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SUBGRID COMBUSTION MODELING FOR LARGE EDDY SIMULATION (LES) OF TURBULENT COMBUSTION USING EDDY DISSIPATION CONCEPT (ECCOMAS CFD 2010)

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Abstract. *Theoretical development of the Eddy Dissipation Concept (EDC) using the turbulence energy cascade model was proposed by B.F. Magnussen and is well established for Reynolds Averaged Navier Stokes (RANS). EDC assumes that the combustion takes place in the fine structure and these fine structure quantities and reaction rates are modeled with turbulent kinetic energy and dissipation. However extension of the EDC for Large Eddy Simulation (LES) is not straightforward, where most of the turbulent kinetic energy is resolved on the grid scales. The formulation of EDC with subgrid kinetic energy and subgrid dissipation will have severe shortcomings and its performances will largely be affected by the chosen subgrid model. In present study the EDC which requires calculation of time scale, fine structure regions and fraction of the fine structure quantity where reaction occurs is studied for the LES and these quantities are modeled with subgrid model. Performance of subgrid EDC with the different subgrid model, such as Smagorinsky and dynamic model is reported. Another issue with reacting flow is a solution of pressure correction Poisson equation with density time derivative term which causes severe time constraint per iteration and is most destabilizing part of the calculation. In the present study a procedure similar to the Echt Konservativer Transport (EKT) is used. In EKT, density was formulated by solving the four pseudo species transport equations in predictor and corrector step whereas in the present formulation density is formulated from species mass fraction which is computationally less expensive. An LES simulation of a turbulent piloted non-premixed methane/air jet flame(Sandia Flame D) for a Reynolds number of 22400 is carried out to estimate the combustion characteristics with the subgrid model and filter width. Subgrid EDC with a simplified one step and a three step-global reaction mechanism is used. The results are compared with an experimental data base and flamelet model. Study shows that the combustion characteristics are highly function of subgrid model and model constant.*

1 INTRODUCTION

Large Eddy Simulation (LES) solves the filtered N-S equations and resolves most of turbulent kinetic energy on the grid scale. In LES, the large geometrically dependent energy-carrying eddies are resolved on the grid scales(GS), whereas effects of the smaller, more universal isotropic scales are modeled using a sub-grid scale (SGS) models. LES is a promising tool for understanding the physics of unsteady turbulent flow at comparatively reduced costs. Although LES captures the large energy carrying eddies but still it does not capture the small dissipative structures where combustion takes place. Direct Numerical Simulation (DNS) resolves all the scales including small dissipative scale, but it is computationally demanding. When DNS is applied to combustion problems, e.g.,[1] the computational requirements are increased by 10-20 orders of magnitude[2] compared to modeling of non-reacting flows. Closure of the spatially filtered source term is still a challenge due to unresolved reactive structure. Although there have been some attempts for the direct closure. DesJardin and Frankel[3] carried out an LES of diffusion flame at a Reynolds number of 1000 with direct closure of the Arrhenius source term with single step chemistry. The agreement with DNS was not so satisfactory. They proposed two subgrid combustion model using the scale similarity assumption, the scale similarity filtered reaction rate model (SSFRRM) and the scale similarity resolved reaction rate model (SSRRRM) for low Reynolds number. The results were not encouraging and the models were not tested for practical Reynolds number.

The LES does not resolve the reactive fine structures and the turbulence-chemistry interactions need to be modeled using a model. Although LES combustion models do not differ considerably from already existing RANS model but LES itself captures the instantaneous quantities and mixing accurately. Over the time different LES combustion models, derived from existing RANS model, have been studied and reported. An LES subgrid combustion model based on equilibrium chemistry was presented by Cook and Riley,[4] where they carried out a LES simulation of a hydrogen diffusion flame. Branley and Jones,[5] Forkel and Janicka[6] also carried out the LES of hydrogen diffusion flame using the equilibrium chemistry and they obtained good predictions. Kempf et al.[7–10] presented LES of Sandia Flame D, Bluff Body flame, Hydrogen Diffusion Flame and counter flow diffusion flame using the steady state flamelet model and they obtained good agreement with experiments. Pitsch and Steiner[11] carried out a LES of the piloted Sandia-D flame using an unsteady Lagrangian flamelet model and they achieved an excellent agreement even for minor species. Conditional Source Estimation a variant of CMC (Conditional Moment Closure), was proposed by Bushe and Steiner[12] and the model was later used for LES of Sandia Flame D.[13] McMurtry et al.[14] formulated Liner Eddy Model(LEM) developed by Kerstein[15] for LES reacting flows. Hu et al.[16] et al carried out an LES simulations of swirling diffusion flames using the Second Order Moment (SOM) and EDC models. The predictions with EDC model were not satisfactory, and they concluded that the EDC model is not good for LES. Similarly, Zho et al.[17] carried out LES of premixed and non premixed flame using SOM, presumed PDF and EDC models and they concluded that presumed PDF method and EDC model do not perform satisfactory. The reason for the unsatisfactory prediction was

that the EDC model employed by Hu et al.[16] and Zho et al.[17] was basic EDC model proposed by Magnussen and Hjertager,[18] which uses model constant based on the RANS. This model does not account for the fine structure region and fraction of the burning structure. An LES study was carried out by Yaga et al.[19] where combination of Arrhenius and EDC model was used and they obtained satisfactory estimate. In the present study, for turbulence-chemistry interaction RANS based EDC model is extended to LES. A Proposal for modifying the model constant is made. In addition to that, formulation for density based on conservation of species mass fraction is also proposed. The formulation is suitable for splitting the conserved variables. Finally, an LES of Sandia Flame D is carried out for which experimental data is available. Influence of subgrid modeling, chemistry and model constant is also studied.

2 Modeling

2.1 Governing Filtered Equations

The governing filtered equation for LES are
The continuity equation

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i}{\partial x_i} = 0 \tag{1}$$

The momentum equation

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right)\right) - \frac{\partial \tau_{sgs}}{\partial x_j} \tag{2}$$

The mass fraction equation for species i

$$\frac{\partial \overline{\rho}\widetilde{Y}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{Y}_i\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\overline{\rho}D_i\left(\frac{\partial \widetilde{Y}_i}{\partial x_j}\right)\right) + \overline{\rho}\widetilde{\omega}_i \tag{3}$$

where $\overline{\rho}$ is a (Favre) filtered density, $\widetilde{u}_i$ is a filtered velocity component, $\overline{p}$ is pressure $\widetilde{Y}_i$ is a species mass fraction for species i, μ is the dynamic viscosity, t is time, τ_{sgs} is subgrid stress and $\widetilde{\omega}_i$ is the chemical source term. The governing equations were discretized with finite volumes technique on a staggered cylindrical grid. Convective and diffusive terms in the momentum equation were discretized using second order central differencing scheme. Convective term in species transport equation were discretized using the Total Variation Diminishing(TVD) schemes. The TVD schemes are bounded schemes, which do not produce undershoot and overshoot in the mass fractions. The SGS term was closed with Smagorinsky subgrid model. The numerical accuracy of current finite volume technique is an order of two in space. The transport equations were integrated in time by an explicit low storage three stage Runge−Kutta method. For further details please refer.[7–10]

2.2 Modeling of the Filtered Reaction Rates

The source term in transport equation is modeled as

$$\omega_i = \frac{\gamma_\lambda^2 \chi}{\tau_\star}\left(Y_i^0 - Y_i^\star\right) \tag{4}$$

where γ_λ is the fine structure region, $\frac{\gamma_\lambda^2}{\tau_\star}$ is the mass exchange between the surrounding and the fine structure region. Superscripts * and ^{0} refer the fine structure and the surrounding state. $\tau_\star$ represent the residence or mixing time. χ is the fraction of the fine structure where reaction take place. The fine structures states are estimated using the reactor modeling. In the present study a perfectly stirred reactor (PSR) is used assuming that the reactor mass is constant at each time step, and reactants are perfectly mixed inside it. The chemistry in the reactor can be modeled either with fast chemistry, equilibrium or chemical kinetics. In the present study reactor is modeled with fast chemistry assumption. The equilibrium and chemical kinetics reactor modeling are computationally expensive.

