
This item was submitted to [Loughborough's Research Repository](#) by the author.
Items in Figshare are protected by copyright, with all rights reserved, unless otherwise indicated.

Unsteady flamelet / progress variable approach for non-premixed turbulent lifted flames

PLEASE CITE THE PUBLISHED VERSION

VERSION

NA (Not Applicable or Unknown)

LICENCE

CC BY-NC-ND 4.0

REPOSITORY RECORD

Sadasivuni, S.K., W. Malalasekera, and Salah S. Ibrahim. 2019. "Unsteady Flamelet / Progress Variable Approach for Non-premixed Turbulent Lifted Flames". figshare. <https://hdl.handle.net/2134/5835>.

This item was submitted to Loughborough's Institutional Repository (<https://dspace.lboro.ac.uk/>) by the author and is made available under the following Creative Commons Licence conditions.



For the full text of this licence, please go to:
<http://creativecommons.org/licenses/by-nc-nd/2.5/>

Unsteady Flamelet / Progress Variable Approach for Non-premixed Turbulent Lifted Flames

S. K. Sadasivuni¹, W. Malalasekera¹, and S. S. Ibrahim²

¹*Wolfson School of Mechanical and Manufacturing Engineering, Loughborough University, Loughborough, LE113TU, Leicestershire, United Kingdom, mmsks@lboro.ac.uk, W.Malalasekera@lboro.ac.uk*

²*Automotive and Aerospace Engineering, Loughborough University, Loughborough, LE113TU, Leicestershire, United Kingdom, S.S.Ibrahim@lboro.ac.uk*

Abstract—The unsteady flamelet/progress variable approach has been developed for the prediction of a lifted flame to capture the extinction and re-ignition physics. In this work inclusion of the time variant behavior in the flamelet generation embedded in the large eddy simulation technique, allows better understanding of partially premixed flame dynamics. In the process sufficient simulations to generate unsteady laminar flamelets are performed, which are a function of time. These flamelets are used for the generation of the look-up table and the flamelet library is produced. This library is used for the calculation of temperature and other species in the computational domain as the solution progresses. The library constitutes filtered quantities of all the scalars as a function of mean mixture fraction, mixture fraction variance and mean progress variable. Mixture fraction and progress variable distributions are assumed to be β -PDF and δ -PDF respectively. The technique used here is known as the unsteady flamelet progress variable (UFPV) approach. One of the well known lifted flames is considered for the present modeling which shows flame lift-off. The results are compared with the experimental data for the mixture fraction and temperature. Lift off height is predicted from the numerical calculations and compared with the experimentally given value. Comparisons show a reasonably good agreement and the UFPV combustion model appear to be a promising technique for the prediction of lifted and partially premixed flames.

1. Introduction

Flame stability has been the utmost criteria for the modern gas turbine combustion systems

in-order to attain lower emissions. Experimentalists in the research of diffusion combustion claim to observe the flame lift-off, re-ignition and extinction phenomena more often. Regulations on emissions from gas turbines also pressurize the research in combustion to develop models which predict close to modern day gas turbine combustors. Pollutants such as NO_x and CO form the prime target for all the combustion models. The combustion models that have been in extensive use for numerical modeling of non-premixed turbulent flames are laminar flamelet model [1], conditional moment closure [2] and joint PDF model [3]. Laminar flamelet model is most widely used for modeling aspects of all practical combustors. Flamelet model is considered as a turbulent diffusion flame as an ensemble of laminar diffusion flamelets subjected to stretch in the turbulent flow. Thermo-chemical state of any flamelet is given as a function of scalar dissipation rate and mixture fraction prior to turbulent calculations. Turbulent mean values of all reactive scalars are obtained from flamelet profiles which are in the pre-processed presumed probability density function data. However, NO_x predictions are not well captured with this model. This formulation of laminar steady flamelets is also termed as steady laminar flamelet model (SLFM). Flamelet theory provides the advantage of lowering the computational cost while considering the coupling of turbulence and chemistry interactions. Turbulent partially premixed combustion is the subject of present research with the application of advanced flamelet modeling known as flamelet progress variable method. Flamelet progress variable (FPV) approach forms the extended development of the SLFM technique. The FPV approach takes the similar theory of the steady flamelet model [4] which employs diffusion flamelets but replaces the scalar dissipation rate with a flamelet parameter based on reaction progress variable to define the flamelet structure. Progress variable approach, developed by Pierce and Moin [5] for the LES based non-premixed combustion not only reduced the computational time for solving the transport equations for all the species but also predicts the right lifted flame dynamics.

The joint filtered PDF of mixture fraction and reaction progress variable was first modeled through a presumed PDF approach by Pierce and Moin [5]. A beta function was assumed for the marginal filtered PDF (FPDF) of mixture fraction and a delta function for reaction progress variable. The FPV approach has proved to predict the stabilization characteristics of a confined turbulent non-premixed swirling flame more precisely than SLFM. Using the direct numerical simulation (DNS) technique Ihme *et al.* [6] made some significant changes to the above methodology by incorporating the beta (β) function for the FPDF of reaction progress variable and also by providing a closure model for the reactive scalar variance term. Modeling of re-ignition phenomena at lower scalar dissipation rates was proved to be inaccurate and therefore lead to the extension of the FPV approach to unsteady flamelet formulation, Pitsch and Ihme [7]. This unsteady flamelet approximation was applied to the confined turbulent non-premixed swirling flames employed previously by Pierce and Moin [8], embedded with progress variable approach giving a new dimension to the flamelet theory termed as unsteady flamelet progress variable (UFPV) approach. The filtered PDF for the progress variable was assumed to be a delta function. A noticeable progress in the predictions of the distribution of mass fraction of CO was observed. In the present work the UFPV approach is used for the first time to predict the behavior of partially premixed turbulent lifted flames. Ihme *et al.* [6] proposed the FPDF to be a beta function distribution, but here due to computational cost a delta PDF is used for the for the progress variable. The beta PDF formulation has been used for the progress variable without the consideration of scalar dissipation fluctuations for lifted flames and found to predict good agreement with the experimental data, Ravikanti [9].

Large eddy simulation demonstrates accurate and more sophisticated methodology for turbulence calculations compared to Reynolds Averaged Navier Stokes (RANS) based modeling. LES resolves the large scale turbulent motions which contain the majority of turbulent kinetic energy and control the dynamics of turbulence, whereas the small scales or

sub-grid scales are modeled. The advantage of resolving the large scale motion is not applicable to chemical source term as the chemical time scales are smaller and therefore combustion needs to be modeled. However, LES seems to have the advantage due to its ability to predict accurately the intense scalar mixing process in any complex flow. UFPV approach with LES takes the advantage of the improved modeling strategy and thus forms the current research issue.

