COMPARATIVE STUDY OF TURBULENCE AND CHEMISTRY MODELS ON SIMULATION RESULTS FOR A METHANE/AIR JET DIFFUSION FLAME

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ABSTRACT

The importance of different submodels in numerical simulations of a turbulent non-premixed flame, is studied. To that purpose, different types of RANS turbulence models are compared: the standard $k - \varepsilon$ model (Jones, 1994), a non-linear $k - \varepsilon$ model with a sophisticated transport equation for the dissipation rate ε (Merci, 2002a, 2002b) and a differential second-moment Reynolds stress model (Jones, 1994). Also different chemistry models are considered, from a (constrained) equilibrium model (Bilger, 1983) to an ILDM method (Maas, 1992; Schmidt, 1996). Finally, the interaction between turbulence and chemistry is described at different levels: the classical pre-assumed β-PDF approach is compared to an extended multivariate pre-assumed PDF method (Repp, 2002; Landenfeld, 2002). It is concluded that for the test case under study (Sandia 'Flame D' (Barlow, 1998; TNF, 2003)), the turbulence model has the major effect on the main results, except when chemical species are of interest.

INTRODUCTION

In simulations of turbulent flows with single-phase combustion, models are used in order to keep computing times reasonably low for practical purposes. In particular, the modelling is applied for the turbulence in the flow, the chemical reactions in the combustion process, the heat transfer and the interaction between these processes.

In this work, advanced reduced chemical kinetics are incorporated through the ILDM-method ('Intrinsic Low Dimensional Manifold') (Maas, 1992; Schmidt, 1996). This allows to describe the complete thermo-chemical state of a gas by means of the mean mixture fraction and two reaction progress variables - mean mass fractions H_2O and CO_2, and the variances of these quantities. For the interaction between chemistry and turbulence, the multivariate pre-assumed beta-PDF ('probability density function') approach is followed as described by Repp *et al.* (2002) and Landenfeld *et al.* (Landenfeld, 2002). It is illustrated by Repp (2002) that good results are obtained for mean quantities in a confined swirling flame with local extinction. In this work, a piloted methane/air jet diffusion flame without local extinction is studied ('Sandia Flame D' (Barlow, 1998)), so that the multivariate beta-PDF method assures

sufficient accuracy for the modelling of turbulence-chemistry interaction. Radiation is neglected, which is justified for the studied flame (Merci, 2001).

Attention is focused here onto the differences in simulation results due to the applied turbulence model. To that purpose, different types of RANS models are compared. On the one hand, two eddy viscosity models are implemented: the standard $k - \varepsilon$ model (Jones, 1994) and an advanced cubic $k - \varepsilon$ model. The latter is the model described by Merci *et al.* (2001), with an improved ε-equation (Merci, 2002a, 2002b) (so that the plane jet - round jet anomaly is resolved for jet flows). For both eddy-viscosity models, the gradient diffusion hypothesis is used for turbulent mixing. On the other hand, a linear second moment Reynolds stress model (Jones, 1994) (RSM) is applied, with their flux transport equations for the turbulent mixing.

With a fixed turbulence model (namely the cubic $k - \varepsilon$ model), the influence of the chemistry and turbulence-chemistry interaction model on the results is also considered. To that purpose, results with a simplified version of the 'constrained equilibrium' model (Bilger, 1983) are included. It is illustrated that, for the test case under study, the turbulence model is more important than the chemistry model for the flow field predictions, as well as for the main thermo-chemical quantities. When specific chemical species are considered, the chemistry and turbulence-chemistry interaction modelling become more important.

TURBULENCE MODELLING

For a complete description of the implemented turbulence models, the reader is referred to previously published work. Only some aspects are highlighted here.

As 'standard' $k-\varepsilon$ model, the formulation of Jones (1994) is used, since it accounts for variable density effects due to chemical reaction.

