ASSESSMENT OF A CONDITIONAL PDF-TRANSPORT METHOD IN THE COMBUSTION-LES CONTEXT

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ABSTRACT

The aim of this work is to combine Large-Eddy-Simulation (LES) and the PDF-transport method for the prediction of turbulent non-premixed flames. On the one hand the motivation is based upon the property of LES to provide a better description of complex flows than RANS (Reynolds-Averaged-Navier-Stokes) methods offer. On the other hand PDF-methods allow for exact treatment of the chemical source term, which provides a possibility to describe strong turbulence-chemistry interaction considering chemical time scales with equal or greater magnitude compared to the turbulent time scales.
The intent of this work is to combine the ability of the LES to predict scalar mixing with high accuracy and the property of PDF transport methods to describe the chemical source term in a closed form.

CONDITIONAL PDF TRANSPORT EQUATION

We consider the transport equation for the species mass fraction Y_i with velocity v, density ρ, diffusion coefficient D_i and reaction rate W_i

$$\frac{\partial Y_i}{\partial t} + v\nabla Y_i - \frac{1}{\rho}\nabla(\rho D_i \nabla Y_i) = W_i \tag{1}$$

Following Pope(1985) and Pope(2001) one can define a fine-grained PDF $P' = \delta(Y(f;x,t) - \psi)$ conditioned on the mixture-fraction f, where the conditional expectation is $\langle P' \rangle = P(\psi|f)$.
Multiplying equation (1) by $-P'$ and differentiating with respect to ψ_i one gets (considering that v is not a funtion of the independent random variable ψ)

$$\begin{aligned}-\frac{\partial}{\partial \psi_i}\left(P'\frac{\partial Y_i}{\partial t}\right) - v\frac{\partial}{\partial \psi_i}\left(P'\nabla Y_i\right) + \\ +\frac{1}{\rho}\frac{\partial}{\partial \psi_i}\left(P'\nabla\left(\rho D_i \nabla Y_i\right)\right) = -\frac{\partial}{\partial \psi_i}\left(P' W_i\right)\end{aligned} \tag{2}$$

Using the properties of the fine-grained PDF

$$\frac{\partial P'}{\partial t} = -\frac{\partial}{\partial \psi_i}\left(P'\frac{\partial Y_i}{\partial t}\right) \tag{3}$$

$$\nabla P' = -\frac{\partial P' \nabla Y_i}{\partial \psi_i} \tag{4}$$

one obtains

$$\begin{aligned}\rho\frac{\partial P'}{\partial t} + \rho v \nabla P' + \frac{\partial}{\partial \psi_i}\left(P'\nabla\left(\rho D_i \nabla Y_i\right)\right) = \\ = -\frac{\partial}{\partial \psi_i}\left(\rho P' W_i\right).\end{aligned} \tag{5}$$

Adding the continuity equation $\frac{\partial \rho}{\partial t} + \nabla(\rho v) = 0$ multiplied with P' results in

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho P'\right) + \nabla\left(\rho v P'\right) + \frac{\partial}{\partial \psi_i}\left(P'\nabla\left(\rho D_i \nabla Y_i\right)\right) = \\ = -\frac{\partial}{\partial \psi_i}\left(\rho P' W_i\right).\end{aligned} \tag{6}$$

Equation (6) still represents the transport equation for the conditional fine grained PDF P'. To obtain the transport equation for the PDF P_f, conditional with respect to the mixture fraction f, averaging equation (6) using the sifting property of the delta function

$$\langle \phi(x,t) P'(\psi; f, x, t)\rangle = \langle \phi(x,t)|\psi\rangle \tag{7}$$

yields

$$\begin{aligned}\frac{\partial}{\partial t}\left(\langle \rho|\psi = Y_f\rangle P_f\right) + \nabla\left(\langle \rho v|\psi = Y_f\rangle P_f\right) + \\ +\frac{\partial}{\partial \psi_i}\left(\langle \nabla\left(\rho D_i \nabla Y_i\right)|\psi = Y_f\rangle P_f\right) = \\ = -\frac{\partial}{\partial \psi_i}\left(\langle \rho W_i|\psi = Y_f\rangle P_f\right).\end{aligned} \tag{8}$$