Present study aims at performance calculation of UFPV model on the lifted flames. The lifted flame selected for the present study includes the experiments performed on a vitiated co-flow burner by Cabra *et al.* [10]. UFPV approach coupled with the in-house LES code developed by Kirkpatrick [11] is used for the simulations of the lifted flame. Complete comparisons of the lift-off height and radial profiles of mean temperature and mean mixture fraction with the experiments have been presented. Flame extinction and re-ignition phenomena are also explained with the scattered data distribution of mixture fraction with the temperature and comparison with the experimental data at different axial locations along the burner.

2. Numerical Modeling

In LES calculations, the large scales are calculated and the small ones are modeled. The box or top hat filter is used in the present code for solving the governing equations of the turbulent reacting flow by considering the equations of mass, momentum, mixture fraction and progress variable. Smagorinsky eddy viscosity model is used for modeling small sub-grid scales which are a prime source in combustion modeling. The dynamic procedure of Piomelli and Liu [12] is used to calculate eddy viscosity constant dynamically.

2.1 Unsteady Flamelet Progress Variable Approach

In the SLFM approach a turbulent diffusion flame is assumed to be an ensemble of laminar diffusion flamelets as mentioned earlier, which parameterizes the flamelets for the steady state

solution of flamelet equations with a conserved scalar, mixture fraction (Z) and its corresponding stoichiometric scalar dissipation rate (χ_{st}). This theory of SLFM forms the basis for the FPV approach. Steady flamelet model predicts neither the flame lift-off, which is typically a common feature in most of the combustion devices nor the extinction and re-ignition which has a considerable effect on the flame structure. The flamelet theory coupled with progress variable approach introduced by Pierce and Moin [5] addresses one of the above drawbacks with the steady flamelet modeling. But the flame extinction and re-ignition effects can only be captured by unsteady behavior of the flamelets. The incorrect representation of flame lift can lead to large discrepancies in flow field predictions, as shown by Pierce and Moin [5] and Pitsch *et al.* [13] which would certainly translate into inaccuracies in the prediction of pollutants. The flamelet progress variable approach can be considered as the initial principle modeling efforts for the development of UFPV approach.

Unsteady flamelet generation replaces the steady flamelet solution, thereby improving the flamelet progress variable approach to a new modeling technique called UFPV model. An unsteady/flamelet progress variable method was developed and formulated as an extension of the steady flamelet/progress variable model for non-premixed turbulent combustion, Pitsch and Ihme [7]. The three main quantities used to parameterize the flamelet solutions are the mixture fraction (Z), stoichiometric scalar dissipation rate (χ_{st}) and flamelet parameter (λ) which is related to the reaction progress variable (C). A presumed joint FPDF is used to model the above quantities. The flamelet parameter is defined from the progress variable in such a way that it is independent of the mixture fraction and scalar dissipation rate. A pre-integrated flamelet library, which includes the filtered quantities for all the scalars as a function of the filtered mixture fraction, the sub-filter mixture fraction variance, the filtered reaction progress variable and the filtered scalar dissipation rate is generated. The transport equation for the filtered reaction progress variable is solved. The filtered chemical source term in the progress

variable transport equation is determined from the flamelet library together with the presumed FPDF of Z , λ and χ_{st} . Hence, a look-up table concept with the flamelet parameter (λ) introduced in the progress variable approach which is the maximum of the summation of mass fractions of the product species like CO_2 and CO (in the present case, C_{max}) is considered. FPV approach considers the replacement of scalar dissipation rate with the flamelet parameter which is a function of reaction progress variable (C) whereas UFPV approach takes into account of the time varying behavior of the flamelet solution. The unsteady flamelet solutions are obtained from FlameMaster code originally developed by Pitsch [14]. The chemistry involved in the code includes GRI 2.11 mechanism with the assumption of unity Lewis numbers for all the species without the radiation effect. In the present study, variations in scalar dissipation rate are neglected considering only single scalar dissipation rate equal to 0.1s^{-1} .

The unsteady flamelet library is constructed by computing extinguished and re-ignited flamelets and is shown in Fig. 1. The entire solution space is represented by all the dotted vertical lines at different scalar dissipation rates. But for the present simulation we consider only one scalar dissipation rate at 0.1s^{-1} taking computational time into account by neglecting the variations in scalar dissipation effects. Inclusion of flamelet parameter eliminates time and therefore making the unsteady flamelet solution as a function of mixture fraction, scalar dissipation rate and flamelet parameter. The flamelet solutions for all scalar quantities in general for UFPV approach is given as

$$\phi = \phi(Z, \lambda, \chi_{st}) \quad (1)$$

The filtered quantities of any scalar is performed by the joint PDF of the above three parameters and is given as

$$\tilde{\phi} = \int_{\lambda^-}^{\lambda^+} \int_0^{\lambda_{\max}} \int_0^1 \phi(Z, \lambda, \chi_{st}) \tilde{P}(Z, \lambda, \chi_{st}) dZ d\lambda d\chi_{st} \quad (2)$$

The presumed PDF of the three parameters is assumed to be independent of each other and therefore can be written as

$$\tilde{P}(Z, \lambda, \chi_{st}) = \tilde{P}(Z) \tilde{P}(\lambda, \chi_{st}) \quad (3)$$

The marginal Favre filtered PDF of the mixture fraction is assumed to be a beta function that includes mean mixture fraction and its variance. The variations in flamelet parameter (λ) and scalar dissipation (χ) are considered as Favre filtered delta PDF functions in order to reduce the dimensionality of the pre-PDF lookup tables and thereby to reduce the computational cost. Therefore both the above parameters are described by delta function PDF, Pitsch and Ihme [7].

