Numerical Simulation of a Turbulent Diffusion Flame

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1 Abstract

In this paper, we have numerically investigated the properties of a diffusion turbulent flame inside a model combustor. Our aim is to compare different numerical methods with the results from experimental data to understand the underlying physics of turbulent diffusion flames. We have first simulated non-reactive flow of air inside a pipe to appreciate the properties of the turbulence independent of combustion. We have then extended the problem to a reactive flow, in which a non-premixed turbulent diffusion flame is formed. It is found that the "species transport" and the "$K-\varepsilon$" are the best models to resemble combustion and turbulent processes, respectively, through comparison to experimental data. The accuracy of the results compared to the experimental data indicates the correctness of the models and the simulation used, which was not acquired with any of the recently done researches.

2 Introduction

Combustion theory is widely used in industrial applications. It has been analyzed extensively by scientists around the world both experimentally and numerically. One of the most noted areas of combustion theory is the diffusion flames. The complicated nature of these flames requires a vast knowledge of fluid mechanics. This complexity is even magnified for the case of turbulent diffusion flames which is usually the case. The solution of these complicated equations is usually obtained numerically, since the analytical solution of these equations is impossible, and the experimental investigation of combustion phenomena is usually destructive and costly. One of the available codes for general purpose fluid simulation is FLUENT, which has been extensively used to investigate combustion problems. The numerical simulation of turbulent diffusion non-premixed flames has been well studied recently. The physical upwinding scheme was first introduced by Schneider and Raw [9]. However, this formulation was encountered with some shortcomings and inabilities in some cases. Those shortcomings were resolved by introducing a second category of velocity components at the cell faces. To enhance the capabilities of their method, they employed the physical upwinding scheme to derive not only the original cell face velocities but also the second of cell face velocities; however, in a two-dimensional domain, Darbandi, et al. [2] extended the two-dimensional physical upwinding scheme to a treatment in the cylindrical coordinates. They solved laminar diffusion flame to evaluate the performance of the extended formulation.

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Most of these simulations are not very accurate and are in bad agreement with experimental data of Smoot and Lewis [6]. A correct numerical simulation is, thus, necessary to be acquired and to be compared with those of experimental. We have investigated the solution of the conventional problem defined by Smoot and Lewis [6] using FLUENT. The simulation is done for two major problems, namely turbulent non-reactive flow in a long axisymmetric pipe and reactive diffusion non-premixed flame in a model combustor. We have performed grid independency check for each and every one of the problems to ensure enough grid resolution. The simulation is done until full convergence is reached. The results are given in the form of diagrams of velocity profiles and mixture fraction. Some useful concluding remarks are reached at the end of the project about the overall simulation.

3 Formulation, simulation, and discussion of results

3.1 Turbulent non-reactive flow inside a circular pipe

The Reynolds number of the turbulent flow inside the axisymmetric pipe is assumed to be 1.1×10^5. This Reynolds number is obtained by the conventional relation $R_e = uD/\nu$. According to this Reynolds number, the inflow velocity to a pipe of length $50m$ and diameter of 1 m would be $1.0m/s$. (See figure (1))

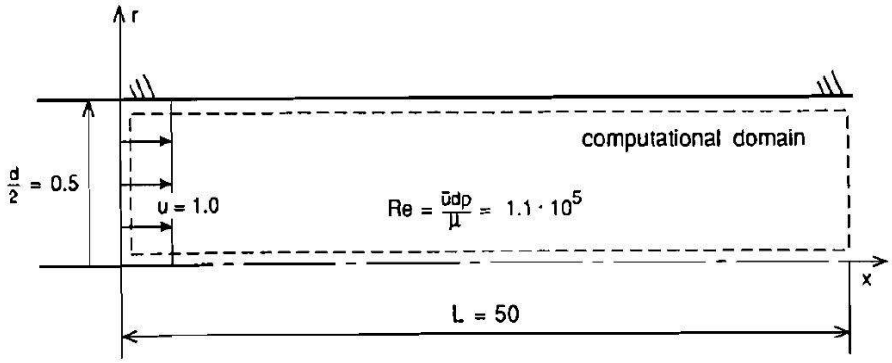

Figure 1: Geometrical and inflow properties of the non-reactive pipe flow.