Considering only high Reynolds number flows, one gets after Favre averaging:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{P_f}\right) + \nabla\left(\overline{\rho}\widetilde{v}\widetilde{P_f}\right) + \nabla\left(\overline{\rho}\langle v''|\psi = Y_f\rangle\widetilde{P_f}\right) + \\ +\frac{\partial^2}{\partial \psi_i \partial \psi_j}\left(\overline{\rho}\langle D\left(\nabla Y_i \nabla Y_j\right)|\psi = Y_f\rangle\widetilde{P_f}\right) = \\ = -\frac{\partial}{\partial \psi_i}\left(\overline{\rho}\langle W_i|\psi = Y_f\rangle\widetilde{P_f}\right)\end{aligned} \tag{9}$$

This equation is very similar to the unconditional PDF transport equation. It shows the same terms for convection, turbulent transport, scalar mixing and the chemical source term, which occurs in a closed form. Due to this similarity, this equation can be solved using a Monte Carlo simulation. Furthermore the stochastic equations are the same as for the unconditional PDF. Basically this method could also be used in a fully coupled manner with LES.

EXPERIMENTAL AND NUMERICAL CONFIGURATION

In this work the performance of a PDF-postprocessing method shall be investigated using the Reynolds averaged flow field, turbulence parameters and mixture fraction field obtained from the LES. The burner configuration investigated was designed by Masri et al(1996). Measurements of scalars and velocities were performed by the groups of Barlow et al. (1998), Karpetis et al. (2002) and Schneider et al.(2003), respectively. A fuel pipe expels a methane-air mixture, which consists of 25 vol.% methane ($f_{stoic.} = 0.35$) and 75% air, respectively at a Reynolds number Re=22400 ($u_{jet,bulk} = 49.6m/s$, $D = 7.2mm$). The jet flame is stabilized via a premixed pilot flame ($u_{pilot,bulk} = 11.4m/s$, $D_{pilot} = 18.2mm$). A laminar coaxial coflow provides air at a rate of 0.9m/s.

LES-calculations have been performed by Kempf et al.(2005) and Flemming et al.(2005). The same code is used for this work. The numerical grid consists of 1025x32x60 nodes in the axial, circumferential, and radial directions, mapping a geometry of 40Dx15D. This very fine grid-spacing was chosen as scalars are mainly transported along the axial direction. For the precalculation within the LES-scope, a steady flamelet model is used to obtain an initial but accurate prediction of density. The PDF substep then offers the possibility to investigate a more detailed chemistry, here covered by an ILDM, developed by Maas and Pope (1992). This ILDM uses the mixture fraction and the mass fractions of water and carbon dioxide as parameters. The LES-code already uses a steady flamelet model thus an initial prediction of density is obtained. The PDF substep facilitates an investigation of more detailed chemistry.

EXTRACTION OF THE MIXTURE FRACTION PDF

The PDF of the mixture fraction is reconstructed from the LES using a presumed β-PDF, depending on the mixture fraction and its variance $\widetilde{f''^2}$:

$$P(f) = \frac{f^{a-1}(1-f)^{b-1}}{\int_0^1 f^{a-1}(1-f)^{b-1}df} \tag{10}$$

with

$$a = \widetilde{f}\left(\frac{\widetilde{f}\left(1-\widetilde{f}\right)}{\widetilde{f''^2}} - 1\right) \tag{11}$$

and

$$b = \left(1-\widetilde{f}\right)\left(\frac{\widetilde{f}\left(1-\widetilde{f}\right)}{\widetilde{f''^2}} - 1\right) \tag{12}$$

For each calculated time step of the LES the mixture fraction and its variance can be extracted for every numerical cell.

As the subsequent PDF-transport method was performed on time-averaged values, a mass weighted average of the β-PDFs had to be built. The averaging process was started after a statistically stationary solution of the LES was obtained. The period of time considered for the averaging process was 0.3s. Within this period 10000 samples were taken for the averaging process. As the flow is axisymmetric for the steady state, additional accuracy can be obtained by averaging in circumferential direction. For demonstration,

