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On proper closures for modeling of turbulent combustion

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Abstract

The subject of this work is the numerical simulation of a turbulent diffusion jet flame fueled with a mixture of CH_4, H_2, and N_2. Simulations have been investigated with various two-equation turbulence models to improve prediction of jet flow fields. The calculations are validated against existing experimental data obtained by Raman and laser Doppler velocimetry. In particular, a comparison of three two-equation turbulence models and their influence on combustion process is presented, namely the Pope corrected k-ϵ model, standard k-ϵ model and the realizable k-ϵ. For combustion modeling the eddy dissipation concept (EDC) model with a 25-step reaction is considered. The numerical results for mean velocity components, temperature, and major chemical species are presented and compared with the experimental data. The goal of the work is to investigate the capabilities of the used turbulence models in proper predicting of the round jet spreading in a nonpremixed jet flame. Simple geometry allows for reliable flow simulations. Calculations were performed using FLUENT 2D and 3D solver. The Pope correction has been applied via the user defined function. The advantages and disadvantages of the models are discussed in detail in the meantime during presentation of the results.

Keywords: Two-equation turbulence; Jet flows; Pope correction; Combustion

1 Introduction

Turbulent combustion exists in industrial applications as well as in nature. It finds applications in energy production, aeronautics, combustion chambers and in some natural phenomena. In the study of this important phenomenon, difficulties related to turbulence closure of momentum and scalar transport equations are

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further compounded by interaction with chemistry in combustion calculations. Therefore proper turbulence modeling remains in the area of improvement.

Today, even with the successful development of direct numerical simulation (DNS) and large eddy simulation (LES) methods for turbulent flows, the most popular models for round jet flows and industrial modeling are the two equation Reynolds averaged Navier-Stokes (RANS) models. While LES offers a promise for the future by directly calculating large scale turbulence, RANS techniques are required especially for the fast analysis of complex nozzle geometries. As a result, there is still a need for work in the area of RANS turbulence modeling for round jets and improvement of the jet flow field. Mameri *et al.* [15] in their paper showed that Pope correction can be successfully used to proper prediction of the spreading rate of the round jet. However there is no comparison of spreading rates calculated with different turbulence models. Additionally, they didn't couple the Pope correction with combustion model so they didn't analyze the influence of corrected flow field on the temperature and species mass fraction distribution.

This form of model is easy to solve, converges relatively quickly, is numerically robust and stable. There is no need for direct empirical input such as mixing-length specification. The standard k-ϵ constants are the only empirical input which, for generality, are supposed to take same values in all fluids. However, this generality is found not to exist.

There are three different regions that can be defined in the round jet, namely the near, intermediate and far-field. The near-field region is located between $0 < x/D < 6$ (where D is the nozzle diameter and x is the downstream coordinate along the jet-stream centerline) and contains the region of potential core where the flow characteristics matches those from the nozzle exit. The far-field region, located at approximately $x/D > 30$, [1], is the fully-developed region. The intermediate-field region lies between the near- and far-fields of the jet. The near- and intermediate-fields comprise the development portion of the jet and significantly influence the downstream evolution of the jet in its numerous applications. In the shear layer vortex cores form, evolve and pair-up to form large eddies because of the large velocity gradient in the radial direction. These large eddies break down and form smaller and smaller eddies, and the turbulence structures decrease in scale. Throughout this process, energy is transferred from the large-scale structures to the smaller scales in the outer layer.

The aim of this work is to compare three turbulence models, and their impact on the velocity profile in the jet flow. Indirectly turbulence affects also temperature field in the flame, because velocity, species mixing and combustion process are strictly related.

In the paper the model of restoring correct value of spreading rate in the round jet flow field is presented, where the standard model constant $C_{\epsilon 2}$ is replaced by

a new variable $C_{\epsilon 2Pope}$ dependent on vortex stretching.