We have used the $K-\varepsilon$ turbulence model to simulate the flow inside the pipe, which is used in the standard form. We have used standard wall functions for near wall flow simulations. For solving the governing equations, implicit formulations with steady state and axisymmetric assumptions are used. The implicit formulation is used here because it guarantees better stability. The use of axisymmetric 2-dimentional space instead of 3-dimensional spaces has significantly reduced the computational cost of simulation. We have considered the flow to be non-reactive and thus there is no need to solve any thermal equations.

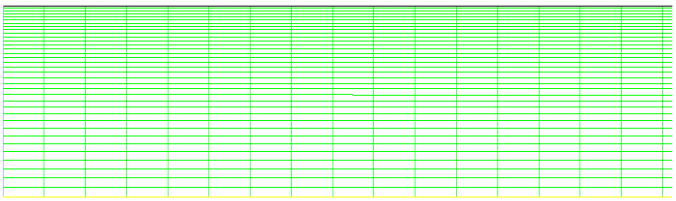

Figure 2: A portion of the grid used for the analysis of the non-reactive pipe flow.

The grid used is a stretched structured mesh. To better capture the boundary layer, the grid has been condensed near the wall. A part of this mesh is shown in figure (2).

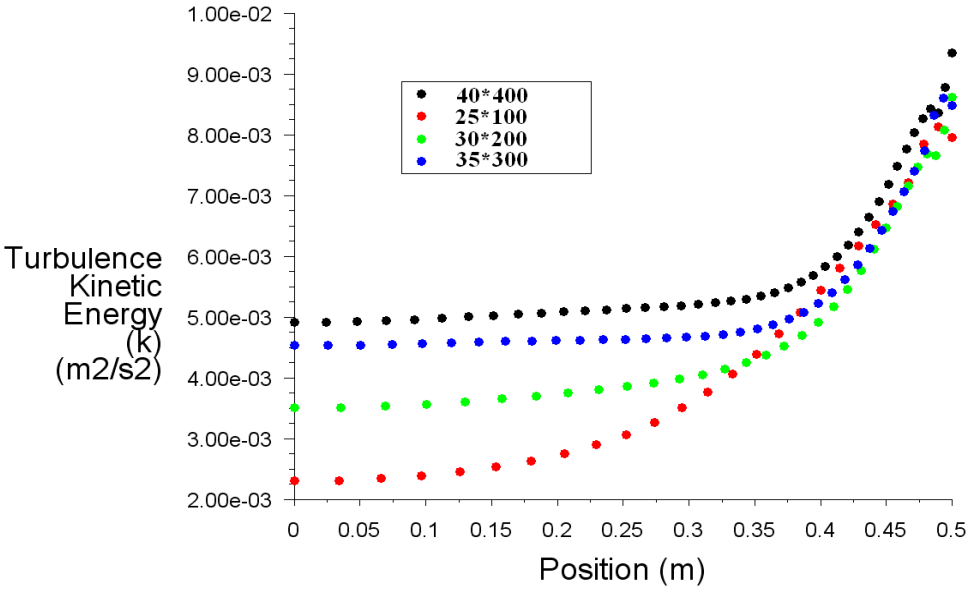

Figure 3: Radial distribution of the turbulence kinetic energy at the outlet of the pipe for 4 different mesh resolutions.

The mesh is 300×35 which adds up to a total number of 10500 cells in finite volume formulations. In figure (3), the radial distribution of the turbulence kinetic energy (which is chosen because it is a highly-sensitive parameter) at the outlet for 4 different mesh resolutions is shown. It is seen that for meshes finer than 300×35 the solution is not significantly different. Therefore, the 300×35 mesh is used as the optimum grid size.

Air is the working fluid in this simulation which is assumed to be incompressible. We have 4 different boundary conditions in this problem, one of them being the air inlet boundary. The inflow velocity and temperature (as seen in figure (1)) are $1m/s$ and $298K$, respectively. Another boundary condition is the axis of symmetry for which we have considered "axis" boundary condition. On the walls we have the "no-slip" condition, stating that the velocity vector is zero on the wall. The air flow is assumed to enter the atmosphere at the outlet of the pipe. Thus pressure-outlet has been applied at the outflow to ensure constancy of the atmospheric pressure.

