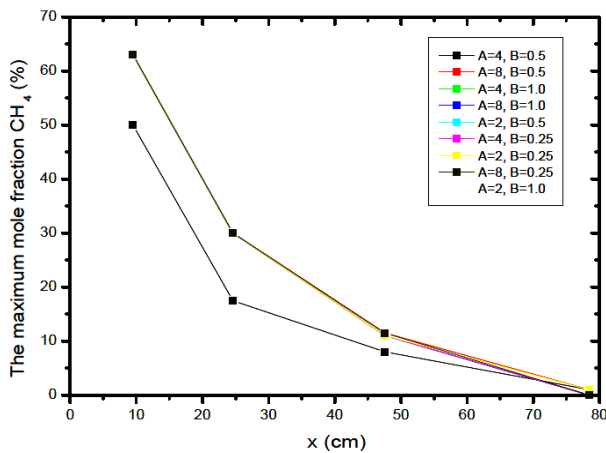


Fig.6. The maximum % CH_4 at different locations with different schemes.

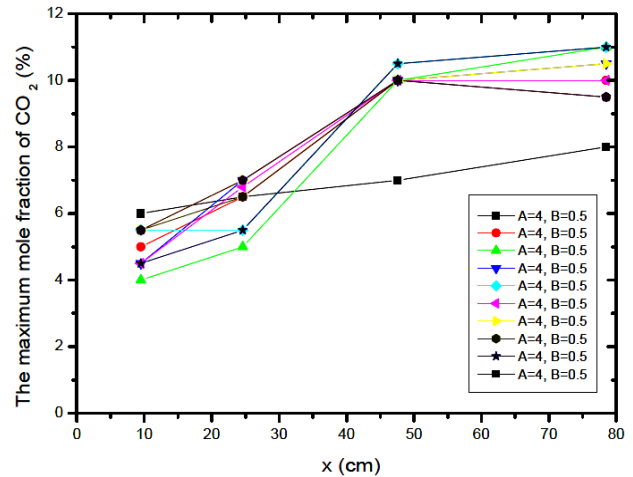


Fig.7. The maximum % CO_2 at different locations with different schemes.

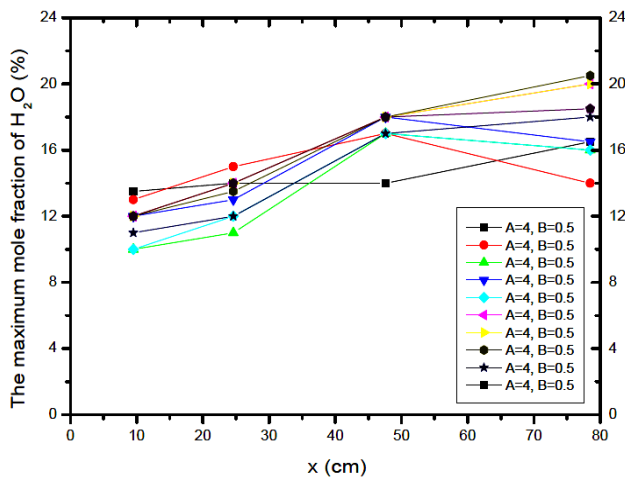


Fig.8. The maximum % H_2O at different locations with different schemes.

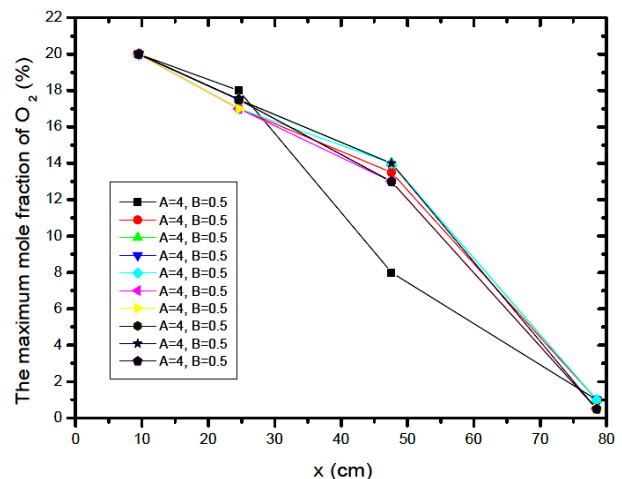


Fig.9. The maximum % O_2 at different locations with different schemes.