2.3 Fine Structure Region for LES

The Eddy Dissipation concept for turbulence combustion proposed by Magnussen et al.[18,20–23] is based on the energy cascade. In the cascade model larger eddies, which extract energy from the mean flow are unstable. These eddies breakdown and transfer their energy to smaller eddies. This process continue until eddies are stable and finally these smaller eddies dissipate their energy due to molecular diffusion. EDC model assumes that the molecular mixing and the subsequent combustion take place on the smaller dissipative eddies which are close to the Kolmogorov length scales and are termed as fine structures. Ivar and Magnussen[24] estimated the characteristic length $L^\star$ and velocity scale $u^\star$ of the fine structure using the cascade theory of turbulence.

$$L^\star = \frac{2}{3}\left(\frac{3C_{D2}^3}{C_{D1}^2}\right)^{1/4}\left(\frac{\nu^3}{\epsilon}\right)^{1/4} = 1.43\left(\frac{\nu^3}{\epsilon}\right)^{1/4} \tag{5}$$

$$u^\star = \left(\frac{C_{D2}}{3C_{D1}^2}\right)^{1/4}(\nu\epsilon)^{1/4} = 1.75\,(\nu\epsilon)^{1/4} \tag{6}$$

where $C_{D1} = 0.134$ and $C_{D2} = 0.5$.[24] ν is the kinematic viscosity and ϵ is eddy dissipation. The scales $L^\star$and $u^\star$ are same order of magnitude as Kolmogorov scales. RANS based EDC assumes that the full cascade take place at each numerical cell and a connection between the fine structure and the larger eddies is achieved through the cascade. The fine structure region is estimated as a function of fine structure velocity and the eddy characteristic velocity $u^{'}$, $\gamma_\lambda = \left(\frac{u_\star}{u^{'}}\right)$. Characteristics of the large eddies such as velocity $u^{'}$ and length scale $l^{'}$ are evaluated using the turbulence model such as $k-\epsilon$. Although this approach is very successful in RANS but in LES most of the turbulent kinetic energy is resolved on the grid scale and only a

small fraction of turbulent kinetic energy termed as subgrid kinetic energy is available. In LES the turbulent kinetic energy is not available explicitly, the EDC model need to be formulated with the subgrid kinetic energy k_{sgs} or eddy viscosity ν_{sgs}. In the current formulation of EDC for LES the amount of the fine structures are evaluated using the subgrid eddy velocity u_{sgs} and fine structure velocity $u_\star$. The ratio between the mass of the fine structure and the total mass of subgrid structure, γ_λ, is expressed as

$$\gamma_\lambda = \left(\frac{u_\star}{u_{sgs}}\right) \tag{7}$$

and using the Equ.(6), the fine structure region can be expressed as

$$\gamma_\lambda = \left(\frac{3C_{D2}}{4C_{D1}^2}\right)^{1/4} \left(\frac{\nu\epsilon}{k_{sgs}^2}\right)^{1/4} \tag{8}$$

where k_{sgs}, subgrid kinetic energy, is modeled using the subgrid turbulent viscosity. $\nu_{sgs} = C_k \triangle {k_{sgs}}^{1/2}$ and similarly the subgrid eddy dissipation rate $\epsilon_{sgs} = C_\epsilon (k_{sgs})^{3/2}/\triangle$ and finally $\nu_{sgs} = C_{\nu sgs} k_{sgs}^2/\epsilon_{sgs}$. Where the dimensionless model coefficients are $C_k = 0.05$ and $C_\epsilon = 1.00$.[25] The fine structure region is represented as.

$$\gamma_\lambda = \left(\frac{3C_{\nu sgs}C_{D2}}{4C_{D1}^2}\right)^{1/4} \left(\frac{\nu}{\nu_{sgs}}\right)^{1/4} \tag{9}$$

Equation (9) is the fine structure region as a function of the molecular viscosity, the subgrid viscosity and the model constants. In case of LES, subgrid viscosity might become zero (local laminarization due to combustion) and in that situation $\gamma_\lambda \to \infty$. The reactor model have no meaning for such large values of the fine structures. This behavior of EDC model is similar to what we observe very close to the wall in the viscous sublayer where turbulent kinetic energy disappears and the molecular diffusion is larger than the turbulent diffusion $(\gamma_\lambda \to \infty)$. In RANS, to avoid numerical problem an upper limit $(\gamma_\lambda < 0.5)$ was proposed.[26] Myhrvold[27] presented a model for calculating the fine structure region close to the wall.

In case of LES a model constant $C_{EDC} = (3C_{\nu sgs}C_{D2}/4C_{D1}^2)^{1/4}$ is proposed. The value of the model constant $C_{EDC} = 1.01$, where $C_{\nu sgs} = 0.05$.[25] A preliminary LES simulation of Sandia Flame D[28] with $C_{EDC} = 1.01$ showed overprediction of the temperature and other chemical species. To establish the model constant a parametric study is performed. In addition to that an upper limit of $(\gamma_\lambda < 1)$ is used when the fine structure velocity is larger than the subgrid velocity. Although in the current formulation, EDC constant is assumed to be fixed, however in realistic problem the model constant need to be computed dynamically. The dynamic evaluation of the EDC constant is under progress.

2.4 Modeling of Fraction of Burning Structure χ

As mentioned, the mixing and subsequent combustion take place in the fine structure. In fast chemistry limit it is assumed that only a fraction of the mixed fine structure reacts and is termed

as fraction of burning structure and denoted by χ. The fraction of burning fine structure χ is inherent with the reactor modeling having detailed kinetics ($\chi = 1$). This has been confirmed by Inge Gran.[26] In case of infinitely fast reaction the fraction of the reactive fine region is computed using the probability function χ.[22,23,26] In case of single step infinitely fast chemistry the global reaction is

$$1 \text{ kg of fuel } (Y_F) + r_F \text{ kg of oxidizer } (Y_O) \Rightarrow (1 + r_F) \text{ kg of product } (Y_P) \tag{10}$$

The fraction of reacting structure can be expressed as,

$$\chi = \chi_1 \chi_2 \chi_3 \tag{11}$$

where χ_1 is the probability of coexistence of the reactants

$$\chi_1 = \frac{\left(\widehat{Y}_{min} + \widehat{Y}_P\right)^2}{\left(\widehat{Y}_F + \widehat{Y}_P\right)\left(\widehat{Y}_O + \widehat{Y}_P\right)} \tag{12}$$