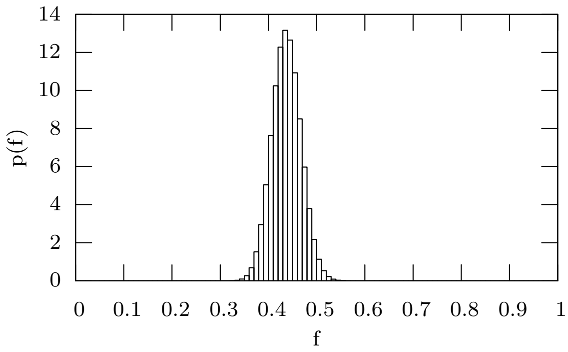

Figure 1: Instantaneous PDF

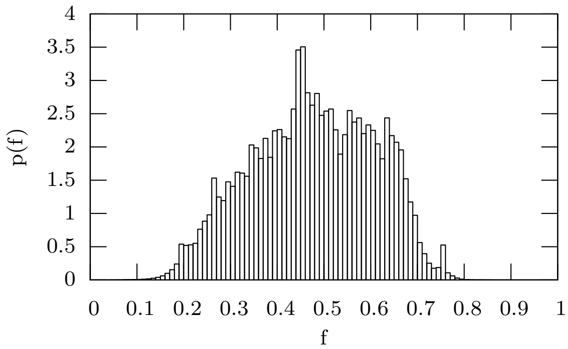

Figure 2: Averaged PDF

figures 1 and 2 show the reconstructed PDFs for a single time step (β-PDF) and after the averaging process .

This PDF was evaluated at a radial distance of one jet diameter and at the axial position of 41.7D.

PARTICLE METHOD

Solving for the conditional PDF

It is possible to solve transport equations of the form of equation (9) for several discrete representations of the mixture fraction. Performing a Monte Carlo simulation however, this would result in an increased amount of stochastic particles and additionally the mixing term of the conditional scalar transport in eq. (9) would need further modelling.

Alternatively a simplified method is used here which is demonstrated in fig. 3. Only one unconditional PDF trans-

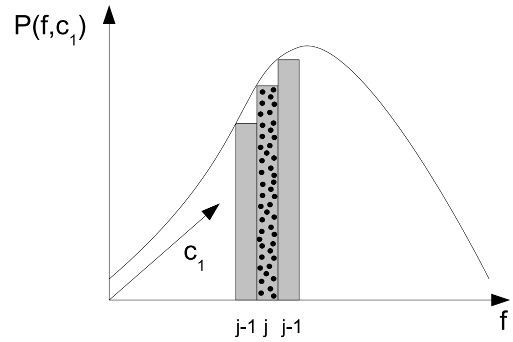

Figure 3: Sorting of Monte-Carlo particles

port equation is solved within the scope of this work. The mixture fraction space is then divided into several bins, corresponding to those used in the above section. For each of those bins the mixture fraction is assumed constant and conditional probabilities for this certain mixture fraction can then be obtained by normalising the local PDF using Bayes' theorem. The conditional PDF is then calculated by dividing by the PDF of the mixture fraction itself

$$P_f(c) = \frac{P(f,c)}{P(f)} \tag{13}$$

where c represents the reaction progress variables. Using the mixture fraction PDF $P_{LES}(f)$ provided by the LES, one can evaluate a new PDF P^* with the marginal PDF $P_{LES}(f)$:

$$P^*(f,c) = P_{f,MC}(c) \cdot P_{LES(f)}. \tag{14}$$

Particle evolution

For axisymmetric problems, particles are propagated in 3D cartesian coordinates and are rotated back into the 2D domain after each convective substep. Convection, mixing (of scalars ξ) and chemical reaction are successively performed in substeps and are described by the following stochastic equations given by Sheiki et al.(2005), where W represents the Wiener increment and l the length of the LES filter:

$$dx_i^+ = \left(u_i + \frac{1}{\overline{\rho}}\frac{\partial \Gamma_t}{\partial x_i}\right)dt + \sqrt{\frac{2\Gamma_T}{\overline{\rho}}}dW \tag{15}$$

$$d\xi^+ = \left(-C_\phi \frac{\Gamma_T}{\overline{\rho} * l^2}\left(\xi^+ - \overline{\xi}\right) + \omega_i\right)dt \tag{16}$$

VALIDATION OF THE CONDITIONING METHOD

To validate the conditioning step of the modified PDF-transport method, results for the calculated mixture fraction in the axial direction and for several axial positions in the radial direction are shown in figures 4 and 5. Each plot shows the results obtained from the LES, the results obtained from the unconditional and conditional PDF-transport method as well as experimental results with errorbars for comparision. One can see that the LES gives a good prediction of the results. Even the unconditional PDF-transport method differs only marginally from the LES. As the mean velocity field is taken from the LES and only turbulent transport is done within the PDF-transport step, this is to be expected.
It can also be seen that the LES-profiles of the mixture fraction almost achieve a perfectly match with the results obtained using the conditional PDF-transport-method. Very small differences are due to the fact that the conditioning step requires the PDF obtained from the PDF-transport model to be non-zero for the whole mixture fraction domain. Except for regions where only intermittency effects occur (which is only the case near the inlet), turbulent diffusion should ensure this; even if the probability density is very small in some intervals. In this work on the other hand the PDF-transport equation is solved via a Monte-Carlo method. Therefore the obtained unconditional PDF which results from this step is discrete and may show areas with zero probability. To minimise this effect, averaging over 2000 particles is performed during the solution process. A steady distribution however cannot be achieved everywhere in the solution domain.