According to the above considerations, two sets of equations must be solved: the flow equations and the turbulence equations. We have chosen to solve the turbulence and the momentum equations using a 1^{st} order upwind scheme. The solution fully converges after around 500 iterations, the residual history of which is shown in figure (4).

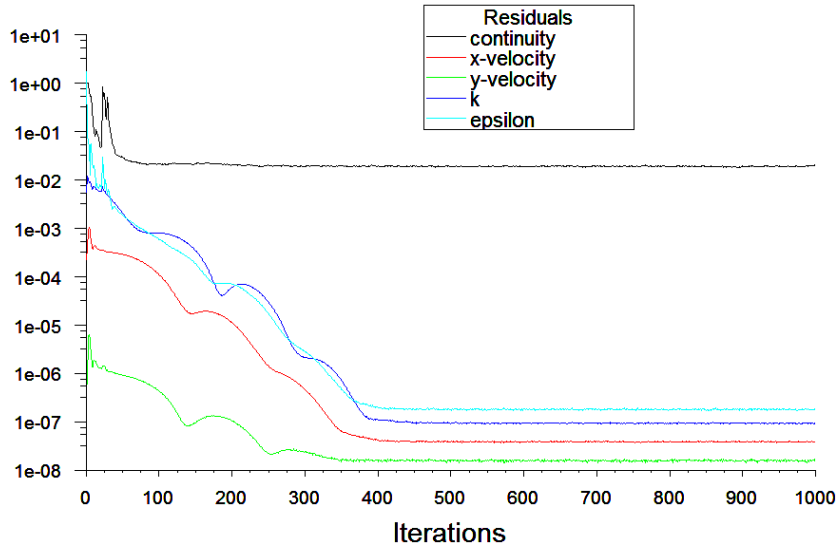

Figure 4: Residual history for the non-reactive pipe flow.

The velocity profile at the outlet of the pipe is plotted in figure (5).

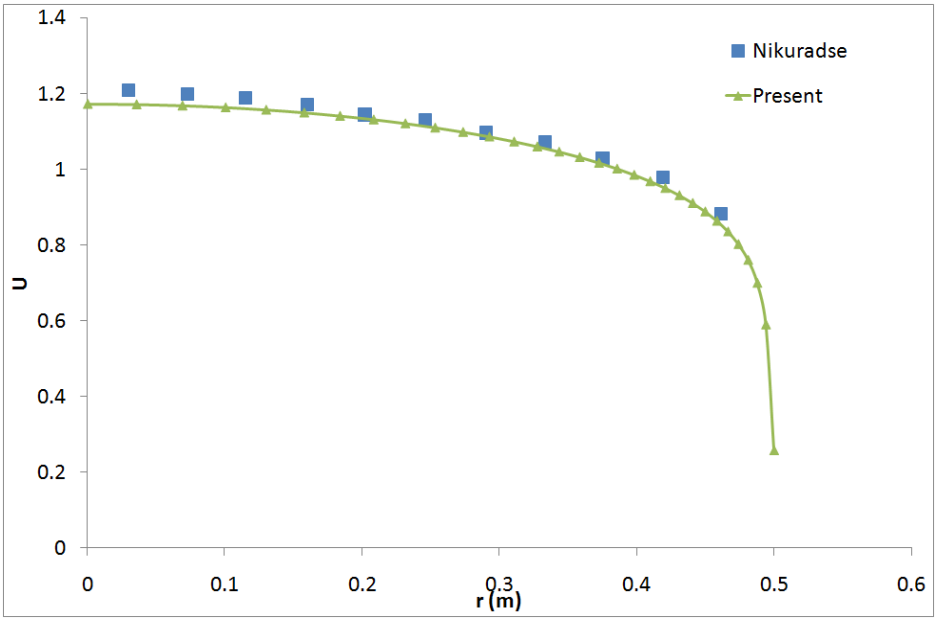

Figure 5: Velocity profile at the outlet of the pipe compared to those of Nikuradse's.