The joint PDF can therefore be written as

$$\tilde{P}(Z, \lambda, \chi_{st}) = \beta(Z; \tilde{Z}, \tilde{Z}''^2) \delta(\lambda - \lambda^*) \delta(\chi_{st} - \chi_{st}^*) \quad (4)$$

But as discussed earlier, the present simulation eliminates the variations in scalar dissipation rate by considering only the flamelet parameter which defines the flamelet solution independent of the mixture fraction. Therefore the joint PDF can be reduced as

$$\tilde{P}(Z, \lambda) = \beta(Z; \tilde{Z}, \tilde{Z}''^2) \delta(\lambda - \lambda^*) \quad (5)$$

The value of χ_{st} is considered as a constant value equal to 0.1s^{-1} . Therefore any filtered scalar can now be defined as

$$\tilde{\phi} = \int_0^{\lambda_{\max}} \int_0^1 \phi(Z, \lambda) \tilde{P}(Z, \lambda) dZ d\lambda \quad (6)$$

Berkeley flame operate under partially premixed conditions with the fuel consisting of a mixture of CH_4 and air in the ratio of 1:3 by volume and at a temperature of 323 K while the oxidizer consists of vitiated air at 1355 K. At these conditions, near equilibrium flamelets possess a partially premixed structure. With variations in time, the flamelets are generated from equilibrium state to mixing limits in a smooth transition with uniform change in time. In the present study, a total of 106 unsteady flamelet profiles have been considered at a single scalar

dissipation rate (0.1s^{-1}) to be converted into table format for the input for scalars in the LES simulation. Fig. 2 shows the flamelet solution for parameters like temperature, density, mass fraction of CO_2 and progress variable with mixture fraction.

A pre-integrated PDF lookup table is thus generated from the above equation in the flamelet parameter space where the filtered scalar can be represented as

$$\tilde{\phi} = \tilde{\phi}(\tilde{Z}, \tilde{Z}''^2, \tilde{\lambda}) \quad (7)$$

This table is further converted to progress variable space and given as the input for the LES when the first two moments of the mixture fraction i.e., mean mixture fraction and its variance and the value of flamelet parameter are known. The filtered mixture fraction is calculated from its transport equation as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z}) + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{u}_k\tilde{Z}) = \frac{\partial}{\partial x_k}\left(\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{Z}}{\partial x_k}\right) \quad (8)$$

The sub-grid scale variance of the mixture fraction is modeled from the scale similarity hypothesis of Cook and Riley [15] and is given by

$$\widetilde{Z''^2} = C_z \left(\widehat{\tilde{Z}^2} - \widehat{\tilde{Z}}^2 \right) \quad (9)$$

The hat symbol used on the R.H.S of the above equation is the test filter operator used in the dynamic procedure of Germano *et al.* [16]. The value of constant C_z is 1. The flamelet parameter varies from 0 to 1 from pure mixing to equilibrium limits. The flamelet parameter or λ space is converted to progress variable or C space thereby eliminating the flamelet parameter λ and hence the re-interpolated table which is a set of independent parameters is used for the simulation. Therefore the flamelet library has the filtered scalars as a function of $\tilde{Z}, \widetilde{Z''^2}$ and \tilde{C} which are all known as a part of LES solution. The filtered reaction progress variable can be quickly obtained from the transport equation as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{C}) + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{u}_k\tilde{C}) = \frac{\partial}{\partial x_k}\left(\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{C}}{\partial x_k}\right) + \bar{\rho}\tilde{\omega}_c \quad (10)$$

The sub-grid scale scalar fluxes in the above equation are modeled by the eddy diffusivity model and the values of Sc and Sc_t are 0.7 and 0.4 respectively. The filtered chemical source term $\tilde{\omega}_c$ is obtained from its pre-integrated look-up-table generated from Eq. 6. The re-mapping or the re-interpolation technique originally developed by Ravikanti [9] is used in the present study for the development of fourth dimension in the lookup table (scalar dissipation rate). The re-mapping procedure involves a constraint equation that satisfies the filtered reaction progress variable \tilde{C} , which is the representative of the above transport equation (Eq.10) to be equal to the progress variable obtained from the integration of the steady laminar flamelet solution from Eq. (6). The elimination of the flamelet parameter and scalar dissipation rate makes the solution procedure simple and less time consuming. The re-mapping of $\tilde{\lambda}$ space to \tilde{C} space and the PDF integration forms the pre-processing stage for the simulation to be set-up.

3. Model Validation

The UFPV approach is used here for the first time to predict the flame lift-off behavior rather than to predict the emissions. Considering the flame extinction and re-ignition effects, the details of the validation work is presented below.

3.1 Experimental Details

The experimental study used in the validation procedure of the simulation is the lifted flame configuration of Cabra *et al.* [10]. The lifted flame with CH_4/Air as fuel with the vitiated co-flow of H_2/Air is considered for the combustion model validation with the LES based calculation. The details of the burner geometry, which has a central jet and the co-flow surrounding the jet with the mixture of gases, can be found from Table. 1. The experimental

burner consists of a central nozzle with inner diameter of 4.57 mm and outer diameter of 6.35 mm. The fuel jet consisting of a mixture of 33% CH₄ and 67% air is issued from the central nozzle. A perforated plate of 210 mm diameter through which vitiated co-flow of air is issued surrounds the central nozzle. A flow blockage of 85% was reported with 2200 holes drilled in it. The vitiated co-flow consists of products of lean premixed H₂/Air flame with an equivalence ratio of 0.4. The entrainment of ambient air into the co-flow has been delayed by incorporating an exit collar which surrounds the perforated plate.

The measured lift off height from the experiments in terms of H/D ratio is found to be 35. The value of H is the axial distance of the flame base where the temperature is cut-off with a value equal to coflow temperature of 1355 K. The jet penetration into the flame makes the flame structure as shown in the Fig. 3 where the lift-off height is H/D and the flame penetration depth is specified as l_c . D is the central jet diameter with the value as given in the above table. The mean temperature and mixture fraction radial profiles are measured at different axial locations and are compared with the computational results that are discussed in the next section. The scattered data of temperature at various axial locations are also provided. The axial locations are normalized with the jet diameter and therefore at Z/D of 1, 15, 30, 40, 50 and 70 are considered for the computational validation.

3.2 Computational Details

The in-house LES code called PUFFIN originally developed by Kirkpatrick [11] as discussed earlier is used in the simulation involving the finite volume scheme. The computational domain has dimensions of 200 x 200 x 410 (all dimensions are in mm). The axial distance of approximately 90 jet diameters and the burner width of approximately 44 jet diameters is used in order to account the independency of flow entrainment from the surroundings. An inlet jet velocity profile is specified with a 1/7th power law profile. Convective outlet boundary condition is used at the outlet surface and all the walls and co-flow boundaries in the domain

have been treated as adiabatic. No-slip boundary condition is used in the near wall flow using log-law wall functions. A Cartesian staggered non-uniform grid distribution of $85 \times 85 \times 150$ in the X, Y and Z directions to discretize the domain has been used to optimize the simulation time. The grid details are depicted in the Fig. 4.

