Comparative Study of Turbulence Modelling in Hydrogen Nonpremixed Turbulent Flame

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ABSTRACT

The goal of this paper is to investigate the predictive capability of two turbulence models which are the k-ε model and the Reynolds Stress Model (RSM) within flamelet approach. A co-flow axisymetric turbulent non-premixed hydrogen flame investigated experimentally by Barlow and Carter (1994) and Flury and Schlatter (1997) is used as a test case. The chemical mechanism of Yetter's and al. (1991) is adopted for the generation of the flamelet library. It consists of 10 chemical species and 21 reactions. The comparisons with experimental data demonstrate that predictions based on the Reynolds stress turbulence model are slightly superior to those obtained using the k-ε model. Overall, profile predictions of axial velocity, turbulent kinetic energy, mixture fraction, flame temperature and major species are in reasonable agreement with data and compare favourably with the results of earlier investigations.

INTRODUCTION

Hydrogen combustion attached much attention recently because of the need for a clean alternative energy. Indeed, unlike hydrocarbon fuels, the combustion of hydrogen does not produce harmful emissions such as CO_2, CO, Soot and unburned hydrocarbons. The only serious pollutant is NO_x, which can be minimized by reducing combustion temperature through carefully designed lean premixed combustors. However, this technique can be dangerous because of the very flammable character of hydrogen. In order to avoid this kind of risks, it is recommended to operate in diffusion flames.

The studies on turbulent non-premixed hydrogen flame are concentrated on combustion modelling and turbulence modelling in hydrogen mixtures (H_2-N_2, H_2-He) and pure hydrogen cases. The most turbulence model used in the calculation of these flames are the k-ε model and the Reynolds stress model (RSM). The overall agreement is strongly dependent on the turbulence model. It is known that the spreading rate and centreline decay are over predicted using these turbulence models in there classical form in the case of the round jet and also in a jet flame. The use of a so-called Pope correction or reducing the constant ($C_{\varepsilon 2}$) or ($C_{\varepsilon 1}$) will overcome this deficiency.

The H_2 flame investigated in this work was studied experimentally by Barlow and Carter (1994) and Flury and Schlatter (1997). This flame is an attractive candidate because it has well defined boundary conditions, measured data of velocity, temperature, major and minor species, high Reynolds number and a visible flame length smaller than one meter. The flamelet approach is particularly adapted to the calculation of this flame because it is still far from extinction and is fully attached to the nozzle.

Flamelet method is a possible way to reduce the computational burden in which the flow field and the scalar field are decoupled. Indeed, in laminar diffusion flamelets, scalar quantities (e.g. species mass fractions, temperature and density) are unique functions of the mixture fraction and scalar dissipation rate that can be precalculated and stored for further use. It is observed that few studies have been done concern to the application of flamelet

approach to the above H_2 flame and especially with Reynolds stress model. For example, Schlatter and al. (1996) studied this flame in the case of 20 % He dilution with the flamelet and the Probabilistic Euler Lagrangian (PEUL) combustion models The flamelet approach include two flamelets obtained for two different strain rates : high strain rate for a section close to the nozzle $x/l_{visible}$ = 1/8, where $l_{visible}$ is the flame visible length measured, and low strain rate at the flame tip. The turbulence model applied was the k-ε model with a so-called Pope's correction. This contribution was aimed at the applicability of the two combustion models to NO_x predictions. It was shown that both combustion models were equally capable to predict the measured temperatures with a reasonable accuracy. The flamelet results on the temperature at the section $x/l_{visible}$ = 1/8, were very close to the experiment because the preferential diffusion is including in the flamelet model but not in PEUL model**.**

The Reynolds stress model and the k-ε closure are widely used with other combustion models in this H_2 flame. Barlow and al. (1999) simulated numerically NO_x formation in this flame under helium dilution (0, 20 and 40 %) in order to draw comparisons between calculations made with the CMC and the PDF combustion models with the same turbulence model (k-ε), a radiation model and a reduced chemical kinetic mechanism. Fairweather and Woolley (2003) applied the CMC closure to this flame. Their predictions were based on both k-ε and Reynolds stress /scalar flux turbulence closures and used three kinetic schemes of varying levels of complexity that employed 5, 24 and 62 reaction steps. Comparison with experimental data demonstrated that the predictions based on Reynolds stress closures were better than those obtained by eddy viscosity-based approach. It was also found that the results were insensitive to the kinetic scheme employed. Obieglo and al. (2001) applies the k-ε model of turbulence with pope correction to this flame where three combustion models are compared. These are : a PEUL model, a PDF model and an eddy dissipation (EDC) model with single one step reaction. It was shown that the precision of the results depend on the choice of combustion model. The both probabilistic methods give better predictions than the standard model.