2 Turbulence modeling

Standard k-ϵ model predicts the velocity field of a two-dimensional plane jet quite accurately, but results in large errors for axisymmetric round jets, overestimating the spreading rate up to 40% [2]. This 'round-jet plane-jet anomaly' takes the origin from numerous simplifying assumptions in all RANS models. In order to obtain accurate calculations of round jets, modification to the classical models is required. Modifications to the turbulence constants have been suggested by McGuirk and Rodi [3], Morse [4], and Launder *et al.* [5]. All modifications involve the turbulence constants becoming functions of the velocity decay rate and jet width defined as a parameter where $y_{1/2}$ is the distance from the centerline to location where the velocity is half the centerline velocity [12]:

$$\delta_{0.5} = \frac{dy_{1/2}}{dx} \, . \tag{1}$$

Pope [2] proposed a modification to standard k-ϵ model by adding another source term in energy dissipation equation, which bases on vortex-stretching invariant defined as

$$\chi = \left(\frac{k}{\epsilon}\right)^3 \omega_{ij}\omega_{jk}d_{ki} \, , \tag{2}$$

with

$$\omega_{ij} = \frac{1}{2}\left(\frac{\partial V_i}{\partial x_j} - \frac{\partial V_j}{\partial x_i}\right), \quad d_{ki} = \frac{1}{2}\left(\frac{\partial V_k}{\partial x_i} + \frac{\partial V_i}{\partial x_k}\right) \, , \tag{3}$$

where d_{ki} is the strain rate tensor components, ω_{ij} rotation tensor components. New source term in transport equation for ϵ is given in the form

$$Pc = C_{\epsilon 3}\frac{\epsilon^2}{k}\chi \, , \tag{4}$$

where $C_{\epsilon 3}$ is a new model constant equal to 0.79. The correction replaces the constant $C_{\epsilon 2}$ with $C_{\epsilon 2Pope}$ defined as

$$C_{\epsilon 2} - C_{\epsilon 3}\chi = C_{\epsilon 2Pope} \, , \tag{5}$$

After transformations the transport equation for ϵ can be written as

$$\frac{\partial}{\partial t}(\epsilon) + \frac{\partial}{\partial x_j}(\overline{v}_j\epsilon) = \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + \frac{\epsilon}{k}\left(C_{\epsilon 1}P_k - \epsilon\left(C_{\epsilon 2} - C_{\epsilon 3}\chi\right)\right) \, . \tag{6}$$

where k – kinetic energy of turbulence, ϵ – dissipation of kinetic energy of turbulence, ν – dynamic viscosity, ν_t – turbulent viscosity, P_k – production of kinetic

energy, $C_{\epsilon 1} = 1.44$, $C_{\epsilon 2} = 1.92$.

The new constant $C_{\epsilon 3} = 0.79$ with the modified version of epsilon reproduces the spreading rate and the velocity profile to the measured value of $\delta_{0.5} = 0.86$. In applied model the correction of Pope was implemented as a user defined function (UDF) into Fluent solver in a form of a source term included to energy dissipation equation. In the Fig. 1 cold flow calculations of jet spreading rates are presented. It can be noticed that modification of epsilon equation decreases the spreading rate and influences the velocity field, while unmodified standard k-ϵ and realizable version of the model over predicts the experimental spreading rate. Figure 2 shows local changes of the $C_{\epsilon 2 Pope}$ constant calculated in the flow field area of the jet. It can be seen that the values are locally changing due to vortex stretching invariant influence.

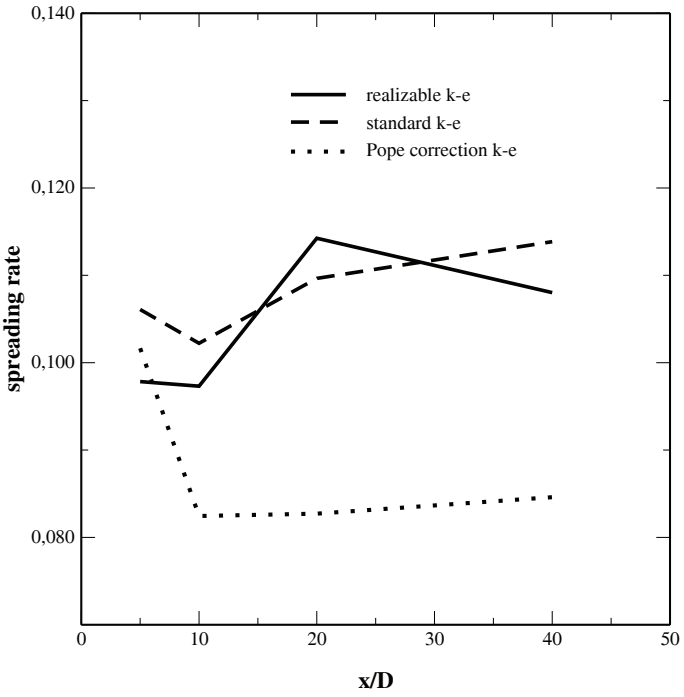

Figure 1. Spreading rate of the jet – $\delta_{0.5}$.