χ_2 is express the degree of heating

$$\chi_2 = \min\left[\frac{\widehat{Y}_P}{\gamma_\lambda\left(\widehat{Y}_{min} + \widehat{Y}_P\right)}, 1\right] \tag{13}$$

and χ_3 limits the reaction due to lack of reactants

$$\chi_3 = \min\left[\frac{\gamma_\lambda\left(\widehat{Y}_{min} + \widehat{Y}_P\right)}{\left(\widehat{Y}_{min}\right)}, 1\right] \tag{14}$$

Here, the notation $\widehat{Y}_F = \widetilde{Y}_F$, $\widehat{Y}_O = \widetilde{Y}_O / r_F$, $\widehat{Y}_P = \widetilde{Y}_P / (1 + r_F)$ and $\widehat{Y}_{min} = \min\left[\widehat{Y}_F, \widehat{Y}_O\right]$ is used

2.5 Time Scale $\tau_\star$

In the RANS version of the EDC model, a mixing time scale or residence time is represented as the rate at which energy is transferred from the larger eddies to the smaller eddies. The residence or mixing time scale is evaluated using the molecular viscosity and the dissipation rate $\tau_\star = \left(\frac{C_{D2}}{3}\right)^{0.5}\left(\frac{\nu}{\epsilon}\right)^{0.5}$. In LES it is assumed that the rate at which energy is transfer is constant through out the cascade. Then the rate at which subgrid eddies transfer energy to fine structure is $\tau_\star$.

$$\tau_\star = \left(\frac{C_{D2}}{3}\right)^{0.5}\left(\frac{\nu}{2\left(\nu_t + \nu\right)}\right)^{0.5}\frac{1}{|\widetilde{S}|} \tag{15}$$

where, ϵ is the eddy dissipation and evaluated using $\epsilon = 2\left(\nu_t + \nu\right)|\widetilde{S}|^2$ and $|\widetilde{S}| = \left(2\widetilde{S}_{ij}\widetilde{S}_{ij}\right)^{1/2}$.

2.6 Chemical Mechanism

In the present simulation in order to reduce computational time the single step and the three step reaction mechanism are used in the framework of infinitely fast chemistry.
The Single Step mechanism used in the present study is

$$CH_4 + 2O_2 \Rightarrow CO_2 + 2H_2O \tag{16}$$

The Three Step mechanism used in the present study is

$$\begin{aligned} CH_4 + 0.5O_2 &\Rightarrow CO + 2H_2 \\ H_2 + 0.5O_2 &\Rightarrow H_2O \\ CO + 0.5O_2 &\Rightarrow CO_2 \end{aligned} \tag{17}$$

2.7 Density Calculation for Splitting the Conserved Variables

In reacting flows, solution of the pressure correction Poisson equation with density time derivative term causes a severe time constraint per iteration and is the most destabilizing part of the calculation. This stability problem mostly dominates near to the nozzle due to sudden heat release. Branley and Jones[5] used a mixing density close to the nozzle to alleviate the stability problem, arguing that using mixing density rather than chemical density close to the nozzle will not have significant influence in downstream region. Another issue which was discussed by Kempf et al.,[10] was splitting of ρf with density in the flamelet approach. A similar problem is also faced while splitting ρY_i with density in the EDC approach. Brizuela[29] discussed an error associated in evaluating the mean density from the Favre-averaged temperature/enthalpy and reactant composition.

$$\overline{p} = \overline{\rho} R \sum_j \frac{\widetilde{TY_j}}{w_j} \cong \overline{\rho} R \sum_j \frac{\widetilde{T}\widetilde{Y_j}}{w_j} \tag{18}$$

$$\overline{\rho}_{chem} = \overline{p}/R \sum_j \frac{\widetilde{T}\widetilde{Y_j}}{w_j} \tag{19}$$

Brizuela[29] pointed out that neglecting the correlation between the temperature and the mass fraction introduced an error. The density computed using Equ. (19) is an approximate Favre filtered density and will not be used for splitting the conserved variable ρY_i in the present study. The density is formulated based on the conservation of species which is an extension of the EKT "Echt Konservativer Transport"[10] or fully conservative transport. The EKT scheme is based on the conservation of fuel ρf and oxidizer $\rho\,(1-f)$. The EKT scheme assumes two pseudo species $X_A = f^+ = f$ and $X_B = f^- = (1-f)$ and the transport equations for the pseudo species are solved in predictor and corrector steps. In the EKT approach the density was formulated as

$$\overline{\rho} = \left(\overline{\rho}\widetilde{f^+}\right)^{n+1^\star} + \left(\overline{\rho}\widetilde{f^-}\right)^{n+1^\star} \tag{20}$$

A similar approach is used here for calculation of the density. In the present formulation the actual species mass fractions were conserved instead of pseudo species.

$$\overline{\rho} = \sum_{i=1}^{i=n} (\rho Y_i)^{n+1^\star} \Big/ \sum_{i=1}^{i=n} (Y_i)^{n+1^\star} \tag{21}$$

where $\sum_{i=1}^{i=n} (Y_i)^{n+1^\star} = 1$. The time derivative density term in the pressure correction equation is evaluated at each time step using the density from Equ.(19) and Equ.(21)

$$\frac{\partial \overline{\rho}}{\partial t} = \frac{\overline{\rho}_{chem} - \overline{\rho}}{\triangle t} \tag{22}$$

3 Present Predictions

3.1 Geometrical and Numerical configuration of Test Case

In the present study the LES of the CH_4/air diffusion flames Sandia Flame D was carried out. The studied configuration has a fuel nozzle with a diameter(D) of 7.6mm which was surrounded by a pilot of a diameter 18.2mm and an air co-flow. The fuel jet consist of a mixture of three parts air and one part CH_4 by volume and the pilot was a lean (ϕ=0.77) mixture of C_2H_2, H_2, air, CO_2, and N_2. The fuel bulk velocity was 49 m/s, which gave a Reynolds number of 22400 based on the nozzle diameter. Flame D has a small degree of local extinction.[28] For the numerical simulation a cylindrical computational domain with 75D in axial direction and 33D in radial direction were employed. The numerical grids of $514 \times 32 \times 57$ were used axially, circumferentially and radially respectively. The grid was equidistant in the axial and circumferential directions. 5 and 11 uniform grid cells were used in nozzle and pilot respectively. Otherwise the grid was stretched radially. The inflow boundary condition was Dirichlet condition where velocity profiles , temperature and species mass fractions were specified.[28] Fluctuations with specified length scales were generated using the turbulence inflow generator developed by Klein et al.[30] and these fluctuations were superimposed over mean velocity profile.[28] On the downstream (outflow boundary) zero gradient conditions ($\partial u_i/\partial x_i = 0.0$) was posed. On the annular surface of the computational domain fixed absolute values of pressure and zero gradients for velocity components were specified. Periodicity was applied to all quantities in the circumferential direction.

3.2 Simulation Cases

In total six simulation cases were carried out to investigate the influence of the constant associated with EDC model, subgrid model and chemistry. Table-1 presents the description of the cases, which are studied to validate the present methodology. The cases 1, 2 and 3 were meant to understand the influence of the model constant or in other words the influence of fine structure region . Cases 3 and 4 were meant to understand the influence of the subgrid model. The final case was to understand the influence of the chemical mechanism.