The implemented non-linear $k-\varepsilon$ model is completely described by Merci (2002a, 2002b) and elsewhere in the current conference's proceedings (Merci, in press (b)). The main aspect for the investigation in this paper, is the (steady) transport equation for the dissipation rate ε:

$$\frac{\partial}{\partial x_j}(\rho \varepsilon v_j) = (1 - f_{R_y})c_{\varepsilon 1}\frac{P_k}{\tau_t} + f_{R_y}C_1 S\rho\varepsilon$$
$$- c_{\varepsilon 2}f_2\frac{\rho\varepsilon}{\tau_t} - c_{\varepsilon 3}\frac{\mu_t}{\rho^2}\frac{\partial\rho}{\partial x_l}\frac{\partial p}{\partial x_l}\frac{1}{\tau_t} \qquad (1)$$
$$+ \frac{\partial}{\partial x_j}[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x_j}] \, .$$

The blending function f_{R_y} goes from zero to one as $R_y = \frac{\rho\sqrt{k}y}{\mu}$ goes from $R_y = 1000$ to $R_y = 2000$ (with y the normal distance to the nearest solid boundary). The blended source term is important for the quality of the ε transport equation. Near solid boundaries ($y \to 0$, $f_{R_y} \to 0$), the 'standard' source term $c_{\varepsilon 1}\frac{P_k}{\tau_t}$ is recovered. In free shear flows ($y \to \infty$, $f_{R_y} \to 1$), the source term becomes $C_1 S\varepsilon$. This corresponds to Shih et al. (1995), where the ε-equation was derived from the enstrophy transport equation. The major improvement is that the plane jet - round jet anomaly is resolved. As already mentioned, the reader is referred to Merci et al. (2002a, 2002b, in press (b)) for more model details.

In the implemented Reynolds stress model (RSM), the local isotropy assumption for the dissipation rate is applied and the Jones-Musonge formulation of the pressure-strain correlation is used (Jones, 1994). More details are given by Landenfeld et al. (2002).

TURBULENCE-CHEMISTRY INTERACTION

The pre-assumed β-PDF method is used, with the concept of the mixture fraction as conserved scalar. Classically, transport equations are solved for the mean mixture fraction ξ and its variance. The PDF is locally reconstructed with the given values for these quantities.

However, in the context of advanced chemistry modelling (see next section), more refined turbulence-chemistry interaction descriptions are possible. A multivariate pre-assumed β-PDF method is described by Landenfeld et al. (2002) in which, beside the mean mixture fraction and its variance, the mean values of the CO_2 and H_2O mass fractions and their variances play a central role. Therefore, modelled transport equations are solved for the mean values and the variances of the mentioned mass fractions. The treatment of the chemical source terms, occurring in those equations, is described by Landenfeld (2002). Linear gradient diffusion is assumed for the turbulent scalar fluxes and the scalar dissipation rates are modelled under the assumption of constant time scale ratio.

The thermo-chemical quantities are tabulated a priori as a function of the mentioned independent quantities. The joint PDF is simplified as a product of one-dimensional PDFs. While the statistical independence of the different arguments is at least very questionable, the results by Landenfeld et al. (2002) are encouraging to justify the approximation and, therefore, to be used in the present work.

CHEMISTRY MODELLING

The multivariate β-PDF method is combined with ILDM modelling of the chemical reaction system. This technique avoids the assumption of infinite Damköhler number. It describes to some extent the chemical system dynamics, with only a few progress variables. Using an eigenvalue analysis in composition space, the chemical reactions are sorted on the basis of their chemical time scale. Reactions which are faster than a critical time scale are assumed to be in equilibrium, while the slowest eigenvalues span a low-dimensional manifold, along which the reactions proceed. The full mechanism and details for the reduced ILDM mechanism are described by Schmidt (1996), resulting in the mass fractions of H_2O and CO_2 as progress variables, as already mentioned.

In order to judge on the importance of the chemistry model, results are compared to what is obtained with the classical pre-assumed β-PDF approach (based on the mean mixture fraction and its variance only), in combination with the simplified version of the 'constrained equilibrium model' (Bilger, 1983), as described by Merci et al. (2001). The composition is assumed to be in complete chemical equilibrium (infinite Damköhler number), under certain constraints (on e.g. CO).

NUMERICAL METHOD

The presented, grid independent, results are generated by two different research groups: the non-linear $k - \varepsilon$ model simulations have been performed at Ghent University, while the standard $k - \varepsilon$ model and the RSM results have been obtained at Darmstadt University of Technology. As a consequence, the numerical methods differ.

At Ghent University, the steady-state solutions are obtained through a time marching method with a second order accurate finite volume technique, as described elsewhere (Vierendeels, 2001; Merci, 2000, 2003). The importance of the inlet boundary conditions (see also further in this paper) has been illustrated by Merci et al. (in press (a)).