Comparing the results obtained here with those of Nikuradse (obtained by analytical solution of the flow equations) shows good agreement. The profile obtained here correctly models the no-slip condition on the wall and gives a maximum velocity of 1.2 in the middle of the pipe.
It is also found that the flow is fully developed in a distance 20 meters from the inlet.

3.2 Turbulent axisymmetric diffusion flame in a model combustor

In the second part of this project, reactive turbulent flow in a conventional combustor is studied. Although the solution has been tried to resemble the experimental setup, there are still plenty of assumptions made to simplify the simulation. The typical combustor we have investigated is shown in

figure (6). Most of the flow and geometrical parameters of the combustor are depicted in the figure. The working fluid, i.e. the oxidant, is air and the fuel is Methane. The combustion starts with a hydrogen igniter after the air and fuel are partially mixed. The air and the fuel inlet velocities are $U_{air} = 34.3\frac{m}{s}$ and $21.3\frac{m}{s}$, respectively. The air inflow temperature is taken to be higher than the fuel to ensure proper combustion by pre-heating the air. The turbulence model used here is again the two-equation $K-\varepsilon$ for which standard coefficients are used and which applies standard wall functions near the wall.

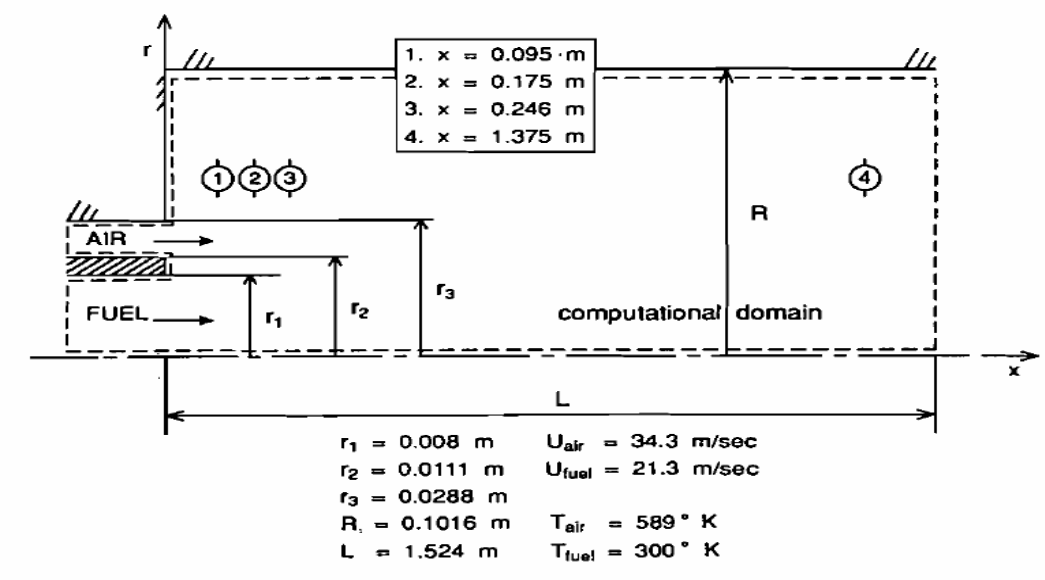

Figure 6: Geometrical and inflow properties of the reactive flow for the combustor.

The reactions are assumed to be volumetric and the combustion-turbulent interaction model is species transport with eddy dissipation.

The conservation equation for the species transport takes the general form

$$\frac{\partial(\rho m_i)}{\partial t} + \frac{\partial(\rho u_i m_i)}{\partial x_i} = -\frac{\partial}{\partial x_i} J_{i,i} + R_i + S_i \qquad (1)$$

in which R_i is the mass rate of creation or depletion by chemical reaction and S_i is the rate of creation by addition from dispersed phases plus any user-defined sources. An equation of this form will be solved for N-1 species where N is the total number of fluid phase chemical species present in the system.

The perfect gas assumption is used here to simplify simulations. All three coefficients of heat capacity, heat conductivity, and viscosity are assumed to have negligible variations with temperature (which is a very rough assumption in combustion problems). We have also assumed to have the 5 major species of CH_4, CO_2, O_2, H_2O, and N_2 and their relevant reactions in the combustion model.