Table 1: Simulation Cases and Description

Cases	Subgrid Model	Combustion Model	EDC constant
LES-R1	Smagorinsky $(C_s = 0.1)^a$	Fast Chemistry Single Step	0.2
LES-R2	Smagorinsky $(C_s = 0.1)$	Fast Chemistry Single Step	0.25
LES-R3	Smagorinsky $(C_s = 0.1)$	Fast Chemistry Single Step	0.3
LES-R4	Dynamic	Fast Chemistry Single Step	0.3
LES-R5	Smagorinsky $(C_s = 0.1)$	Fast Chemistry Three Step	0.25

[a] where C_s is the Smagorinsky constant

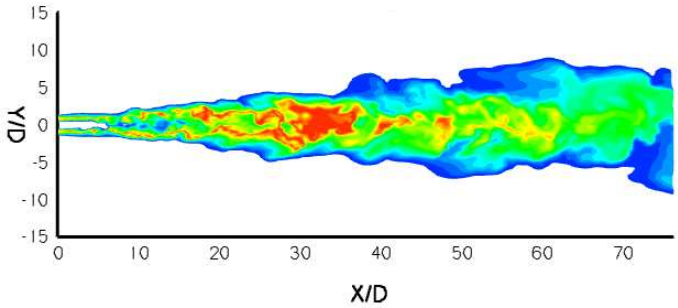

Figure 1: Axial Distribution of χ

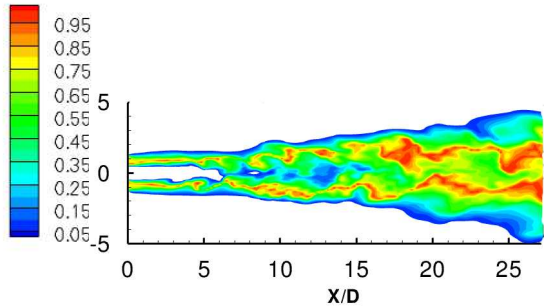

Figure 2: Axial Distribution of χ

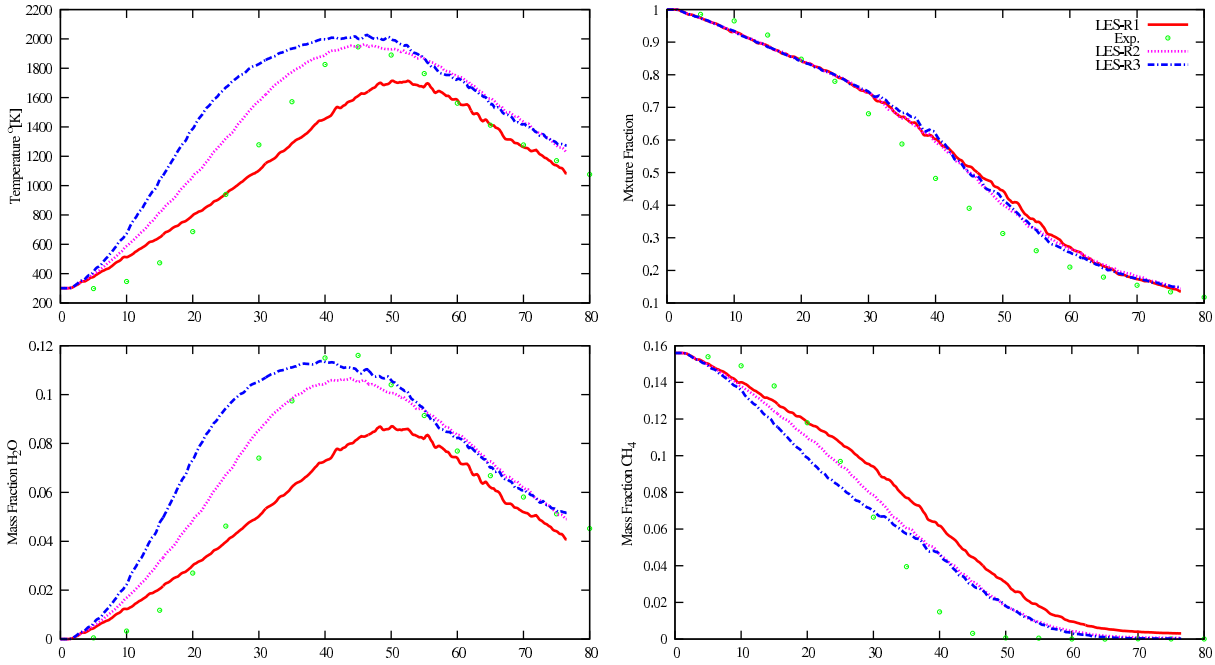

Figure 3: Mean mass fractions of H_2O, CH_4, Temperature and Mixture Fraction along the centerline

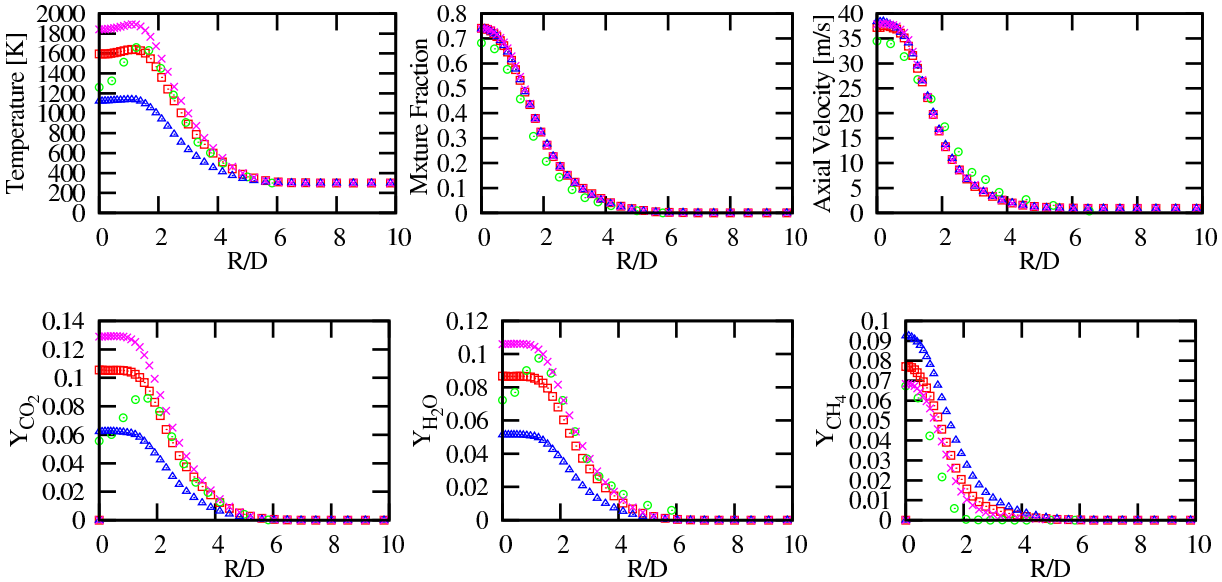

Figure 4: Mean mass fractions of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 30$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