3 Burner and flame description

To achieve a better understanding of the complex processes in turbulent combustion, the concept of using 'standard flames' has been developed. A standard flame has to be operated in a well-characterized burner, under well-documented

Figure 2. Local changes of $C_{\epsilon 2Pope}$ in the axisymmetric coflowed jet.

conditions and rather simple flow filed. The German Aerospace Center (DLR) provided measurements on a simple standard flame DLR-A [11]. The diffusion flame configuration used in this study has been experimentally investigated by Bergmann *et al.* [6].

The flame burner consists of a straight stainless steel tube (length 350 mm, and inner diameter 8 mm) with a thinned rim at the exit. The tube was surrounded by a contoured nozzle (*i.d.* = 140 mm) supplying the lower part of the flame with co-flowing dry air at the exit velocity of typically 0.3 m/s (Fig. 3). The fuel had a composition of 22.1% – CH_4, 33.2% – H_2, and 44.7% – N_2 and a mean exit velocity of 42.2 m/s, corresponding to the Reynolds number Re = 15.200. The stoichiometric mixture fraction about 0.167, and the adiabatic flame temperature about 2130 K. The ambient pressure during the measurements was 95.3 kPa. Hydrogen was added to stabilize the flame, without changing the simple flow field of the round jet, as in case of piloted flames.

4 Combustion modeling

For combustion modeling the eddy dissipation concept (EDC) [7] has been used. In the classical approach, rates of reaction were assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations could be avoided. For the EDC model the net rate of production of species is given by the smaller of these two terms: the eddy-dissipation rate and the Arrhenius rate, i.e., the net reaction rate is taken as the minimum of these two rates. The EDC model assumes that reaction occurs in small turbulent structures called the fine scales [8]. The

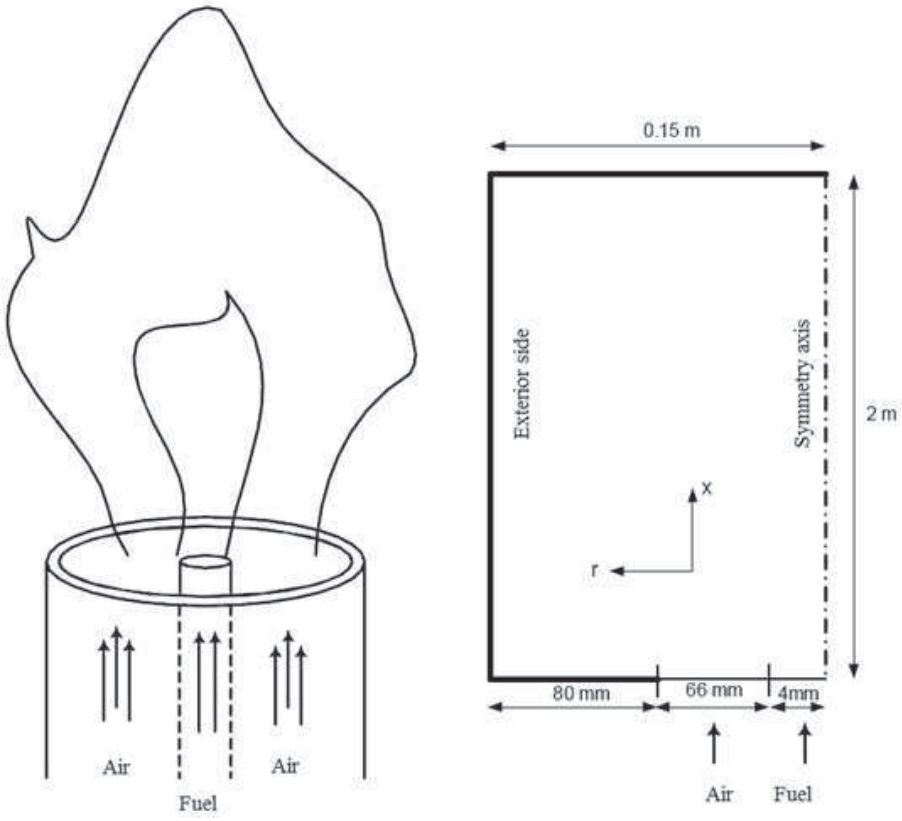

Figure 3. Geometry of the DRL-A burner.