RESULTS

Since the applied post-processing method works on averaged properties obtained from the LES, one has to focus on statistical values. Figure 6 shows the radial distributions of the mean values for temperature at several axial positions. To compare the different methods, results gained by the

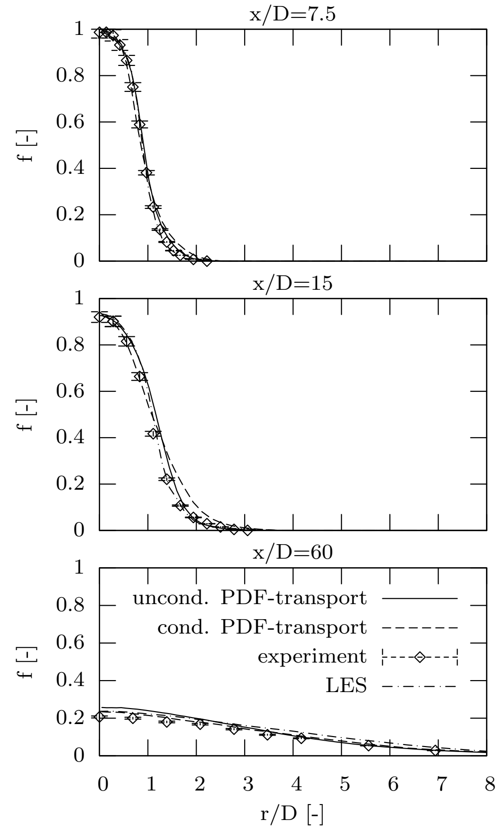

Figure 4: Radial profiles of mixture fraction

LES, the unconditional PDF-transport method and the conditional PDF-transport method are listed as well as experimental data. It is apparent that all methods give accurate results. In particular the conditional method shows a significant improvement concerning the prediction of temperature for axial positions smaller than x/D=60. As the mixture fraction distribution calculated by the LES is mapped to the mixture fraction distribution of the PDF-transport method via conditioning, this effect is mainly due to the improved treatment of chemistry of the new method.
For further comparison of the methods the mass fractions and its variances of the species OH, H_2O and CO_2 are shown in figure 7. Concerning the prediction of OH, two observations can be made. For the first, the prediction of the mean profile of the OH mass fraction is superior to that of the LES, particularly for the downstream range x/D 45. Secondly, the prediction of the OH mass fraction fluctuation is better than the LES, but values are overpredicted in the range 60 > x/D > 30. As the mixture fraction is the same for the LES and the conditional-PDF method, this is due to the different transport of the species H_2O and CO_2, which are additional parameters for the ILDM and therefore for the postprocessing step.
The prediction of H_2O is slightly worse than the LES, whereas CO_2 shows a qualitatively better trend, particularly in the downstream range x/D 30. The evolution of the temperature in the axial direction is shown in figure 6. The simulations yield similar results. Excellent agreement with experimental data and a significant improvement of predicition quality compared to the LES and to the unconditional PDF-transport method is obtained at x/D=7.5 and x/D=15. Here the mixture fraction is also predicted very accurately by the LES, thus the ILDM chemistry prediction also performs very well. Even for the downstream range