The solver, like the case of the pipe, is unsteady, segregated, axisymmetric, and implicit. Besides the two inflows of air and fuel, we have 3 important boundary conditions to implement, one of them being the wall adjacent to the air inlet which is assumed to be adiabatic. Another thermal boundary condition is the combustor wall which is assumed to have a constant temperature of 1140 Kelvins [6]. The outflow is assumed to be discharged to the atmosphere and thus pressure-outlet boundary condition is applied. The computational mesh, as shown in figure (7- left), is stretched and structured.

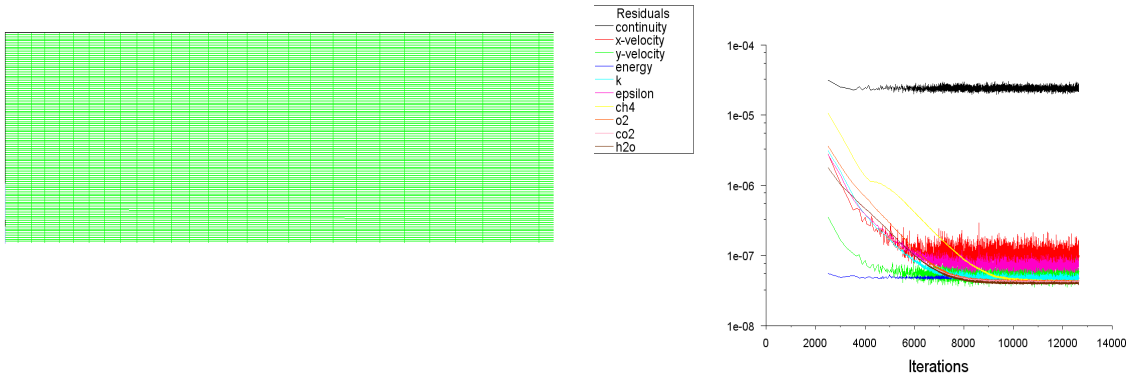

Figure 7: left: Grid used for the analysis, Right: residual history of the reactive flow inside a combustor.

The mesh, consisting of 6120 cells, is finer at initial parts of the combustor to more accurately model the mixing and combustion process. It is important to note that the resolution of the grid is optimized like the case of the flow in the pipe.

In addition to the flow, turbulent, and energy equations we have to solve 4 transport equations for the present species. All these equations are discretized using a 1st order upwind scheme.

In figure (7 - right), you can see the residual history of the solution of the ten governing equations. The simulation is continued until solution converges. It is seen to converge after about 12000 iterations. The oscillations in the residual history, after the convergence, are due to the unsteady nature of turbulent combustion.

For a non-premixed combustion problem, *mixture fraction* could be an appropriate parameter to investigate properties of fluid flow, which is defined as

$$f = \frac{\left[Y_f - \left(F/O\right)_{st} Y_O\right]_M + \left(F/O\right)_{st} Y_{O,A}}{1 + \left(F/O\right)_{st} Y_{O,A}} \qquad (2)$$

in which the subscripts A and M correspond to inflow and the present section of the combustor, respectively. The indices f, O denote fuel and oxidant, respectively and $\left(F/O\right)_{st}$ is the stoichiometric fuel-air ratio.