An ignition source is provided with the progress variable of 0.7 patched in the region of best mixed fuel air mixture. Simulations are run for sufficient length of time before capturing the statistics. A total time of 50 ms is allowed to run in order to have a periodic behavior of flow with the fixed limits for the Courant number. The time integration of the scalar equations is accomplished through Crank-Nicolson scheme. Bi-conjugate Gradient Stabilized (BiCGStab) solver with Modified Strongly Implicit (MSI) pre-conditioner has been employed in this simulation for the pressure correction equation.

Images from the experiments are captured for the flame lift-off and lift-off height is normalized with the jet diameter and specified as H/D ratio. The experimentally found value of H/D is 35. This lift is considered as the lowest position of flame luminosity.

4. Results and Discussion

The measured values of mean mixture fraction and mean temperature at various axial locations are compared with the numerical results. The lift-off is measured from the boundary line of the temperature which differentiates the hot gases and co-flow temperature. The distance from the jet base to the position where the temperature is 1355K as shown in the Fig. 3 is considered as the lift-off height. The lift-off can also be specified from the simulation results based on the maximum chemical source term. But in the present section we represent the value of H/D with the temperature boundary line of 1355K. The scattered data of temperature is also compared with the experimental results for the close prediction of flame extinction and re-ignition. The instantaneous snapshots of temperature at the mid plane of the domain will give a clear picture

of the flame re-attachment and extinction at various times. The present simulation results are compared with the FPV- δ function model developed by Ravikanti [9] applied to the same burner geometry. Comparison of UFPV and FPV makes a clear distinction for the modeling capabilities of UFPV approach. Both the models are based on delta function PDF for the progress variable. Thus the UFPV- δ function model is tested for the flame structure predictions rather than for any emissions comparison. The FPV- β function model is also tested and compared by Ravikanti [9] with the FPV- δ function model. But the present paper discusses the assessment of modeling strategy of the UFPV- δ with FPV- δ function model.

4.1 Flame Structure

The flame surface lifting location is described by the temperature contour plot. The lift off height is obtained as 44.11 in terms of H/D ratio from the numerical results. Fig. 5 shows the contours of the temperature at the mid plane ($X=0$). The flame lift is defined by the value of T_c which is equal to 1355K, the co-flow temperature, which distinguishes the higher flame temperature zone. The experimental data shows the lift off height, H/D equal to 35. There has been 20 % over-prediction in the numerical solution for the lift off height.

The above result is from the UFPV model with a scalar dissipation rate of $0.1s^{-1}$ with the time variations in the flamelet solutions. The scalar dissipation rate close to zero resembles the complete set of unsteady solutions from pure mixing to equilibrium (Ref. Fig.1) and therefore a scalar dissipation rate of $0.1s^{-1}$ is considered for the present study. The UFPV model with the scalar dissipation rate fluctuations makes the simulation problematic with the additional dimension of scalar dissipation rate in the pre-PDF lookup tables, but has the capability to predict the extinction and re-ignition physics. Considering the computational cost, UFPV model with a single scalar dissipation rate is taken as the initial task for its validation. FPV and UFPV models are compared with the available experimental data. The FPV approach with the delta PDF for progress variable have found to predict a lift off height, H/D equal to 17.5,

Ravikanti [9]. This under-prediction of 50 % in the lift off height is due to the assumption of steady laminar flamelets which does not consider the time variations in the flamelet profiles eventhough the flamelet PDF lookup table included all the steady flamelets along the S-Curve as depicted in the Fig. 1 for the FPV model. UFPV on the otherhand, has the advantage of the unsteady effects of the flamelet equations to predict a better solution compared with the steady solution space. Therefore, the addition of unsteady solution makes the UFPV model to overpredict the lift-off height in terms of H/D ratio.

4.2 Radial Mean Temperature Plots

A total time of 20ms is considered for the collection of statistics and data averging is done for this time period. The radial mean temperature plots at Z/D locations of 1.0, 15.0, 30.0, 40.0, 50.0 and 70.0 are depicted in Fig. 6. The locations far away upstream, Z/D = 40.0, 50.0 and 70.0 are the positions where the flame stability resides and therefore a close match with the experiments in these locations gives a better indication of the performance of the combustion model.

The results are compared with the experiments, as well as with the results obtained from the FPV- δ function PDF by Ravikanti [9]. At the initial two locations both the models predict very well. At the location Z/D=30.0, the comparison of UFPV is much closer to the experimental data. In the case of FPV- δ model due to under prediction of the lift off the temperature profile show an over prediction. At the locations at Z/D =30.0 and 40.0 the UFPV approach gives better results. But there is still some under-prediction in the temperature as we go along the radial direction in the UFPV model. This becomes much severe at the next location at Z/D=50.0 where the FPV- δ model over-predicts due to short lift-off in the flame and UFPV- δ under-predicts due to more lift-off than expected. At the last location, both models seem to predict a similar profile.

4.3 Radial Mean Mixture Fraction Plots

The radial mean mixture fraction plots are compared with experiments as shown in Fig. 7. The numerical mean mixture fraction shows good match with the experimental results at all the locations. The centreline mixture fraction values at locations $Z/D=1.0$ to 40.0 are overpredicted with a little margin. Also at these axial locations, the radial profiles over-predict to a marginal extent. But the temperature at the same locations (Fig. 6) show a close match with the experiments. The decrease in the mixture fraction from fuel rich ($Z=1$) to oxidizer rich ($Z=0$) mixture increases the temperature and attains the maximum value at the stoichiometric mixture fraction (Z_{st}) equal to 0.17 . Therefore, till the axial location equal to $Z/D=50$, the mixture fraction profiles vary slightly with the experimental results. But at the locations $Z/D=50$ and 70 numerical results are close to the experiments in the entire radial band as the centreline mixture fraction comes closer to Z_{st} . The relation between the two parameters, mixture fraction and temperature which is given as the input to LES is specified in the form of PDF lookup tables. The interrelation between the above two parameters also depend on the chemical mechanism (GRI 2.11) used.