In this study, the numerical simulations are performed of an axisymmetric turbulent jet diffusion hydrogen/air flame under the atmospheric pressure, by using a detailed chemistry of Yetter and al. (1991) in a combustion model which is, here, flamelet approach. The simulations are performed with the code Fluent which solves the Navier-Stokes equations with finite volume method.

The article consists of five parts. Starting with a brief explanation of the flame experimental setup, a general description of the governing equations then followed. The turbulence modelling is then discussed. After the introduction of the combustion model adopted, the results together with a discussion are presented. The conclusion summarizes the findings of the presented work.

PROBLEM DEFINITION

The examined flame is a vertical turbulent non-premixed diffusion jet flame with an exactly defined coaxial air stream. The experiments have been performed by Barlow and Carter (1994) for the temperature and species concentrations and by Flury and Schlatter (1997) for the flow field. The inner diameter of the tube is 3.75 mm, the outer is 4.8 mm. The air velocity has been fixed at 1 m/s for all measurements.

TURBULENT FLOW CALCULATIONS

The flow and mixing fields were resolved by the solution of the 2-D, axisymetric forms of the density-weighted fluid flow equations, supplemented with the k-ε model in the first instance, and with a Reynolds stress closure in the second. These equations were solved in conjunction with the conservation equations for the mean and variance mixture fraction.

A so-called Pope correction and buoyancy contributions are added to the ε equation for Both k-ε and RSM turbulence models. Solution of the transport equations is achieved using the Fluent CFD code.
For the turbulence models constants $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$, a standard values are adopted which are respectively : 1.44, 1.92 and 0.79.
For the Schmidt number, Sc_t, in the mixture fraction transport equation, a value of 0.85 is taken. The same value is usually chosen on hydrogen flames. The Fluent default value is also the same.
Flame radiation is modelled using the assumption of optically thin transfer between the hot combustion gases and the cold surroundings (Barlow and al., 2001). The radiating specie considered is H_2O.

COMBUSTION MODELLING

The flamelet equations (Pitsh and Peters, 1998) are solved in pre-processing in the Fluent program "prePDF". The stationary solution were stored in tables containing the profiles of temperature, mass density and mass fractions for all chemical species in dependence on mixture fraction, scalar dissipation and enthalpy for a non-adiabatic case. The scalar dissipation rate at stoichiometric condition, χ_{st}, is used as the external parameter in these equations and values from 0.01 up to quenching are considered.

Preferential diffusion is important in the near field region. flamelet approach is interesting for this type of flows as the model could take diffusion effects into account which play an important role on the near field region. To emphasise these effects two flamelet library are considered corresponding to these two situations : unity Lewis number for all the species (situation 1) and fixed Lewis numbers for all the species (situation 2).
It was observed that calculations corresponding to situation 2 leads to unrealistic results. For this reason, the flame simulations were conducted with the assumption of unity-Lewis number for all the species involved in the chemical model ($Le_i = 1.0$, i = 1,…,N) in the flamelet library generation. Note that, for $Le_i = 1$, the number of flamelets generated is 12 (χ_{st} = 0.01, 0.1, 1, 2, 5, 10, 20, 50, 100, 125, 137, 143.75) and 9 flamelets for fixed Le_k (χ_{st} = 0.01, 0.1, 1, 2, 5, 10, 20, 35, 35.4688). The corresponding quenching limits are different.

CHEMICAL MODEL

The reaction mechanism adopted in this work contains 10 chemical species and 21 reactions (Yetters and al., 1991). The formation of NO_x is not taken into account. This mechanism was succefully utilized, in previous work of Papas and al. (1994), for the predicting of the quenching strain rate in a counter flow non-premixed hydrogen-air flames.

BOUNDARY CONDITIONS

The measured velocity profile at the inlet stream is not used because with the mesh resolution, it is not possible to achieve the same profile. This is mainly due to Fluent's scheme interpolation. Also, it was found deviations from fully developed pipe flow profiles and experimental data. This is why; a preliminary calculation was conducted in the injector alone in order to determine the injector length corresponding to the measured momentum. It was observed that with this inlet conditions, the center line velocity is not well reproduced, especially with the RSM model.

The computational domain has been discretized considering several zones with different grid nodes distributions. From nozzle exit, the computational domain is 267 nozzle exit diameter in the axial direction and 80 exit diameter in the radial direction. At the inlet of

the nozzle, masse flow condition is imposed with hydraulic diameter and intensity of turbulence. The coflow air is entering the computational domain with a uniform velocity of 1 m/s. At the outlet region, outflow condition is assumed.