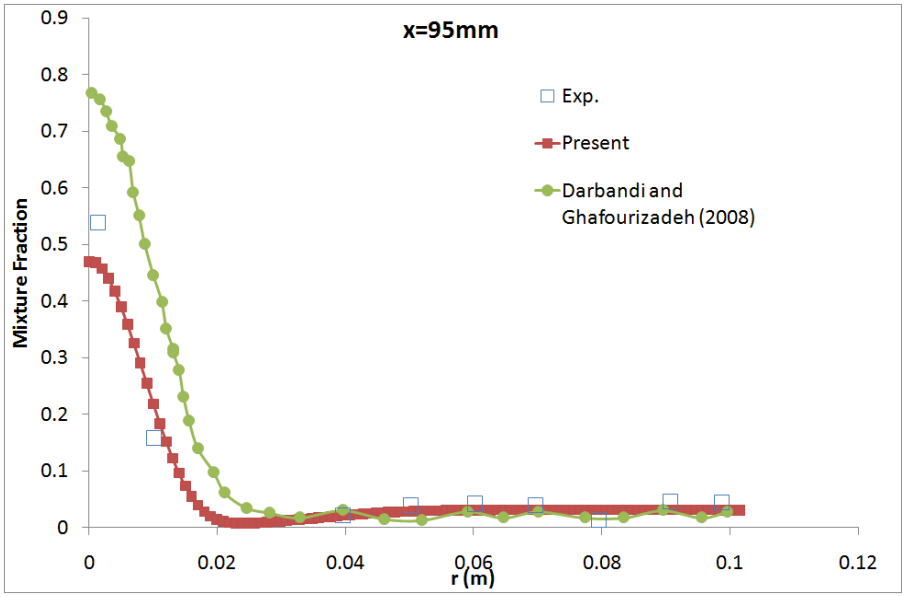

Figure 8: Radial distribution of the mixture fraction compared to that of Darbandi and Ghafourizadeh [2] and experimental data [6].

The radial distribution of mixture friction in a distance of 95 mm from the air inlet is shown in figure (8). It is seen in the diagram that the results obtained are in good agreement with the experimental results of Smoot and Lewis [6] and gives more accurate results than that of Darbandi et al [2]. The variation implies that there is more fuel near the axis of symmetry of the combustor than there is Oxygen. At around one fifth of the radius from the axis of symmetry, the fuel has greatly diminished which is the area of reaction. It is also inferred from the diagram that there is more fuel near the combustor wall than there is in the reaction zone which implies the presence of a large circulation of fluid in the combustor.

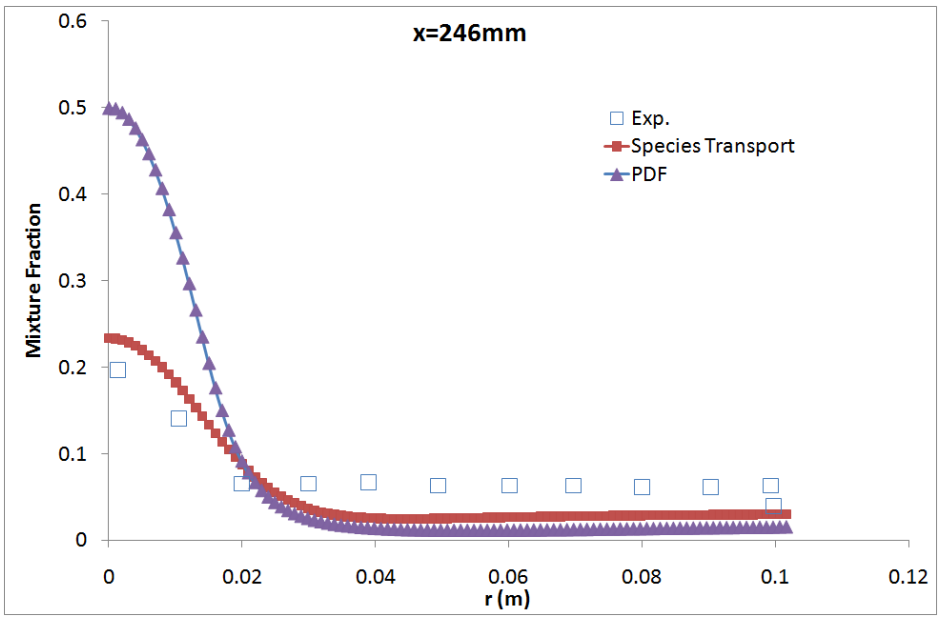

Figure 9: Radial distribution of the mixture fraction using the species transport and the PDF models.

We have also simulated the problem using the PDF (probability density function) combustion model and the result is compared to those of the species transport model. We have plotted the radial distribution of mixture fraction in a section 246 mm distant from the air inlet obtained by the two models along with the experimental result of Smoot and Lewis [6].