length fraction of the fine scales is modeled as

$$\xi^* = C_\xi \left(\frac{\nu\epsilon}{k^2}\right)^{1/4} , \tag{7}$$

where * denotes the fine-scale quantities, C_ξ is the volume fraction constant equal to 2.1377, and ν is the kinematic viscosity. Species are assumed to react in the fine structures over the time scale:

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon}\right)^{1/2} , \tag{8}$$

where C_τ is a time scale constant equal to 0.4082.

In ANSYS FLUENT [16], the combustion at the fine scales is assumed to occur as a constant pressure reactor, with initial conditions taken as the current species and temperature in the cell. Reactions proceed over the time scale, τ^*, governed by the Arrhenius rates and are integrated numerically using the ISAT

algorithm [9]. The source term in the conservation equation for the mean species i is modeled as

$$R_i = \frac{\rho\,(\xi^*)^2}{\tau^*\left[1-(\xi^*)^3\right]}\,(Y_i^* - Y_i)\ , \tag{9}$$

where Y_i^* is the fine-scale mass fraction after reacting over time τ^*, Y_i is the spices mass fraction, and ρ is the density.

Local unsteadiness and stormy chemical reactions, especially in the combustion process, are the sources of flow turbulence. This kind of coupling has not always been reflected in mathematical and numerical modeling. Badur *et al.* [14] has shown that even a simple chemistry-turbulence coupling improves the accuracy of simulations. The EDC model can incorporate detailed chemical mechanisms into turbulent reacting flows, however, typical mechanisms are invariably stiff and their numerical integration is computationally expensive. To include detailed chemical mechanisms in EDC model a 25-step reduced mechanism based on the work of Smooke [10] has been imported from CHEMKIN file. Typical spices modeled in the mixture are: H, O_2, OH, O, H_2, H_2O, HO_2, CO, CO_2, CH_3, CH_4, HCO, CH_3O, CH_2O, H_2O_2, N, and N_2. For flow calculations the ideal-gas assumption has been used and buoyancy effects were also included.

The experimental data for temperature and species mass fractions have been taken from Bergmann *et al.* [6]. The species mass fractions have been determined by the single point Raman spectroscopy measurements, and those of temperature by the single-point Raman and Rayleigh spectroscopy measurements. Two-component laser Doppler velocimetry (LDV) measurements at locations in the flames corresponding to the scalar measurements and at additional locations closer to the nozzle were conducted at TU Darmstadt [11].

5 Results

The calculated results of the mean axial velocity and static temperature are compared to the experimental data along the centerline in Fig. 4. The axial velocity calculated with the Pope correction is in a good agreement with experimental data. The obtained results for Pope correction should be regarded as satisfactory in spite of existing differences between the results from numerical codes and experiment measurements. It is also presented that the realizable k-ϵ model better predicts spreading rate of the jet than the standard model (Fig. 4), however the species mass fraction will be compared only on the base of measurements and results obtained by use of standard k-ϵ Pope correction. The radial velocity (Fig. 5) profiles indicate that the spreading rate is calculated quite accurately. From the radial temperatures at $x/D = 5$, 40, 60 locations shown in Fig. 5 we can notice

that calculated flame temperatures of the near-centre profile are overestimated. This is related to a high nonlinearity of Arrhenius equation in the reaction rate equation. The mean reaction rate calculated on the bases of the mean temperature, can differ few orders of magnitude from the reaction rate calculated using the base of instantaneous temperature [13]. Figures 6 and 7 show the numerical results for the CO, H_2, CH_4 and CO_2 mass fraction validated against measurements. Since influence of radiation phenomena is omitted, the calculated flame temperature is overestimated. The highest temperature of the flame is 2060 K, located in position of $x/D = 65$. Due to higher temperature field, spices transported in the flow tends to react a little faster than they are supposed to, according to the measurements.

