Contribution to Numerical Modelling of Turbulent Non-premixed Flames

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Abstract

The effects of turbulence and combustion modelling on turbulent non-premixed flames characterized by high density ratios of the air coflow and the fuel jet as well as high injection velocity are investigated. These flames configurations are H_2 / Air and (CH_4-H_2-N_2) / Air. Two turbulence models which are k-ε and RSM (Reynolds Stress Model) are used in conjunction with SLFM (Steady Laminar Flamelet Model) and EDC (Eddy Dissipation Concept). Discrepancies between the prediction and the measurements are observed in the near-field region. They are attributed to the fact that turbulence is not fully developed in this region and also to differential diffusion in the case of (CH_4-H_2-N_2) / Air. In addition, in this region, the RSM model gives better results than the k-ε model predictions. Finally, in the far field region, the results compare reasonably well with published experimental data. It is shown that the predictions depends on the values adopted for turbulent Schmidt number in the transport equations for mixture fraction in the case of SLFM model and species mass fraction in the case of EDC model.

1 Introduction

Fuel blending represents a promising approach for reducing both NO_x and particulate emissions from combustion systems. The addition of hydrogen to hydrocarbon fuels affects both chemical and physical combustion processes. These changes affect among others flame stability, combustor acoustics, pollutant emissions and combustor efficiency. Only a few of these issues are understood. Therefore, it is important to examine these characteristics to enable using blend fuels in practical energy systems productions. The experimental approach is restricted, in general, to specific operating conditions (temperature, pressure, H_2 percentage in the mixture, etc.) due to its high costs. However, the numerical simulation can represent a suitable less costly alternative. However, prior to study numerically the effect of hydrogen addition on flame structure and pollutants formation, it is necessary to validate the numerical approach by testing reasonably simple configurations. The flames configurations tested in the present study are H_2 / Air and (CH_4-H_2-N_2) / Air. In addition, discrepancies between the numerical predictions and experimental data very close to the nozzle exit are noted by several investigators. In order to better understand these discrepancies, the effects of turbulence and combustion modelling on the computations are investigated in the present work. The combustion is modelled by using either the Steady Laminar Flamelet Model (SLFM) or the Eddy Dissipation Concept (EDC) while turbulence is modelled by using the standard k-ε model or the Reynolds Stress Model (RSM).

The combustion models discussed above are continuously evolving. In addition, the EDC model is introduced because it allows taking into account differential diffusion. The RSM turbulence model is also tested because it is well known that this model is able to describe the anisotropy of the flow resulting from strong streamline curvature in the vicinity of the jet as the model include pressure-strain correlation and vorticity terms.

The present analysis is conducted following three steps. In the first step, the interaction between combustion and turbulence is handled by using the stationary laminar flamelet model with the assumption of unity Lewis number in the flamelet library generation. The aim is to investigate the performances of turbulence models, particularly, in the region close to the nozzle exit. The flamelet library is considered with the assumption of unity Lewis number for all the species involved in the chemical mechanism. This assumption is adopted because predictions taking into account the effects of differential diffusion may lead to overpredicting flame characteristics. In the second step, the above mentioned turbulence models are coupled with the EDC model. The aim here is to investigate the effects of turbulence modelling with this combustion model. In the third step, the predictions of the two combustion models mentioned above are compared in the case of k-ε turbulence model in order to assess the capabilities of the combustion models especially near the jet exit.

2 Test conditions

Two flame configurations are numerically investigated. The first configuration is the one performed by Barlow and Carter [1] for the temperature and species concentrations and by Flury and Schlatter [2] for the flow field. The inner and outer diameters of the fuel tube are 3,75 mm and 4,8 mm respectively. The co-flowing air velocity has been fixed at 1 $m.s^{-1}$ for all measurements. The mean inlet velocity of the fuel jet is 296 $m.s^{-1}$. The Reynolds number of the flame is 10000. The flame has a visible length of 675 mm. The second flame configuration is an axisymmetric turbulent diffusion flame of (CH_4-H_2-N_2) in low coflow which is studied experimentally by Bergman *et al.* [3]. The fuel is issued from a stainless steel pipe having an inner diameter of 8 mm with a jet velocity of 42,2 $m.s^{-1}$ and a coflow velocity of 0,3 $m.s^{-1}$. A summary of the characteristics of these two flames configurations are reported in table 1, where m and R_ρ are the velocity and density ratios at the injection location respectively.