We can see in figure (9) that the species transport models this combustion process much more accurately than the PDF, which overestimates the value of mixture fraction. In fact, the latter implies, according to equation (2), that there is less oxygen present near the axis of symmetry, which is in contrast with experimental results. In other words, in the regions of high mixing, it is the species transport model that best describes the flow properties.

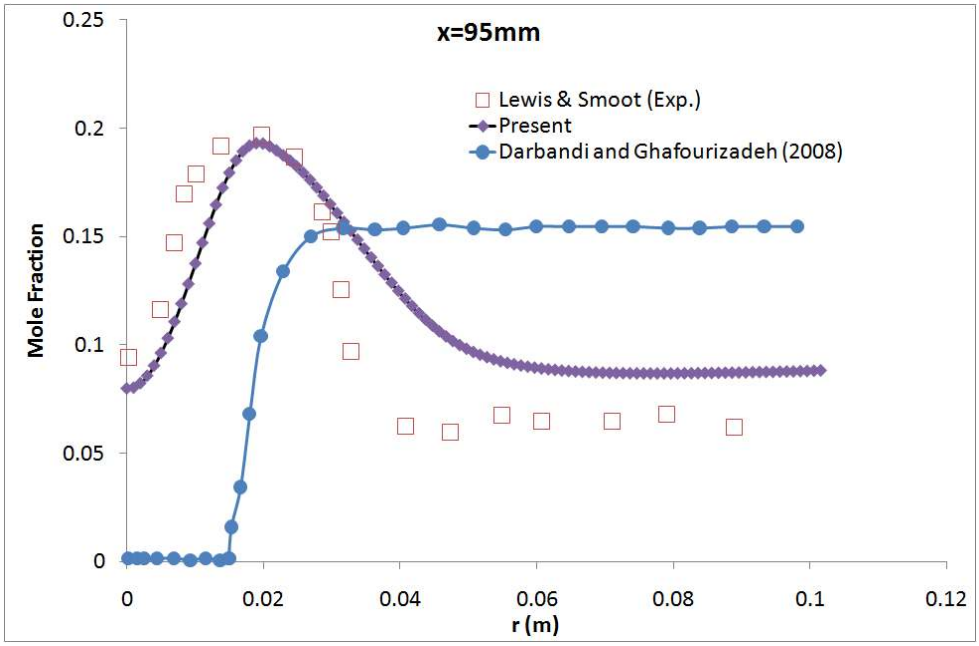

Figure 20: Radial distribution of the mole fraction compared to that of Darbandi and Ghafourizadeh [2] and experimental data [6].

One of the most important parameters in combustion problems is the mole fraction of Oxygen which is somehow indicative of the progress of the combustion. The radial distribution of the mole fraction of Oxygen at distance of 95 mm from the air inlet is shown in figure (10). The profile shows good agreement with experimental data. It is inferred that there exists some Oxygen even at the axis of symmetry of the combustor, which is due to the rapid mixing properties of the turbulent flows. The mole fraction of Oxygen increases in the radial direction due to the high speed air inflow. Finally, expansion of air in the upper region of the combustor accounts for the decrease in the number of Oxygen molecules and consequently its mole fraction. Since the combustion starts right after the mixing of fuel and air near the air inflow, we are having less Oxygen in the upper region of the combustor, in contrast to the result obtained by Darbandi et al [2].

Conclusions

Through a project, we simulated the reactive and non-reactive flows in a model combustor. This area of combustion is well numerically studied but the accuracy of the solutions obtained is usually unacceptable. The inaccuracy exists even in recently published papers, which makes the models used

quite invalid. Hence, there is a need to find the best model out of the many models used both in turbulence and combustion. Through investigating the turbulent flow properties in a non-reactive flow we came to the conclusion that the $K-\varepsilon$ model produces acceptable results. Furthermore, the grid was checked to have an optimum size regarding computational cost. Modeling the combustion with two methods of species calculation showed that the species transport model gives more accurate results than the PDF model for this special problem. The presence of Oxygen in the axis of symmetry of the combustor is well predicted by the species transport model used. This phenomenon is due to rapid mixing properties of turbulent flows.

References

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