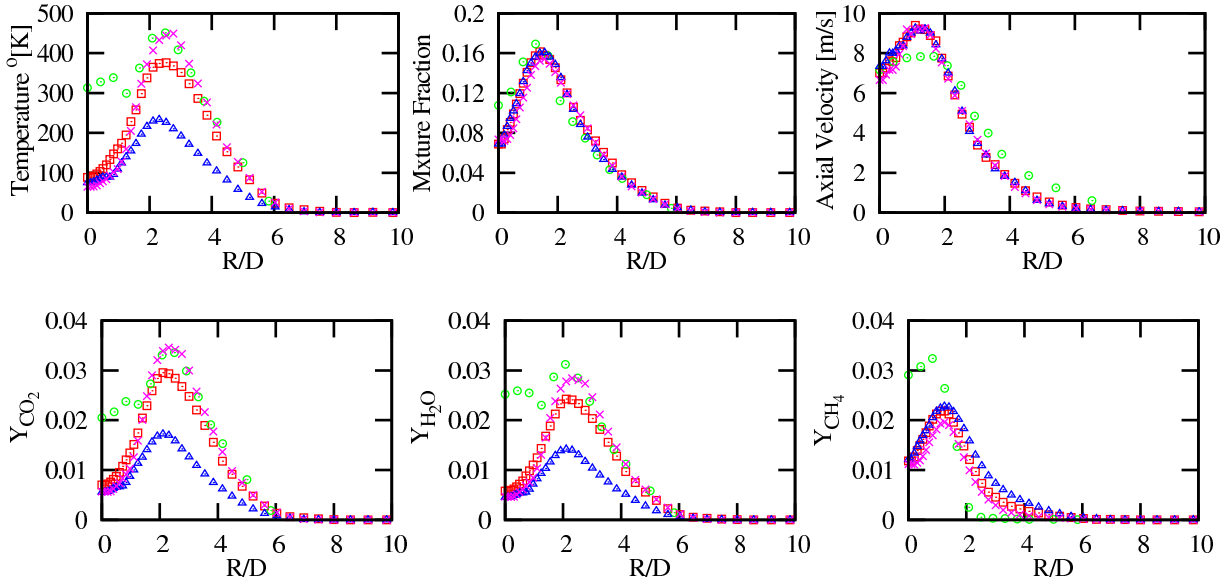

Figure 5: Root Mean Square (RMS) values of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 30$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

4 RESULTS AND DISCUSSION

A preliminary investigation showed that neglecting χ produced too fast reactions especially close to the nozzle. The predictions were completely wrong compared to the experiments. In the previous study,[16,17] where χ was not accounted, the predictions were not satisfactory compared

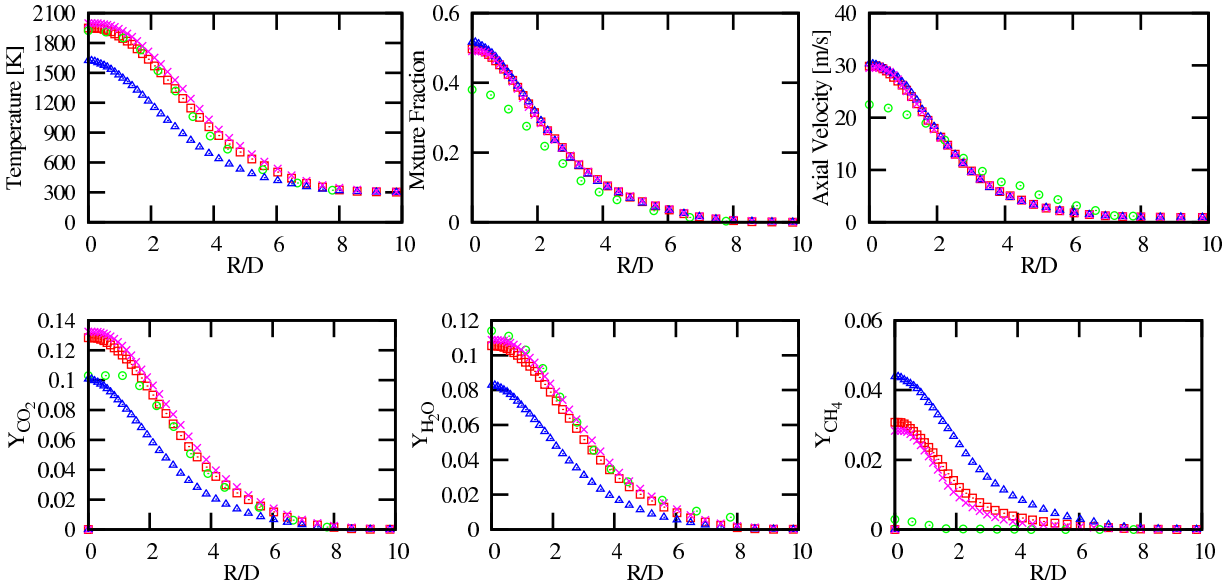

Figure 6: Mean mass fractions of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 45$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

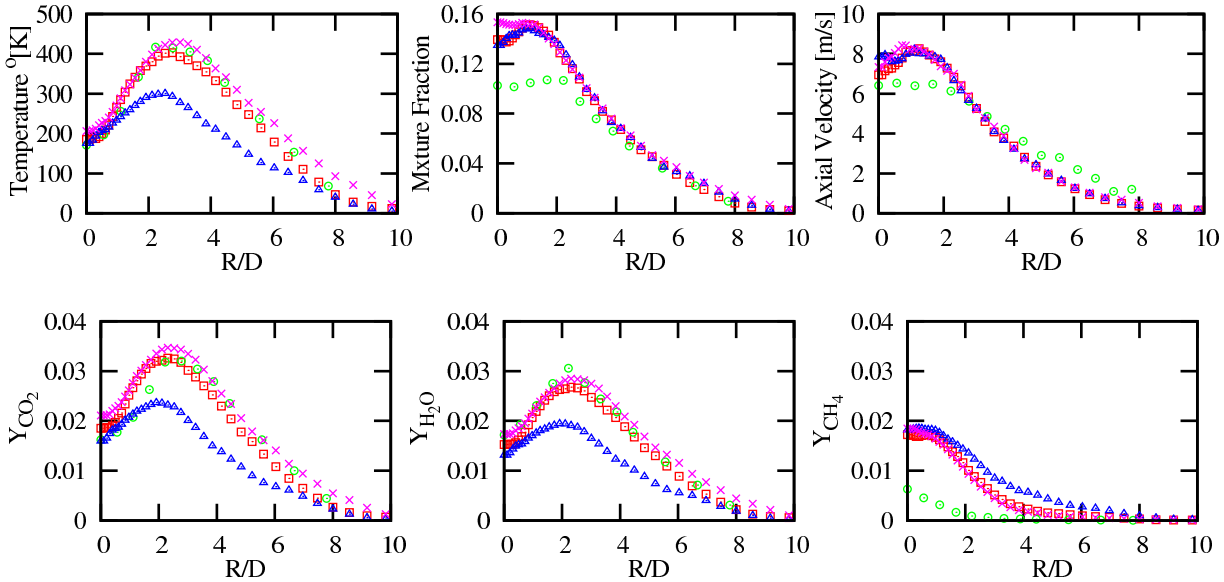

Figure 7: Root Mean Square (RMS) values of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 45$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

to the experiments. LES, which is computationally demanding, reactor modeling of the fine structure with chemical kinetics makes still more expensive. The computational cost can be reduced by modeling the reactor with fast chemistry assumption with appropriate χ. Figure 1 shows the instantaneous contour plot of the χ and Fig. 2 gives an enlarged view of the near field region at the same instance. It can be seen that χ is comparatively larger especially at the thin