Consequently the use of Pope correction and detailed multistep combustion model, can obtain more accurate numerical results, in comparison to simple solution methods [15,16,17].

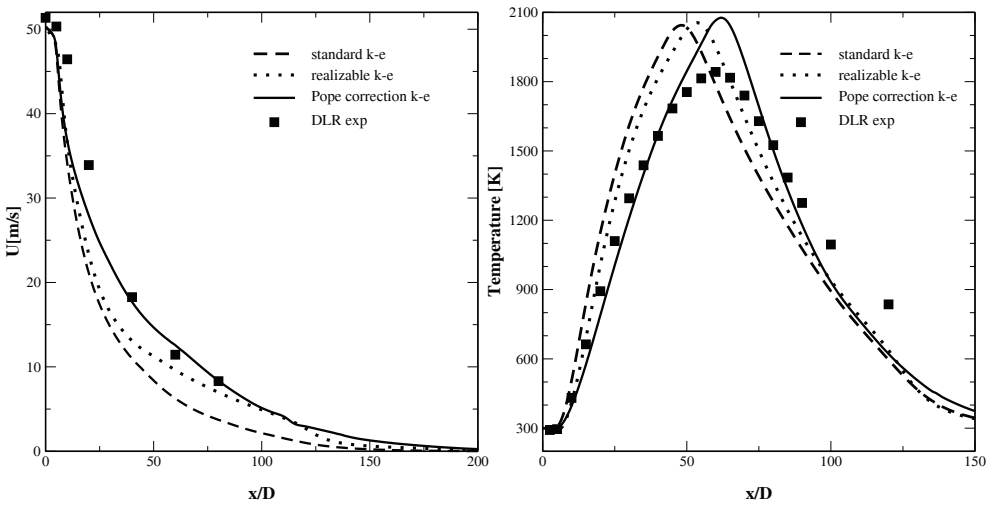

Figure 4. Axial velocity and temperature in the centreline.

6 Conclusions

The results of this study imply that the development of a generalized RANS model is still needed. Improvement of the standard k-ϵ model provided by Pope correction reproduces the spreading rate in the far-filed to measured values and therefore indicates better velocity and temperature predictions. However it was also found that beyond the potential core in the region of intermediate-field the rate of jet decay is faster relative to experimental data. Turbulence models based on standard k-ϵ approach cannot account for the laminar mixing layer region

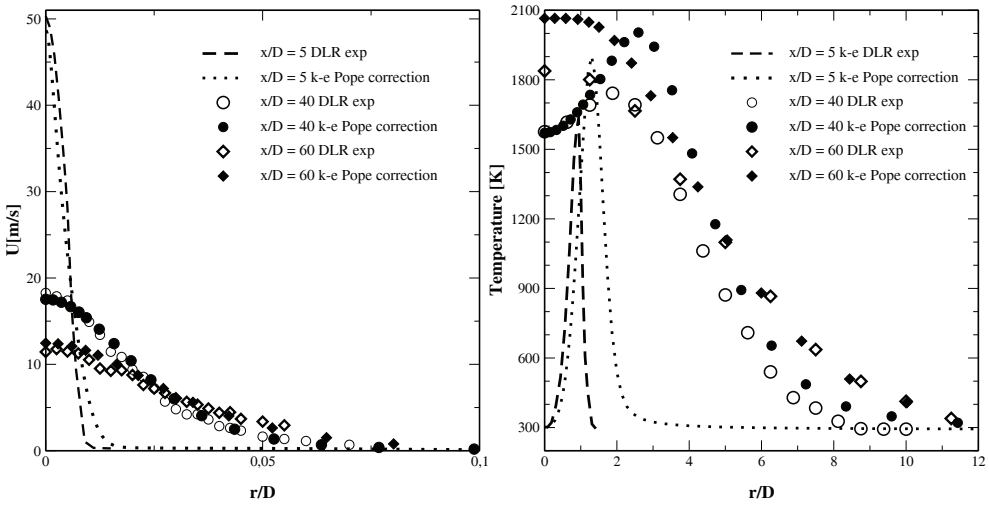

Figure 5. Radial velocity and temperature at $x/D = 5$, $x/D = 40$ and $x/D = 60$ locations.