4.4 Instantaneous Temperature Comparison

The flame extinction and re-ignition phenomena is expected to be captured with the UFPV approach. The visualization of the flame structure at various times is done with the instantaneous temperature snapshots to study the flame extinction and re-ignition. Scattered data of the temperature with the mixture fraction, which is available from the experimental results for various axial locations also provide an understanding of the above mentioned phenomena. The numerical results from FPV and UFPV models are compared with the scattered experimental data and is shown in Fig. 8. The experimental results are available at the same axial locations of $Z/D=1.0, 15.0, 30.0, 40.0, 50.0$ and 70.0 . It has been observed that UFPV model predicts most of the mixing till the axial location of $Z/D=40$. Therefore the

combustion models, FPV and UFPV are compared only at the last two locations of $Z/D=50$ and 70 with the experiments. The scattered data for the temperature versus mixture fraction shows the complete combustion zone from pure mixing limits to equilibrium limits (Fig.8b). The dotted line represents the stoichiometric mixture fraction location.

The above data comparison shows both advantages and drawbacks of the present UFPV model under study. At the location $Z/D=50$ (Fig. 8f), UFPV model is able to capture the mixing line, which is an indication of some locations at this axial plane where the fuel and oxidiser are still in the unburnt state. From Fig. 5 it can be observed that at the axial location $Z/D=50$, the flame structure has most of the region covered with mixing limit temperature profiles of 1355K . At the centreline, the flame has the temperature rise which can be supported from Fig. 8e where the scattered data lies with an increased temperature values near to 1800K . But the drawback at this location from UFPV model should also be emphasized. The equilibrium limit is not predicted well when compared with both FPV model and experiments, considering the maximum temperature limits as shown in Fig. 8b and 8d. At the location $Z/D=70$, both the combustion models and experimental data resemble a good match. The fuel and oxidizer are no more in the pure mixing state and therefore the temperature rise occurs and the maximum temperature can be seen to occur at stoichiometric mixture fraction. FPV- δ model has the mixture fraction limits extended to a maximum of 0.4 (Fig. 8c) whereas the experimental data shows a maximum near to 0.3 mixture fraction (Fig. 8a). UFPV model is able to predict close to experimental values but the maximum temperature is slightly under-predicted. This under-prediction in temperature is caused due to higher lift off height predicted by the UFPV approach.

7. Conclusions

Inclusion of unsteady flamelets to the PDF solution space allowed capturing the dissipation to a

much better extent. UFPV model with the delta PDF for progress variable is found to be more accurate than the steady solution of laminar flamelets. The flame lift-off is improved with an over prediction which is due to more dissipation effects of the unsteady behavior of the flamelet solution. The numerical results compared well with the experiments for temperature and mixture fraction. The UFPV model will be extended for the complete solution space considering all the scalar dissipation rates as a next step. This paper clearly gives an indication of the improvisation and advancement in the flamelet modeling with the UFPV approach. The lifted flame behavior which is difficult to predict is numerically reproduced with the UFPV approach and therefore can be applied to non-premixed turbulent lifted flames of other categories.

8. Acknowledgements

The author is very thankful to Dr. Murthy Ravikanti for providing the baseline code for PDF table generation and for his valuable comments throughout this work. Also very grateful for the support provided by Dr. H. Pitsch, Stanford University, US, with his FlameMaster code for the generation of unsteady flamelets.

References

- [1] Peters N. Laminar Diffusion Flamelet Models in Non-Premixed Turbulent Combustion // Progress in Energy and Combustion Science. 1984. Vol.10, P. 319-339.
- [2] Klimenko A.Y., Bilger R.W. Conditional Moment Closure for Turbulent Combustion // Progress in Energy and Combustion Science. 1999. Vol.25, P. 595-687.
- [3] Pope S.B. PDF methods for Turbulent Reactive Flows // Progress in Energy and Combustion Science. 1985. Vol.11, P. 119-192.
- [4] Bray K.N.C., Peters N. Laminar Flamelets in Turbulent Flames // In Turbulent Reacting Flows (Edited by P.A. Libby and F.A. Williams). 1994. Academic Press London, P. 63-113.
- [5] Pierce C.D., Moin P. Progress-Variable Approach for Large Eddy Simulation of Non-premixed Turbulent Combustion // Journal of Fluid Mechanics. 2004. Vol.504, P. 73-97,
- [6] Ihme M., Cha C. M., Pitsch H. Prediction of Local Extinction and Re-ignition Effects in Non-premixed Turbulent Combustion by a Flamelet/progress Variable Approach // Proceedings of the Combustion Institute, 2005. Vol.30, P. 793–800.
- [7] Pitsch H., Ihme M. An Unsteady/Flamelet Progress Variable Method for LES of Non-premixed Turbulent Combustion // AIAA Paper. 2005. P. 2004-557
- [8] Pierce C. D., Moin P. Large Eddy Simulation of a Confined Coaxial Jet with Swirl and Heat Release // AIAA Paper. 1998. Vol. 98, P. 2892.
- [9] Ravikanti V.V.S.M. Advanced Flamelet Modeling of Turbulent Non-premixed and Partially Premixed Combustion. PhD Thesis. Loughborough University, UK, 2008.
- [10] Cabra R., Chen J.-Y., Dibble R.W., Karpetis A.N., Barlow R.S. Lifted Methane-Air Jet Flames in a Vitiated Coflow // Combustion and Flame. 2005. Vol.143, P. 491-506.
- [11] Kirkpatrick M.P. A Large Eddy Simulation Code for Industrial and Environmental Flows. PhD Thesis. University of Sydney, Australia, 2002.
- [12] Piomeli U., Liu J. Large Eddy Simulation of Rotating Channel Flows using a Localized Dynamic Model // Physics of fluids. 1995. Vol.7, P. 839-848.
- [13] Pitsch H., Chen M., Peters N. Unsteady Flamelet Modeling of Turbulent Hydrogen/air Diffusion Flames // Proceedings of the Combustion Institute. 1998. Vol.27, P. 1057–1064.
- [14] Pitsch H. A C++ Computer Program for 0-D and 1-D Laminar Flame Calculations. RWTH Aachen, 1998.
- [15] Cook A.W., Riley J.J. Subgrid-Scale Modeling for Turbulent Reactive Flows // Combustion and Flame. 1998. Vol.112, P. 593–606.
- [16] Germano M., Piomelli U., Moin O., Cabot W.H. A Dynamic Subgrid Scale Eddy Viscosity Model // Physics of fluids. 1991. A3 (7), P. 1760-1765.