Conclusion

The following conclusions are obtained:

1. The 4-step reduced mechanism of Jones and Lindstedt was successfully implemented into the CFD solver Fluent. The precompiled mechanism was linked to the solver by the means of User Defined Function (UDF). This implemented was tested with the Lewis and Smoot (Natural-gaz) flame.
2. In general, mixing plays a more important role than chemical reaction in turbulent flow. The change in the coefficients A and B is better than decreasing A and B.

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References

- [1] Guessab A., Ais A., Bounif A., Gokalp I., Numerical Analysis of Confined Laminar Diffusion Flame: Effects of Chemical kinetic Mechanisms. International Journal of Advanced Research in Engineering and Technology (IJARET). Volume4, Issue 1, Januray 2013, pp.59-78. www.iaeme.com
- [2] Davidenko D. M., Gökalp I., Dufour E., Magre P. (2005) Numerical simulation of supersonic combustion with CH₄-H₂ fuel, *European Conference for Aerospace Sciences (EUCASS)*, Moscow, Russia, 4-7 July.
- [3] Westbrook, C. K., Applying Chemical Kinetics to Natural Gas Combustion Problems, Report No. PB-86-168770/XAB, Lawrence Livermore National Laboratory, Livermore, Cal., USA, (1985).
- [4] Glarborg, P., Miller, J. A., Kee, R. J., Kinetic Modeling and Sensitivity Anal y sis of Nitrogen Oxide or mation in Well Stirred Reactors, *Combustion and Flame*, 65 (1986), 2, pp. 177-202
- [5] Miller, J. A., Bow man, C. T., Mechanism and Modeling of Nitrogen Chemistry in Combustion, *Progress in Energy and Combustion Sciences*, 15 (1989), 4, pp. 287-338.
- [6] Konnov, A. A., De tailed Reaction Mechanism for Small Hydrocarbons Combustion, (2000) Release 0.5, <http://homepages.vub.ac.be/~akonnov/>
- [7] Huges, K. J., *et. al.*, Development and Testing of a Comprehensive Chemical Mechanism for the Oxidation of Methane, *International Journal of Chemical Kinetics*, 33 (2001), 9, pp. 515-538.
- [8] Dagaut P. (2002), on the kinetics of hydrocarbon oxidation from natural gas to kerosene and diesel fuel, *Phys. Chem. Chem. Phys.*, Vol. 4, p. 2079–2094.
- [9] The Leeds methane oxidation mechanism, <http://www.chem.leeds.ac.uk/Combustion/methane.htm>.
- [10] <http://maemail.ucsd.edu/~combustion/cermech/olderversions/sandiego20030830/>
- [11] GRI-Mech v.3.0, http://www.me.berkeley.edu/gri_mech.
- [12] GRI-Mech v.1.2, http://www.me.berkeley.edu/gri_mech.
- [13] Westbrook, C. K., Dryer, F. L., Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames, *Combustion Sciences and Technologies*, 27(1981), 1-2, pp. 31-43.
- [14] Jones, W. P., Lindstedt, R. P., Global Reaction Schemes for Hydrocarbon Combustion, *Combustion and Flame*, 73 (1988), 3, pp. 233-249.
- [15] Kazakov A., Frenklach M., Reduced Reaction Sets based on GRI-Mech 1.2, <http://www.me.berkeley.edu/drm/>
- [16] Yungster S., Rabinowitz M. J. (1994), Computation of shock-induced combustion using a detailed methane-air mechanism, *Journal of Propulsion and Power*, Vol. 10, No. 5, p. 609-617.
- [17] Petersen E. L., Hanson R. K. (1999), Reduced kinetics mechanisms for ram accelerator combustion, *Journal of Propulsion and Power*, Vol. 15, No. 4, p. 591-600.
- [18] Hyer P., Stocker D. and Clar I.O., Gravitational Effects on Laminar Diffusion Flames, *Creare. X Users' Group Meeting Proceedings*, pp. 345-372, 1991.
- [19] Li S. C., Williams F. A. (2002), Reaction mechanisms for methane ignition, *Journal of Engineering for Gas Turbines andPower*, Vol. 124, p. 471-480.



- [20] Lewis M.H. and Smoot L.D., Turbulent Gaseous Part I: Theory and Local Species Concentration Measurements, J. of Propulsion and Power, Vol. 42, pp. 183-196, 2001.
- [21] Pope S. B. (1978). An explanation of the turbulent round/plane jet anomaly, AIAA Journal, Vol. 16, No. 3, p. 279-281.
- [22] Magnussen B, Hjertager BH (1976) *16th symposium (int.) on combustion*, 719-729, The Combustion Institute, Pittsburgh.
- [23] FLUENT. 2009. "Theory Guide: Release 12.0." Last modified January 23, 2009.