The Darmstadt University group has used a two-dimensional elliptic finite volume CFD code with staggered grid arrangement employing the SIMPLEC velocity-pressure coupling algorithm. The inflow profile for the turbulent kinetic energy dissipation rate ε has been specified assuming an equality of turbulent production and dissipation and neglecting the axial gradients of the mean velocity.

TEST CASE

Simulations have been restricted so far to 'Sandia flame D' (Barlow, 1998), which has been a target flame in the series 'International Workshop on Measurement and Computation of Turbulent Non-Premixed Flames' (TNF, 2003). The experimental data for the thermochemical quantities have been provided by Sandia National Laboratories, while the flow field measurements have been performed at Darmstadt University of Technology.

Flame D consists of a piloted jet diffusion flame with Reynolds number $Re = 22400$, based on bulk jet velocity $U_b = 49m/s$ and nozzle diameter D. In the central fuel jet, methane is premixed with air ($25\%CH_4 - 75\%$ air by volume). It is surrounded by a hot pilot stream ($U_{pilot} = 11.4m/s$), which stabilises the flame. This system is embedded in co-flowing air ($U_{air} = 0.9m/s$). A complete test case description can be found in TNF (2003).

The computational domain has dimensions $100D \times 25D$ and contains 112×80 cells. The inlet boundary is positioned at the burner nozzle exit.

RESULTS

Comparison of Turbulence Models

In fig. 1, profiles along the symmetry axis are presented for the different turbulence models with the ILDM method. A first striking feature is the strange 'cusp' in the mean velocity and mixture fraction profiles with the cubic $k - \varepsilon$ model. This is due to an unfortunate combination of the chemistry model, turbulence model and inlet conditions, since this cusp is absent when a different chemistry model is used with the same turbulence model and inlet conditions (fig. 4).

This being stated, differences between the turbulence models are small when the mean velocity is considered. Larger differences are observed in the mean mixture fraction profiles (thick lines and triangle symbols). Clearly, the RSM model and the cubic $k - \varepsilon$ model are comparable beyond the cusp. The axial position of stoichiometric conditions ($\xi_{stoich} \approx 0.35$) is well predicted, in contrast to the standard $k - \varepsilon$ model, which suffers from excessive diffusion. This is confirmed in the temperature profiles. This is not surprising, since the mean mixture fraction has the major influence on the mean temperature. It is observed that the temperatures with the cubic $k - \varepsilon$ model are comparable to the RSM model's, only for $x > 40D$. Closer to the nozzle exit, the temperature is underestimated with the $k - \varepsilon$ model. Again, this is due to the mentioned combination of factors, resulting in the 'cusp', as is illustrated in fig. 4: when a different chemistry model is applied, the temperature underprediction disappears.

The mixture fraction variance (thin lines and square symbols) is best reproduced with the cubic $k - \varepsilon$ model (correct position of peak variance and good agreement with absolute values). Again the strange dip disappears when a different chemistry model is used (fig. 4).

Finally, the profiles for CO_2 (thick lines and triangle symbols) and H_2O (thin lines and square symbols) mass fractions, illustrate the quality of the cubic model and the RSM model once more (correct peak position and good absolute agreement with experimental data). Needless to say, the delay in increase in the mass fractions disappears when a different chemistry model is used. It is noteworthy that the mean mass fractions of CO_2 and H_2O are obtained from transport equations here.

Figures 2 and 3 show radial profiles at $x/D = 45$ (i.e. around stoichiometric conditions). For all quantities, differences between the cubic $k - \varepsilon$ model and the RSM model are small. They are in good agreement with experimental data, except perhaps for the turbulent shear stress. The standard $k - \varepsilon$ model only yields acceptable results for the flow field variables. In all thermo-chemical profiles, excessive diffusion is observed in their spreading.