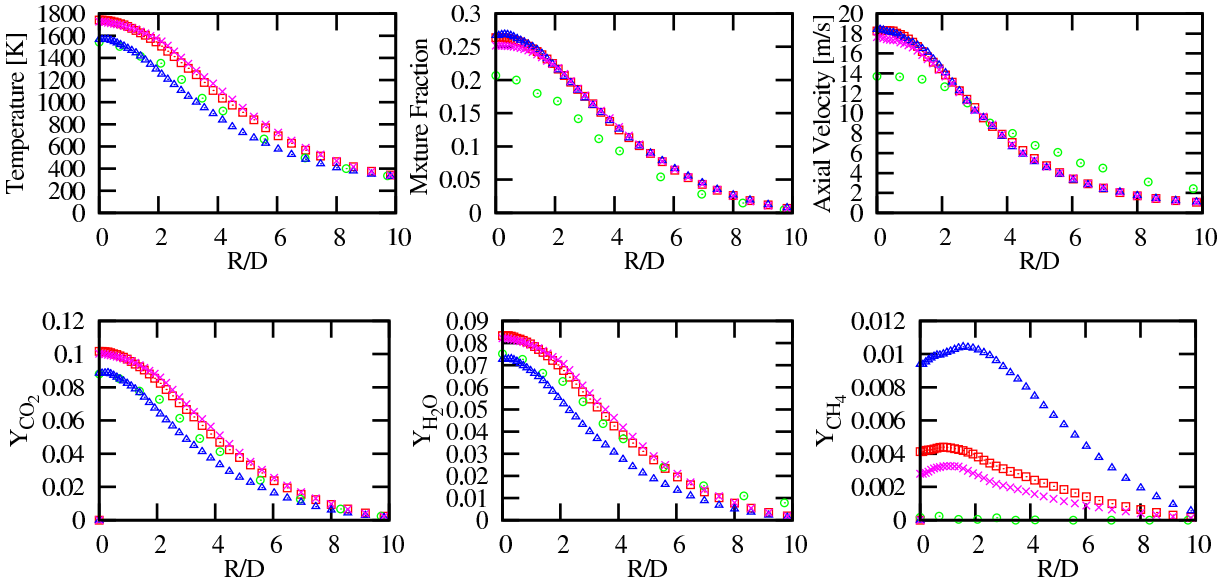

Figure 8: Mean mass fractions of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 60$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

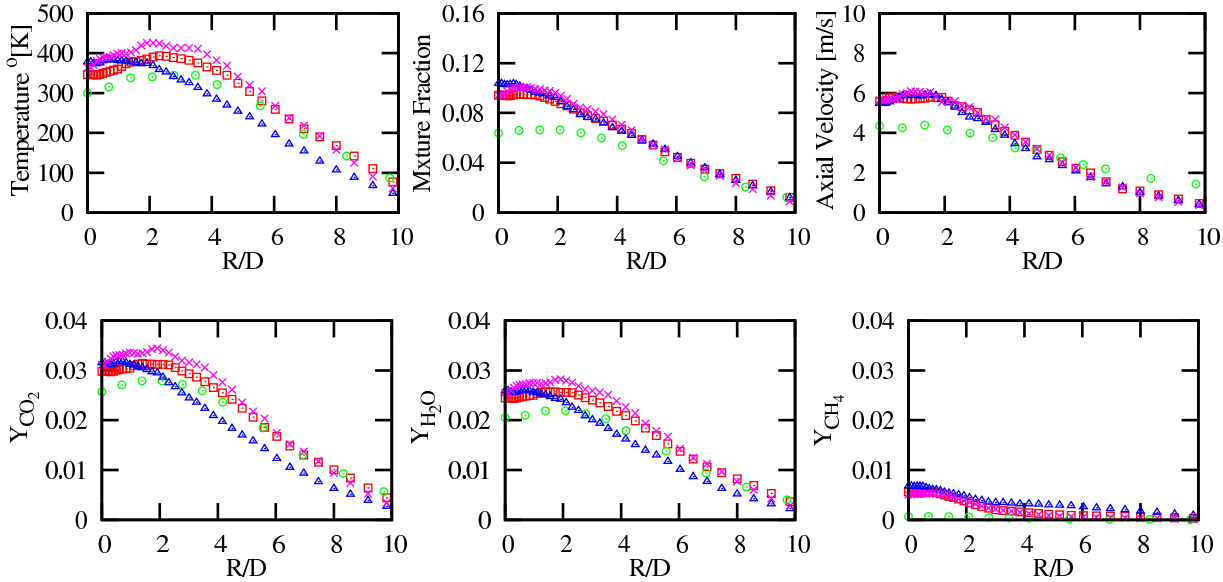

Figure 9: Root Mean Square (RMS) value of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity at $\frac{R}{D} = 60$, where $\odot$, $\triangle$, $\square$ and $\times$ represent Experimental, LES-R1, LES-R2 and LES-R3 respectively

reaction zone between the pilot and jet. The main reaction zone which ranges from 30D-45D is also well represented by χ.

The instantaneous quantities are averaged over time. To understand the flame characteristics mean quantities are plotted and compared with experiments. The calculated mean mass fractions of H_2O, CH_4, temperature, and mixture fraction along the centerline are shown in

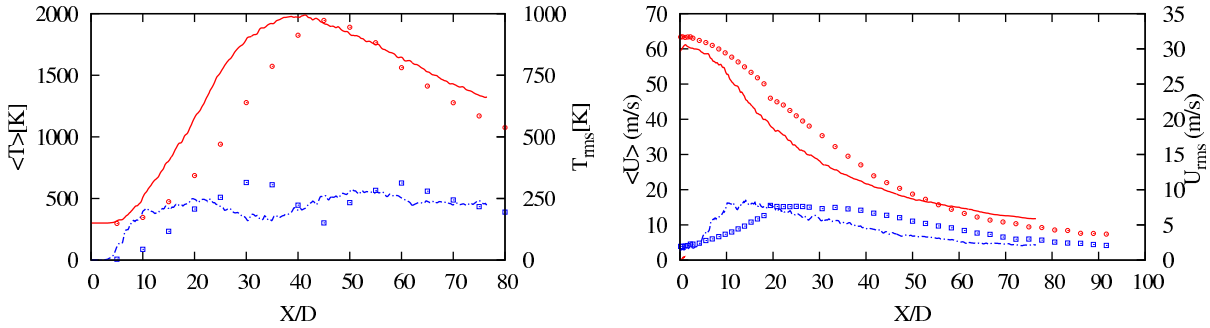

Figure 10: Profiles of Mean and Root Mean Square(RMS) of Temperature and Axial velocity for LES-R5 compared with experiments, where ⊙ and □ are the mean and RMS experimental results respectively; solid line and dashed line are the mean and RMS computed results respectively

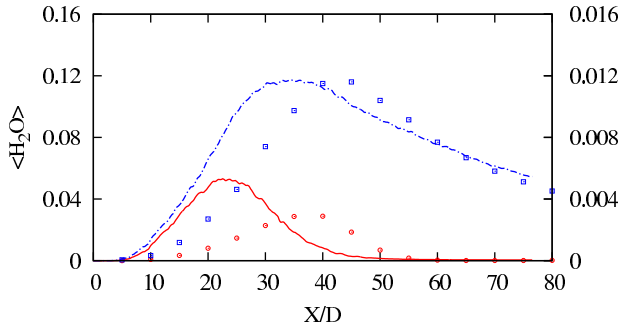

Figure 11: Profiles of mean mass fractions of H_2O and H_2 for LES-R5 compared with experiments, where ⊙ and □ are the mean experimental H_2 and H_2O respectively; solid and dashed line are the mean computed H_2 and H_2O respectively