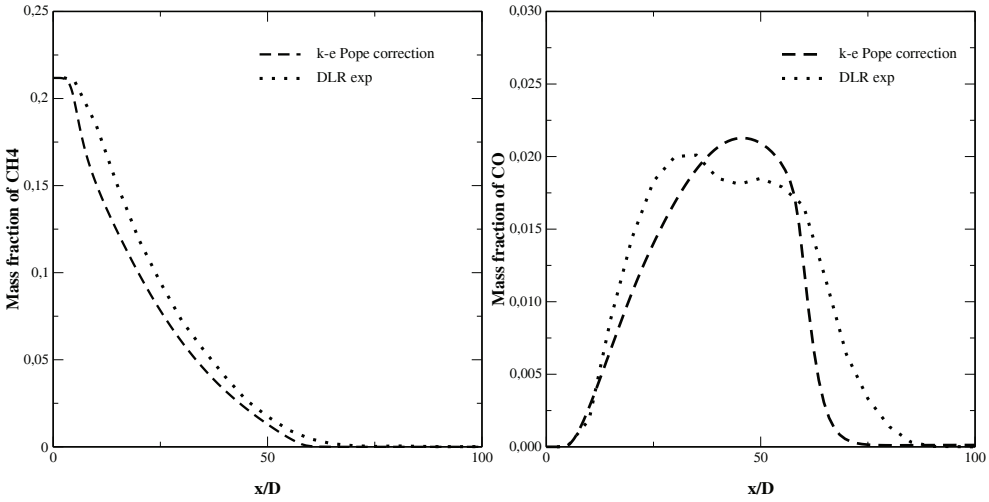

Figure 6. Mass fraction along centreline data, for CH_4 and CO.

close to the nozzle. This results in the increase of mixing rate in this region and therefore consumption is faster. In order to validate the effects of laminar mixing layer the variable diffusion has to be employed. This new approach assumes that, as long as the jet reveals a potential core, there is no turbulent diffusion of chemical species occurring within the mixing layer. The Pope correction and detailed multistep combustion model for both velocity and thermal fields is a simple and reliable way to obtain fast and correct solutions for engineering applications. It should be pointed, however, that more attention is needed when temperatures are investigated. In view of predicted results, especially for temperature of near-

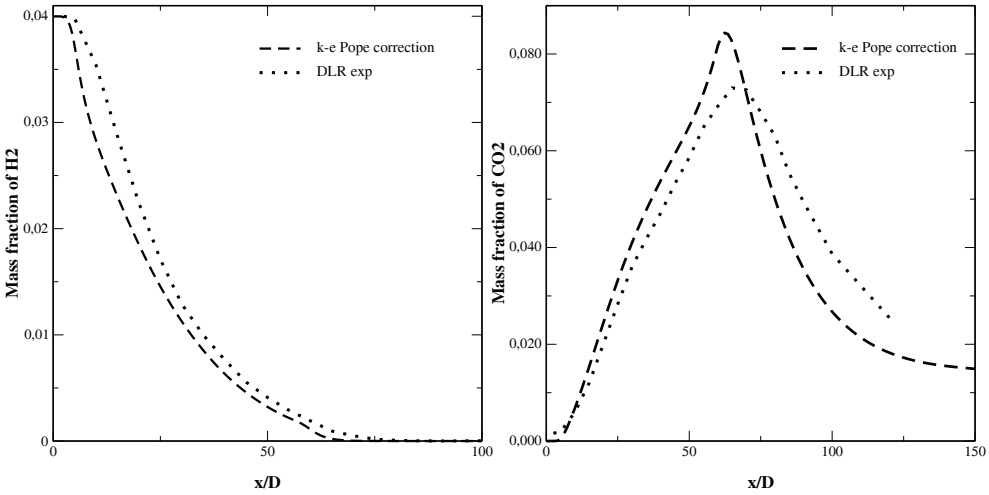

Figure 7. Mass fraction along centreline for H_2 and CO_2.

centre profile, all the processes which are responsible for generation and dissipation should be properly accounted for.

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