Comparison of Chemistry Models

Fig. 4 shows the impact of the chemistry model on axial profiles, obtained with the cubic $k - \varepsilon$ model. As already mentioned, the cusps disappear. Further, it is noticed that differences in all axial profiles are small, except when the chemical species are considered. For the mass fraction of H_2O (thin lines and square symbols), differences are still relatively small: the position of peak mass fraction remains unaltered. For CO_2 (thick lines and triangle symbols) on the contrary, larger differences are observed. Except for the underprediction for small x, agreement with experimental
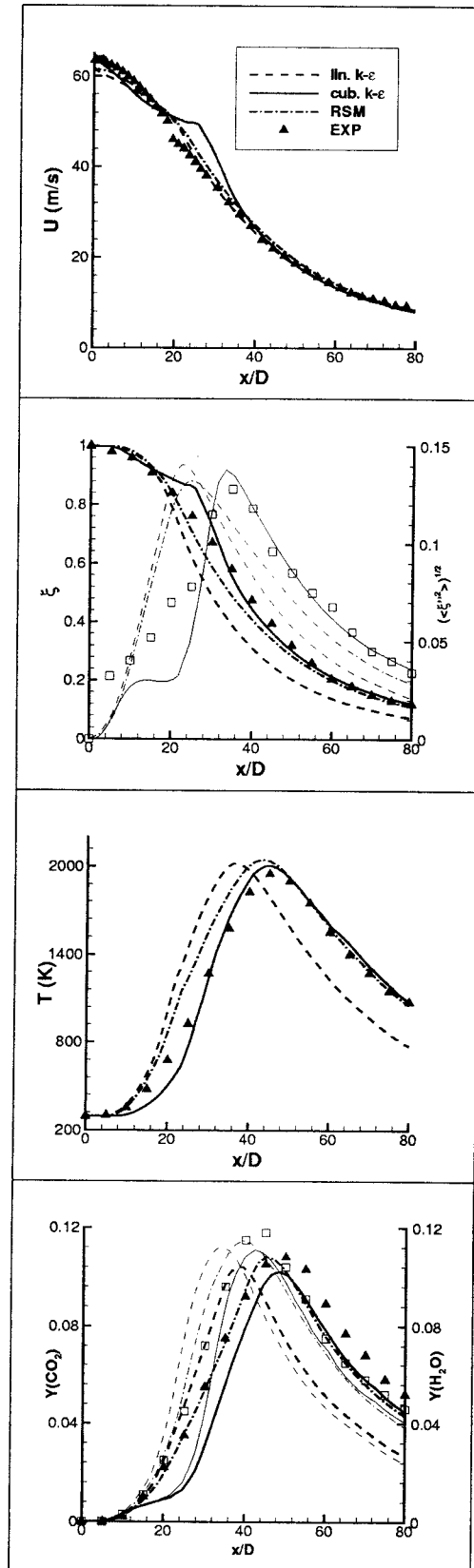

Figure 1: Axial profiles with different turbulence models.

Figure 2: Radial profiles at $x/D = 45$ with different turbulence models.
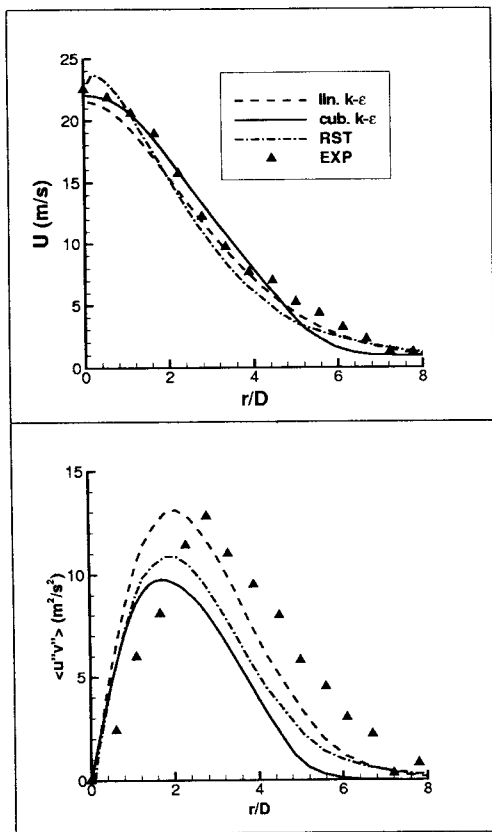

Figure 3: Radial profiles at $x/D = 45$ with different turbulence models.

data is better with the ILDM model and the multivariate PDF method. Note that the mass fractions of CO_2 and H_2O are obtained from transport equations for that model.

The radial profiles at $x/D = 45$ (figs. 5 and 6) confirm this. It is noted that the higher temperature with the constrained equilibrium model is reflected in a higher mass fraction of CO_2 and vice versa. Indeed, the mass fraction CO_2 is an indicator for the 'completeness' of combustion predicted by the chemistry model.