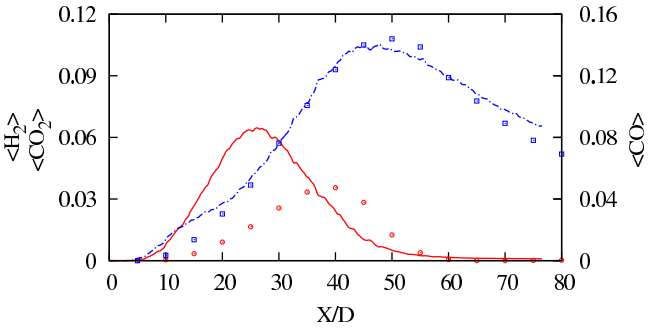

Figure 12: Profiles of mean chemical species CO_2 and CO for LES-R5 compared with experiments, where ⊙ and □ are the mean experimental CO and CO_2 respectively; solid and dashed line are the mean computed CO and CO_2 respectively

Fig.3 for three different constant associated with EDC model. It is observed that the mean temperature changes drastically with increase in the model constant C_{EDC}. The model constant $C_{EDC} = 0.2$ under predicts the temperature as well as mass fraction but on the other hand model constant $C_{EDC} = 0.3$ over predicts the mean quantities. Prediction with the model constant $C_{EDC} = 0.25$ is in reasonable accordance with experiments.

Mixture fraction shown in Fig.3 is calculated using Barlow and Frank[28] formulation. It is observed that the computed mixture fraction is independent of model constant. Explanation for this behavior can be given like this, in the present study density is formulated using Equ. (21), where the transport Equ.(3) for conserved variables ρY_i are summed. In transport Equ.(3) the sum of source terms $\left(\sum_{i=1}^{i=n} \omega_i = 0\right)$ and that leads to the model constant C_{EDC} independent density. It is observed from Fig.3 that the mean values of temperature and mass fractions are overpredicted up to $X/D = 30$. That is because of the early jet break up, which causes substantial mixing and enhancement in reaction rate upstream.

The radial profiles of the calculated mean mass fractions of CO_2,H_2O, CH_4, temperature,

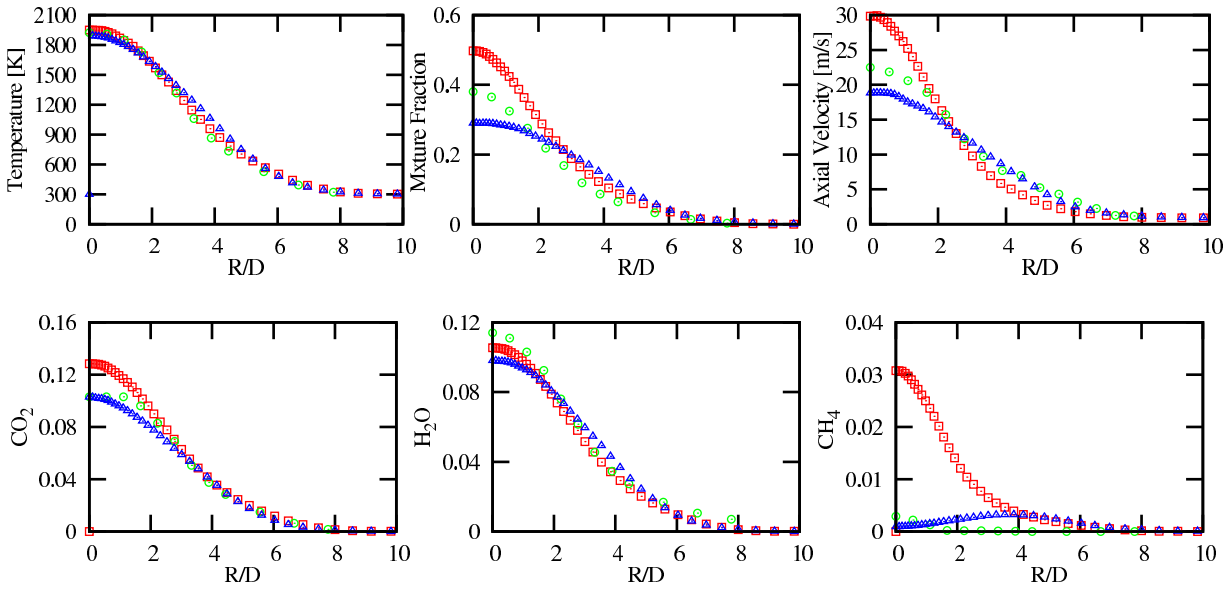

Figure 13: Mean mass fractions of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity, at $\frac{R}{D} = 45$, where ⊙, □ and △ represent Experimental, LES-R2 and LES-R5 respectively

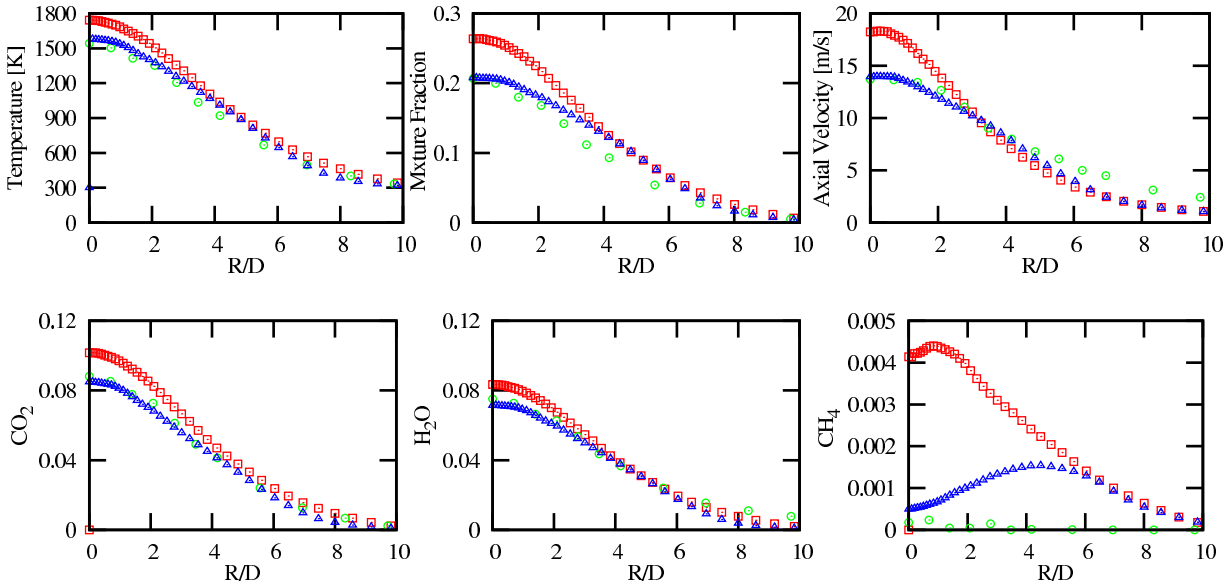

Figure 14: Mean mass fractions of CO_2,H_2O, CH_4, Temperature, Mixture Fraction and Axial velocity, at $\frac{R}{D} = 60$, where ⊙, □ and △ represent Experimental, LES-R2 and LES-R5 respectively

and mixture fraction at $R/D = 30, 45$ and $R/D = 60$ are compared with experiments and plotted in Fig.4, Fig.6, and Fig.8, respectively for LES-R1, LES-R2 and LES-R3. The comparison is relatively better for $C_{EDC} = 0.25$, and it is observed that the computed velocity and mixture fraction profiles do not change with changing the model constant. The reason for this behavior has been mentioned previously. The root mean square (RMS) value of the calculated