NUMERICAL METHODOLOGY

The mathematical model is discretized using the finite volume technique on cylindrical staggered grid. Central differences are employed for the evaluation of the diffusion terms, while a first order upwind scheme is used for the evaluation of the convective one. A time-marching SIMPLE (Patankar, 1980) algorithm is employed to couple velocity-pressure fields. Discretized equations are solved in a segregated manner using a multigrid solver. The convergence of the time-marching iterative procedure is truncated once normalized residuals are below 10^{-8}.

RESULTS

1. Axial profiles

The centerline decay for velocity (figure 1) is well reproduced by the *k-ε* model than the RSM. The results obtained by the RSM deviate from measurements starting from $x/l_{visible}$ = 1/8 and until $x/l_{visible}$ = 3/4. In this region, the center axis velocities calculated are lower than those measured. The same behaviour is observed for the *k-ε* model results but the values obtained in this case are slightly lower than the measures. This trend leads to the underprediction of the spreading rate of the jet and to the overprediction of the flame length. This behaviour is also observed by Pitsch et al. (1998) calculations with Fluent using flamelet approach with *k-ε* model and RSM in the same flame.

Both turbulent models are equally capable of predicting the measured temperature with reasonable accuracy in figure 2. Because of the underpredicted spreading rate, the point of maximum temperature is shifted downstream.

The two models results slightly overpredicted the maximum temperature; the temperature is about 50 K higher.

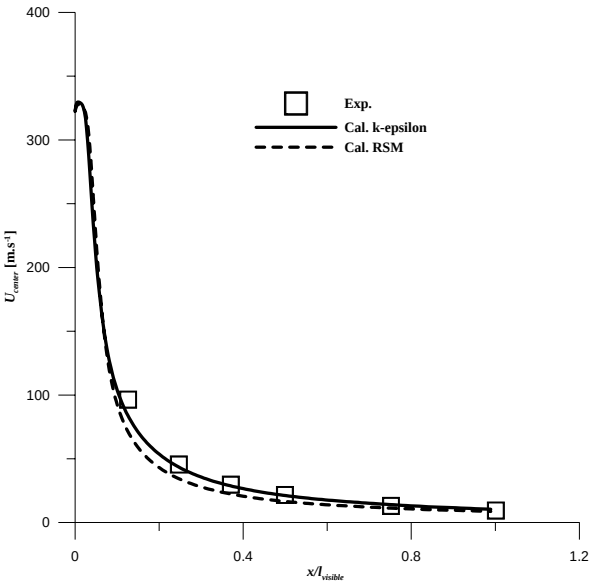


Figure 1 : Centerline velocity

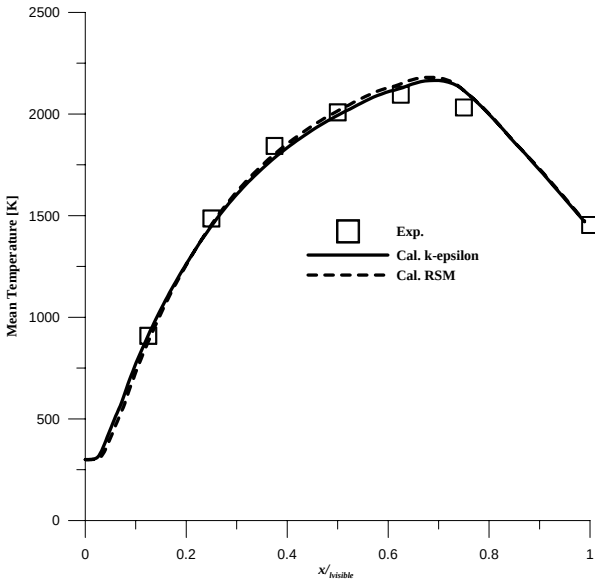
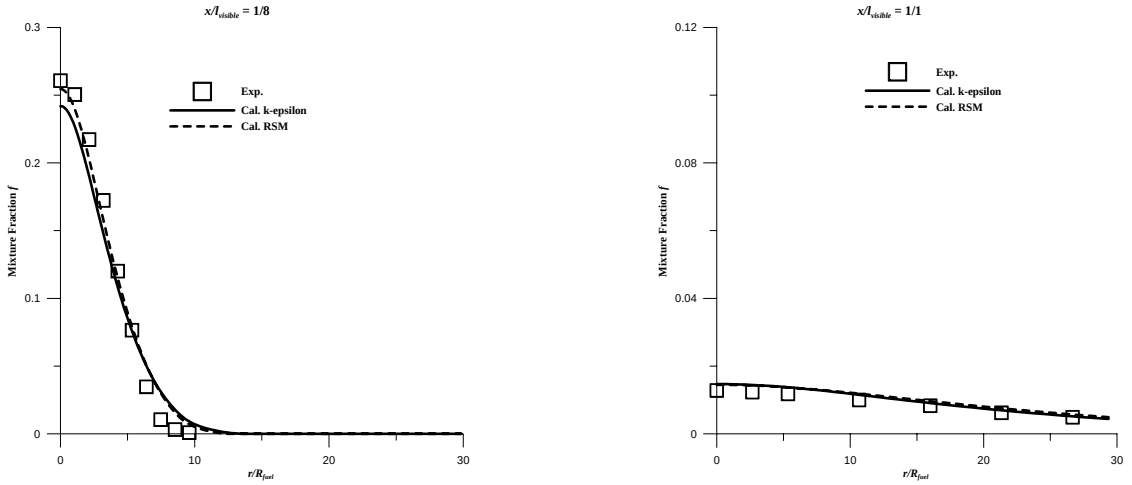