Table 1.Details of Flame and Flow Conditions

Parameter	Jet Conditions	Co-flow Conditions
Re	28,000	23,300
d (mm)	4.57	210
V (m/s)	100	5.4
T (K)	323	1355
X_{O_2}	0.15	0.12
X_{N_2}	0.52	0.73
X_{H_2O}	0.0029	0.15
X_{OH} (ppm)	<1	200
X_{H_2}	0	100
X_{CH_4}	0.33	0.0003
ϕ	-	0.4

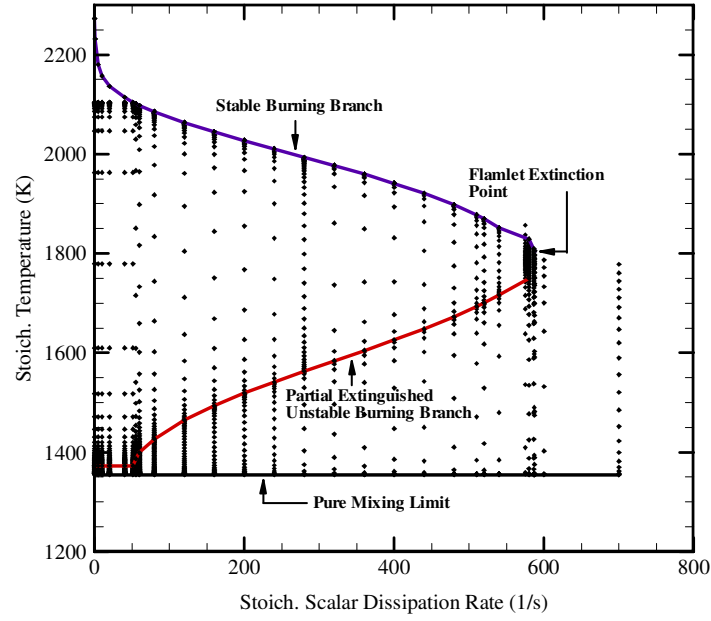


Figure 1 Unsteady Flamelet Solution

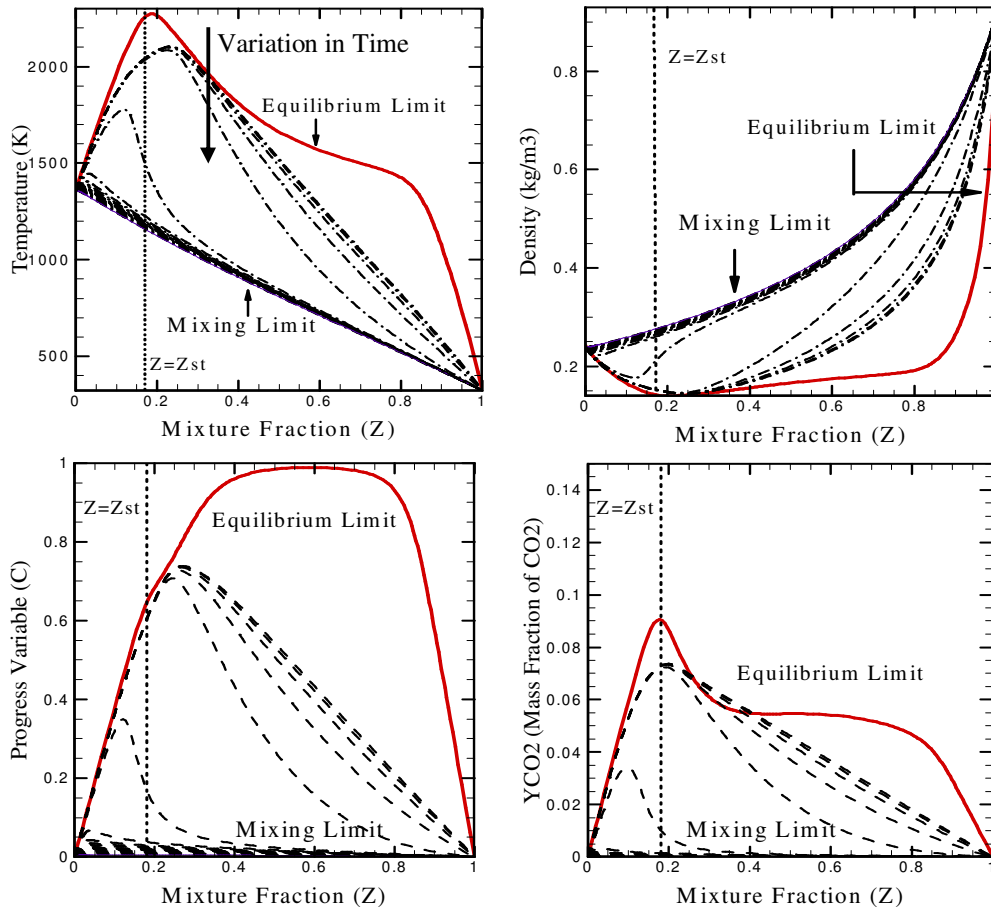
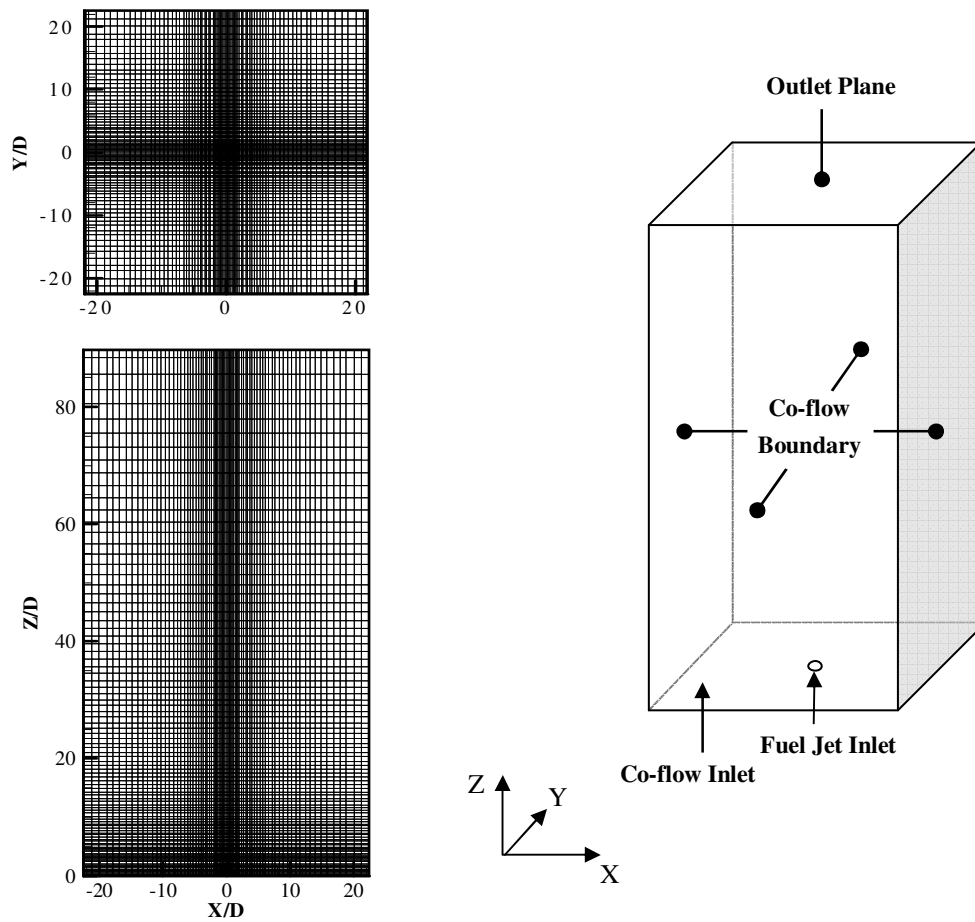
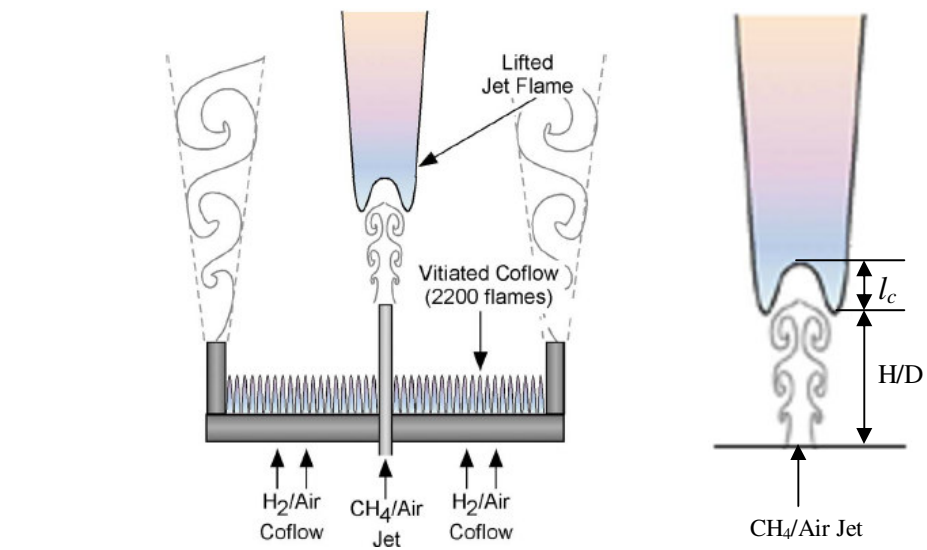