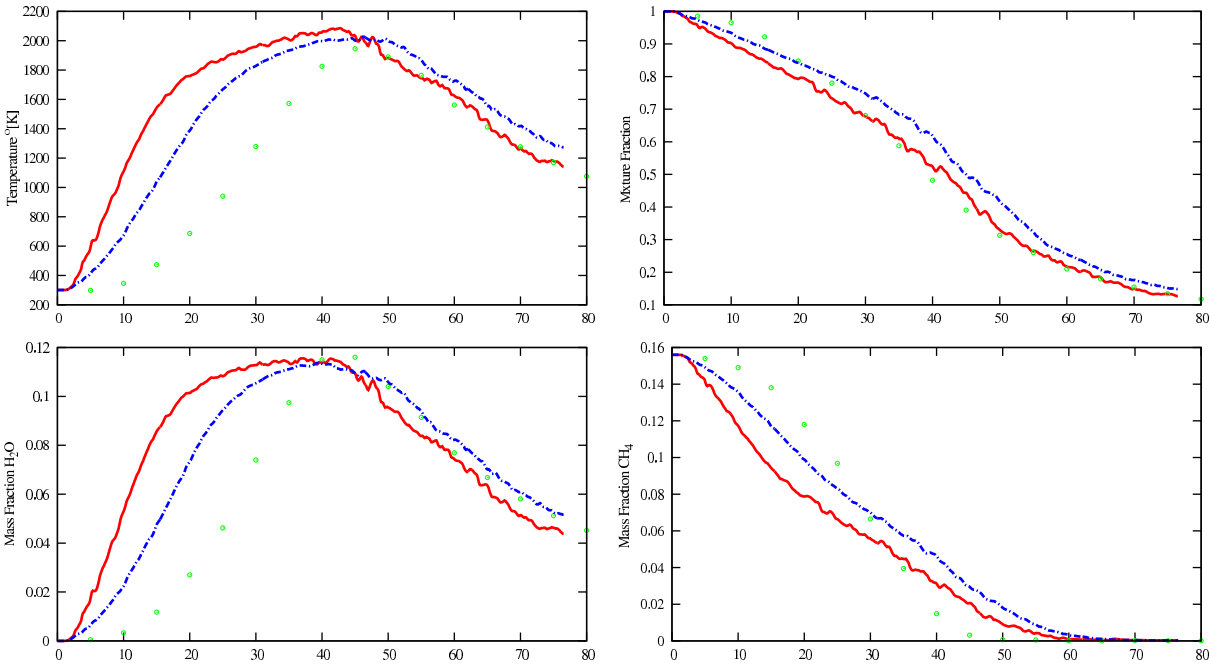

Figure 15: Mean mass fractions of H_2O, CH_4, Temperature and Mixture Fraction for a LES-R3 (dashed line) and LES-R4 (solid line) compared with Experiments(⊙)

mass fractions CO_2, H_2O, CH_4, temperature, and mixture fraction at $R/D = 30, 45$ and 60 are shown in Fig.5, Fig.7, and Fig.9. The agreement between the experiments and computed results is reasonable. The agreement is excellent at $R/D = 45$ and $R/D = 60$ especially for the temperature and mass species. Otherwise the peak in RMS values have been captured reasonably well.

In order to establish the influence of chemical mechanism in the present study, two reaction mechanisms, a single step, Equ. (16), and a three step, Equ. (17), with the fast chemistry is studied. Figure. 10 shows the predicated mean and RMS profiles of the temperature and axial velocity along the centerline compared with experiments. Figure. 11 shows the mean profiles of the chemical species H_2O and H_2 along the axial direction compared with experiments and Fig.12 shows the mean profiles of the chemical species CO_2 and CO along the axial direction compared with experiments. The mean values of temperature, axial velocity, CO_2 and H_2O are predicted satisfactory but species CO and H_2 are over predicted and the peak is also shifted upstream. The overprediction and shifting of the CO and H_2 were caused by early jet break up and fast chemistry assumption. It can been seen from Fig.10 that the peak of the variance of temperature and velocity is shifted upstream. That is because the fluid near to the nozzle is strongly decelerated due to instantaneous mixing which causes sudden heat release and thus expansion. The boundary condition at inflow is a fixed velocities and then sudden heat release and expansion near the nozzle leads to the production of momentum and turbulent kinetic energy, as observed in Fig. 10. In addition the central differencing scheme used for convective terms tends to produce high fluctuations especially close to the nozzle. Simulating upstream nozzle using

immersed boundary condition along with higher order diffusive scheme might improve the solution. Assuming the fast chemistry assumption for partially premixed (CH_4/air) jet with EDC model leads to the overprediction of CO and H_2. It is also observed from Fig.10 that although the temperature RMS profile is shifted upstream but the general trend well captured especially the decrease in the temperature RMS around the maximum mean temperature. Figures 13 and 14 show the radial profiles of the mean mass fractions CO_2, H_2O, CH_4, temperature, and mixture fraction at $R/D = 30$ and 60, respectively. The predictions are in reasonable agreement with the experimental data.

The influence of χ have been studied and is shown in Fig 1. As it was mentioned that with proper modeling of the χ the prediction might improve. The present formulation of χ does not account the finite rate kinetics effects and these effects might be included in future version of χ. In the present study a constant value of the C_{EDC} is assumed and then fine structure region, γ_λ, is entirely a function of the subgrid viscosity. To account for the effects of instantaneous parameters a dynamic version of the model constant C_{EDC} is required and that will definitely improve the prediction.

To understand the influence of subgrid models two LES simulation with dynamic and Smagorinsky subgrid model were carried out. Figure 15 shows the calculated mass fractions of H_2O, CH_4, mean temperature, and mixture fraction along the centerline. The dynamic model tends to produce too fast reactions upstream, that is because the viscosity computed with dynamic model is smaller than the Smagorinsky model. It is also observed that the predictions of axial velocity improves with the dynamic model.

5 CONCLUSIONS

In RANS, the EDC model has been been used successfully for the wide range of the problems with out changing the model constant. However extension of the EDC model for LES requires proper modeling of the fine structure region. An empirical formulation for the fine structure region based on the molecular and subgrid eddy viscosity is proposed. The importance of modeling the fraction of the reactable fine structure is discussed. A preliminary EDC model has been formulated for Large-eddy simulations as a combustion model. The model has been applied in a large-eddy simulation of a turbulent methane/air flame Sandia flame D. A Proposal for modifying the EDC model constant is made. The model constant $C_{EDC} = 0.25$ gave reasonable results for Sandia Flame D. The prediction will improve with the dynamic version of the model constant. The current work further emphasizes the role of EDC model constant, subgrid models and chemical mechanism. The results are compared with experimental data for the velocity, major species including CO and H_2, the mixture fraction etc. The agreement is reasonable for all quantities. The density formulation based on the conservation of species is presented. The present approach gives better stability especially close to nozzle. The density computed with this approach does not include the effects of the chemical source term which makes mixture fraction and velocity predictions independent of the EDC model constant.

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