Figure 2 : Centerline temperature

2. Radial Profiles

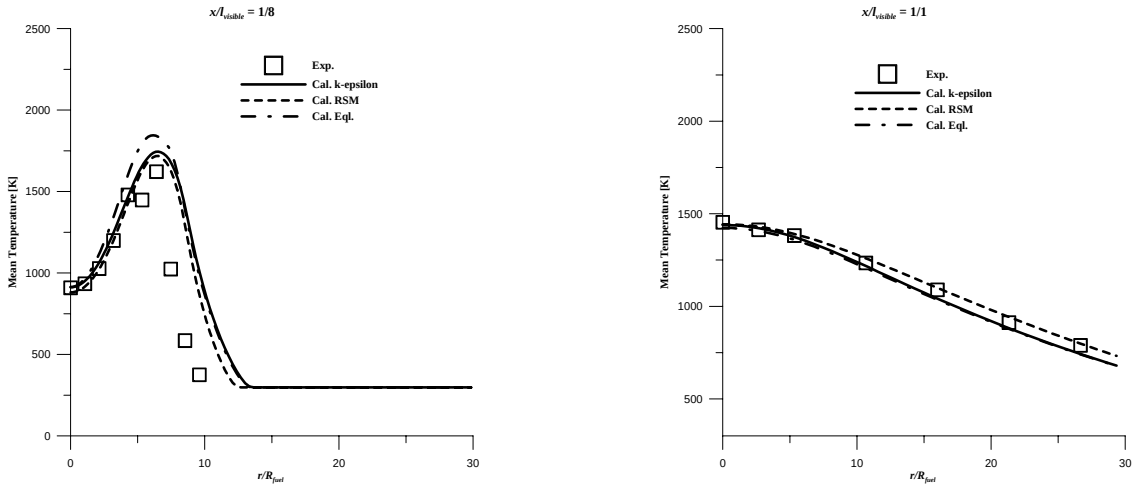
The results derived from the two turbulence approach for the mixture fraction (figure 3) are in good agreement with the experimental data at all locations. At the stations close to the nozzle ($x/l_{visible}$ = 1/8), the RSM predictions are slightly better. Downstream, the opposite phenomenon is noticed. The mixture fraction is calculated from it transport equation assuming unity Lewis number. The stoichiometric value of the mixture fraction is 0.028.

For the temperature profiles, the RSM predictions for the first ($x/l_{visible}$ = 1/8) and the last station ($x/l_{visible}$ = 1/1) are accurate than those obtained from the k-ε closure. Further from the nozzle, radial temperature corresponding to the k-ε model improves slightly over RSM model predictions. It is observable for both models, however, that the temperature profiles decays too slowly over the radius of the flame with this effect decreased with downstream distance. The equilibrium calculations with the k-ε model are also added to this figure. Note that experimental data of the turbulent flame is near but not equal to the equilibrium limit at all axial positions.



(a) **(f)**

Figure 3 : Profiles of mixture fraction



(a) **(f)**

Figure 4 : Profiles of temperature

CONCLUSION

The results obtained demonstrate that flamelet predictions based on the Reynolds stress turbulence model are, in general, slightly superior to those obtaining using the k-ε

model. Indeed, close to the nozzle and the flame tip, the RSM predictions are better than those obtained by the k-ε model. Further downstream, the results are slightly in favour of the k-ε model. In addition, turbulent kinetic energy profiles, hydrogen mass fraction profiles are well reproduced by RSM than k-ε model. Helium dilution leads to an improvement of the calculations in the first location ($x/l_{visible}$ = 1/8).
Overall, predictions of turbulent kinetic energy, mixture fraction, major species and temperature in the flame sections considered are in reasonable agreement with experimental data.
For the prediction of NO_x pollutants, it was found that the integration of the NO_x formation in the chemical processes lead to unrealistic results. An extension of modelling these pollutants in post processing is planned.

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