Figure 2 Unsteady Flamelet Solutions at Scalar Dissipation Rate of 0.1s^{-1}



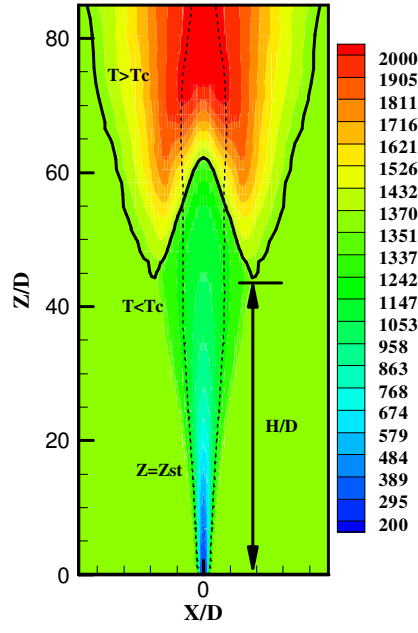


Figure 5 Mean Temperature Contour Plot at X=0 Plane

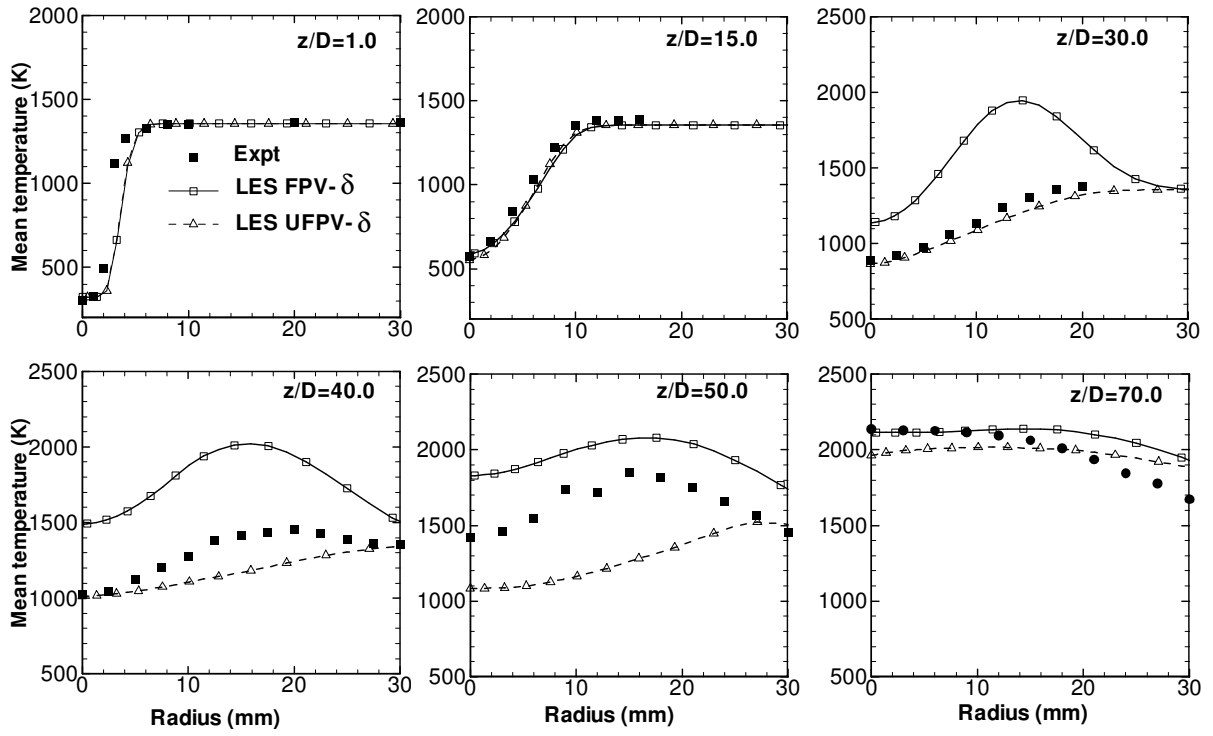


Figure 6 Radial Mean Temperature plots at various axial locations