CONCLUSIONS

It has been illustrated for the test case under study that the simulation results strongly depend on the turbulence model. The turbulence model indeed determines the flow field, which on its turn governs the chemical activity through the turbulent mixing. Since there is little local extinction, the turbulence model is the most important submodel for the considered test case. In general, the quality obtained with the cubic $k - \varepsilon$ model is comparable to the RSM model.

The impact of the chemistry model on the flow field is small. Only when thermo-chemical quantities (like temperature or species mass fractions) are investigated, the differences between the chemistry models become clear. The refined ILDM model with the multivariate pre-assumed PDF method yields accurate results.
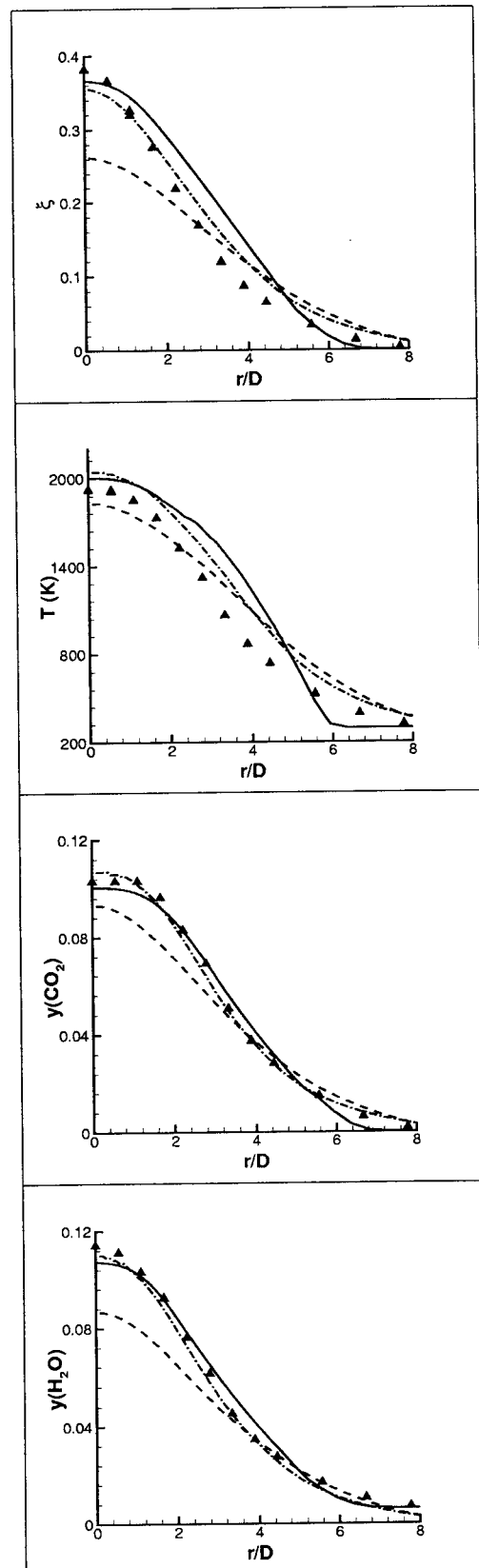
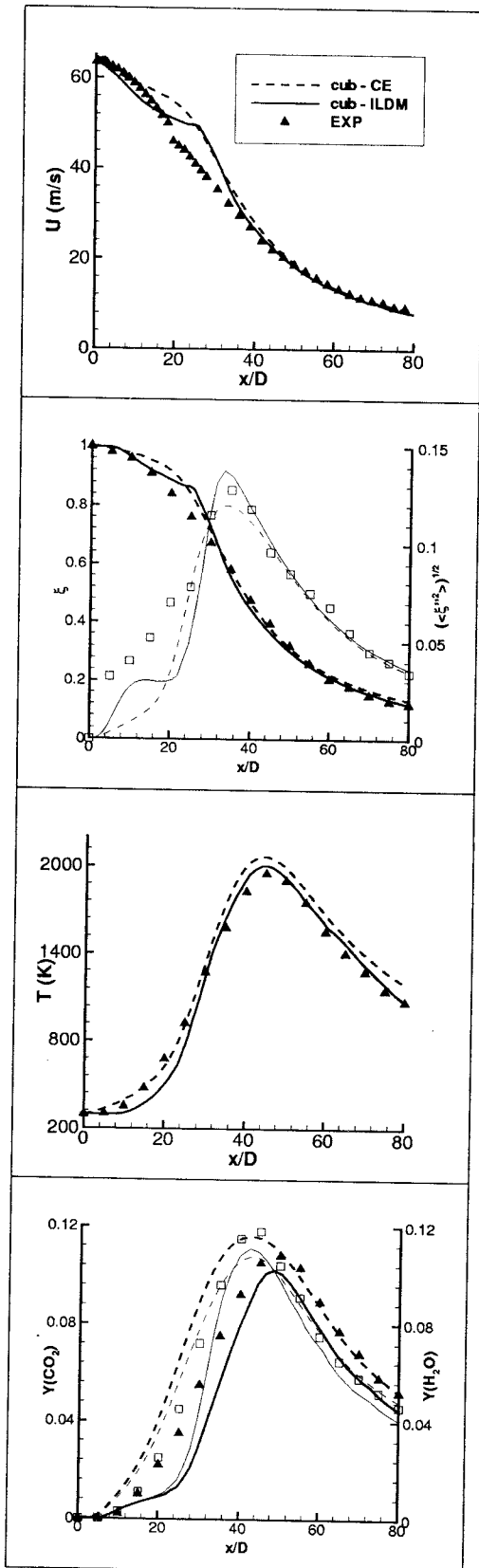Figure 5: Radial profiles at $x/D = 45$ with different turbulence models.