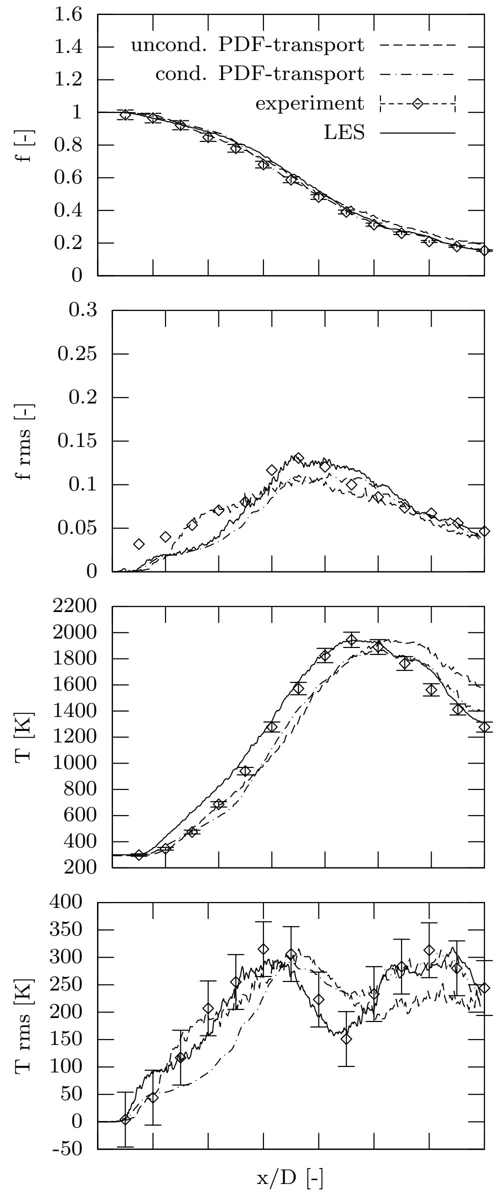

Figure 5: Axial profiles of mixture fraction and temperature

x/D 30, the conditional method shows to be satisfactory.

DISCUSSION AND OUTLOOK

The aproach described above shows a new possibility to use a Lagrangian PDF-method combined with LES calculations of a turbulent flow.
In contrast to FDF (Filtered Density Function) methods, this is achieved conserving the marginal PDF of the mixture fraction obtained from the LES. Thus the form of the mixture fraction PDF obtained from the LES is conserved. Furthermore the chemical source term occurs in a closed form. In the context of this work, a non coupled postprocessing on combustion-LES calculations is performed. Velocity and turbulence properties are provided by the LES.
As the computational costs for a better treatment of chemical reactions increase greatly within the LES context, the presented method offers a possibility for an aftertreatment of LES-results with more sophisticated chemistry models at reasonable additional costs. The results are very promising and show that the conditional method works in principle.

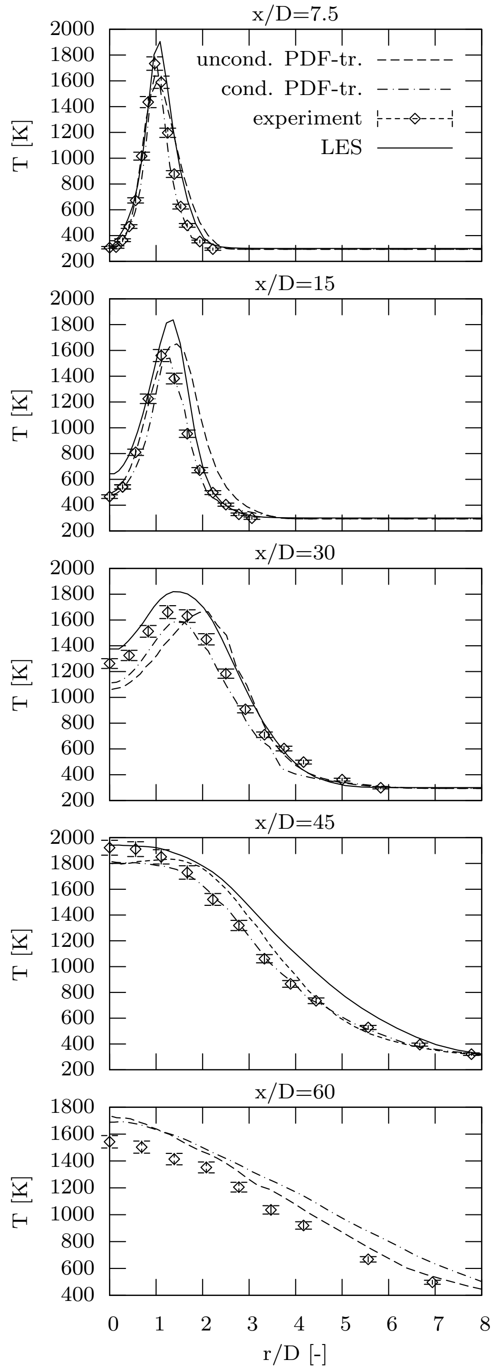

Figure 6: Radial profiles of temperature

Prediction quality seems to be very good and a significant improvement of the LES results can be noticed for many regions.
Nevertheless there are still regions where the pure LES is superior to the conditional-PDF method. Firstly this is based upon the fact that within this work a relatively simple chemistry model via a three parameter ILDM is used. Since the PDF-transport method provides the possibility to use an arbitrarily complex chemistry, it is planed to investigate this dependency in the near future.