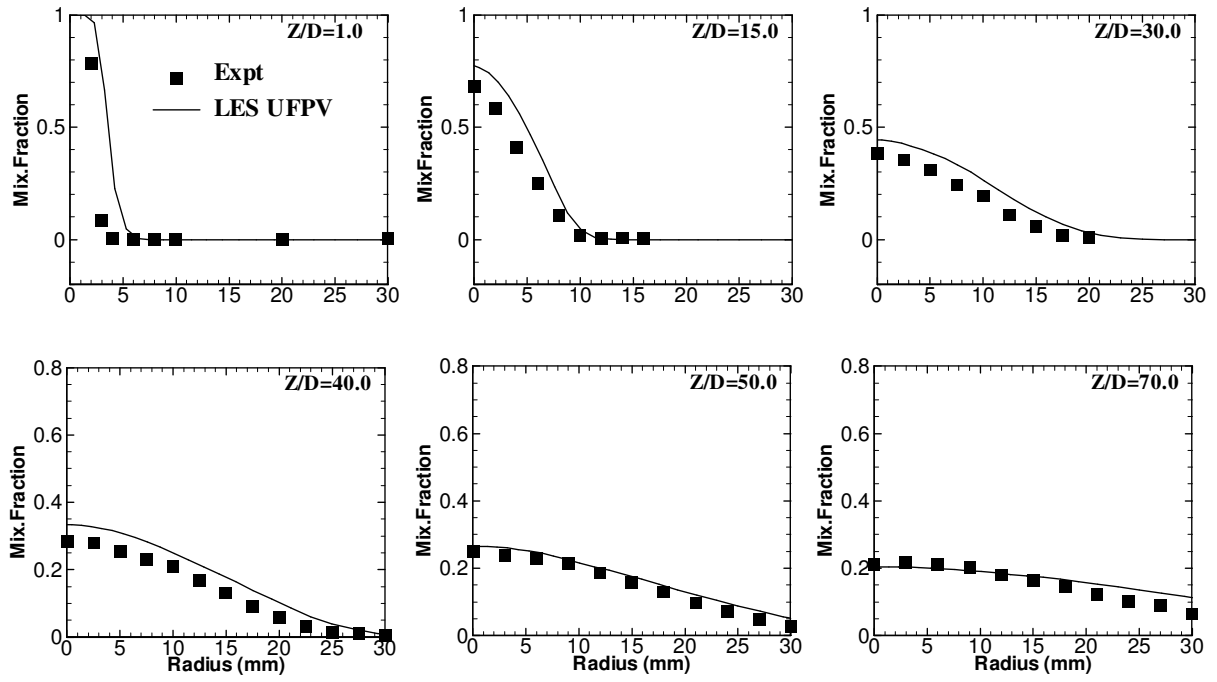


Figure 7 Radial Mean Mixture Fraction plots at various axial locations

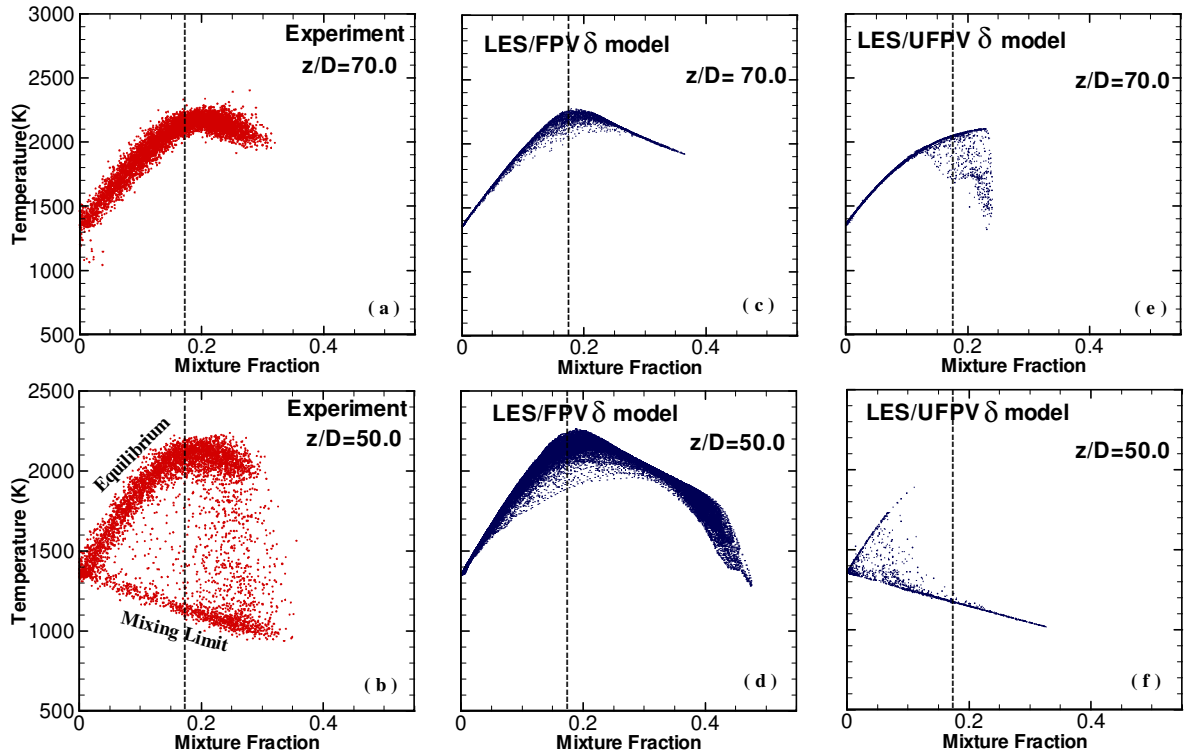


Figure 8 Scattered Temperature Distribution at two axial locations