ACKNOWLEDGMENT

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Figure 4: Axial profiles with different chemistry models.

x/D = 45

cub - CE
cub - ILDM
▲ EXP

0.3

0.15

0 2 4 6 8
r/D

x/D = 45

2000

1500

T (K)
1000

500

0 2 4 6 8
r/D

0.12

0.08

y(CO₂)

0.04
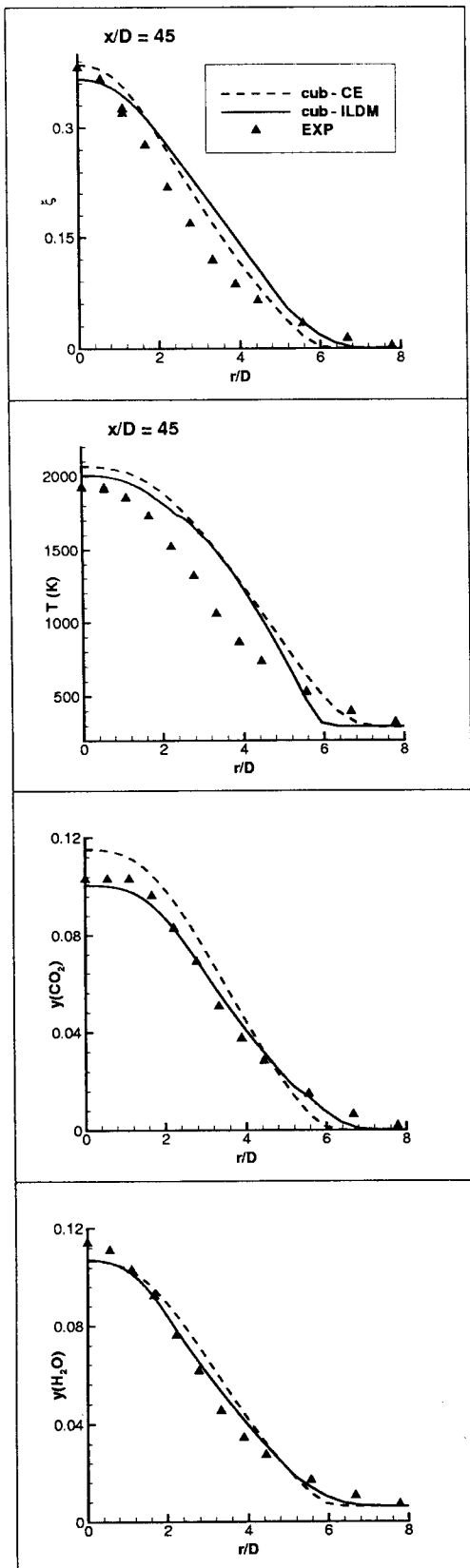
0 2 4 6 8
r/D

0.12

0.08

y(H₂O)

0.04

0 2 4 6 8
r/D

Figure 6: Radial profiles at $x/D = 45$ with different turbulence models.

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