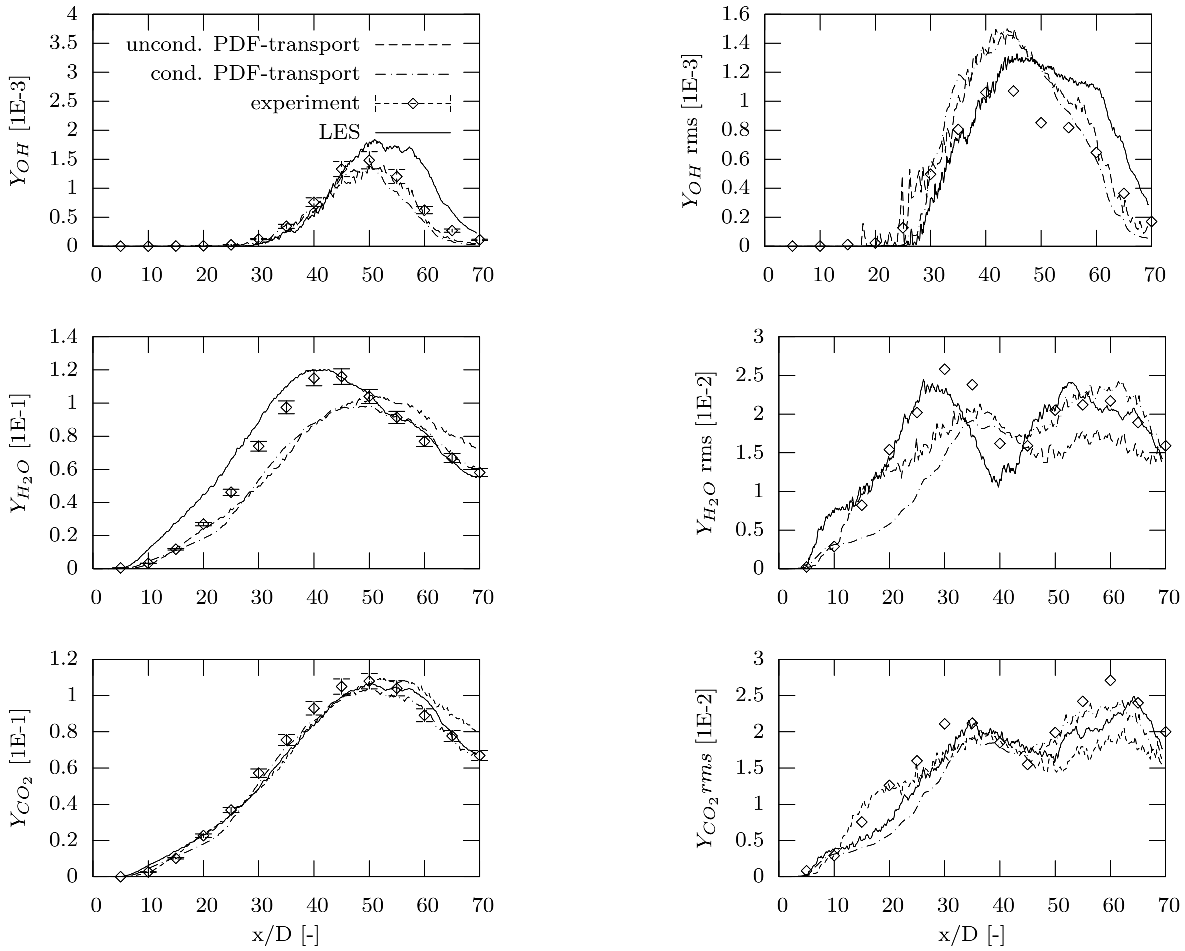

Figure 7: Radial profiles of species mass fractions and its variances

An additional source of error might be the conditioning procedure applied within the scope of this work. A more sophisticated way would be to divide the mixture fraction space into several bins and to solve a PDF-transport equation for each of those bins. Additionally one then has to model the conditional mixing term in equation (9). The methods which are provided by Conditional Moment Closure could be useful for this task.

Furthermore the method could be used on a directly coupled basis with the LES using the strength of the LES to predict scalar mixing accurately and on the other hand the possibility to treat the chemical source term unclosed via a PDF-transport method. Further work has to be done in this area and is in preparation at the authors' institute.

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