Flames configurations	U_J [$m.s^{-1}$]	U_e [$m.s^{-1}$]	ρ_J [$Kg.m^{-3}$]	m	R_ρ
H_2 / Air	296	1	0,082	0,0034	15
(CH_4-H_2-N_2) / Air	42,2	0,3	0,678	0,0071	1,8

Table 1 : Flames characteristics

3 Gas-phase governing equations and numerical method

The flamelet formulation used in this study developed by Pitsch and Peters [4], permit an exact description of differential diffusion. The main difference to previous formulations is the definition of a mixture fraction variable which is not related to any combination of the reactive scalars, but defined from the solution of a conservation equation with an arbitrary diffusion coefficient and appropriate boundary conditions. Using this definition, flamelet equations with the mixture fraction as the independent coordinate are derived without any assumptions about the Lewis numbers for chemical species. The flamelet equations [4] are solved in pre-processing. The stationary solution is stored in tables containing the profiles of temperature and mass fractions for all chemical species as function of the mixture fraction, its variance and the scalar dissipation rate. The coupling of chemistry and flow field is performed via the mixture fraction, its variance and the scalar dissipation which were provided from the flow field calculations. These values at each computational cell are used to extract mean scalar properties from the chemistry lookup tables. The flow field properties are updated and iterations continue until the imposed convergence criteria are met.

The eddy dissipation concept (EDC) [5] applied here is an extension to Eddy Dissipation Model (EDM). This model assumes that chemical reactions occur within the smallest turbulent structures, called fine structures. These are treated as perfectly stirred reactor (PSR) which exchange mass with the surrounding fluid. The overall reaction rate in each PSR is controlled by chemical kinetics. The properties of the fine structures are derived

from a step-wise energy cascade model and expressed with quantities related to the main flow, such as turbulent kinetic energy, k, and the turbulent dissipation rate, ε. This model takes into account differential diffusion.

The chemical reaction mechanism with the two combustion models adopted is GRI-MECH 1-2.

The flow and mixing fields are resolved by solving the 2-D, axisymmetric density-weighted fluid flow equations. Turbulence stress term is handled by using k-ε model in the first step and the RSM model in the second one. A so-called Pope correction and buoyancy contributions are added to the turbulent dissipation rate, ε, equation. Solution of the transport equations is achieved by using the Fluent CFD code.

The governing equations are discretized using finite volume method in an axisymmetric cylindrical coordinates. The SIMPLE numerical scheme is used to handle the pressure and velocity coupling. The diffusion terms in the conservation equations are discretized by using the central difference method and the convective terms are discretized by using the upwind difference method. The governing equations of momentum and energy are solved in a fully coupled fashion at each control volume.

For the H_2 / Air flame, the computational domain starts at the exit plane of the burner and extends 1 m downstream in the axial direction and 0,3 m in the radial direction. The mesh is dynamically refined during numerical iterations using user-specified gradient and curvature boundaries. The mesh characteristics are 200 nodes in the axial direction and 165 nodes in the radial direction. The numerical accuracy is checked by comparing the predicted results by using the grid mentioned above with those obtained by using a coarser grid with 160 nodes in the axial direction and 120 nodes in the radial direction. It is found that the two sets of results are very close to each other and therefore may be regarded as grid independent.

The computational domain for (CH_4-H_2-N_2) / Air flame covers an area that extends from 0 to 1 m in the axial direction and 0 to 0,0775 m in the radial direction. This result in 120(z) × 80(r) nonuniform grids in the simulations with finer grids placed in the primary reaction zone, near the fuel nozzle exit region as well as near the wall. It has also verified that further increase in grid does not significantly influence the simulation results.

For both flames, the mass flow rate, total temperature, turbulence intensity and hydraulic diameter of the fuel pipe are specified for the inlet boundary. At the outlet region, outflow condition is assumed and the symmetry condition on the side boundary.

7 Results

Some preliminary tests are performed in order to analyse the application of Pope correction to the RSM model which is found to produce overall fair predictions of flow characteristics in the near as well as in the far field. At the same time, this correction enables to keep the original coefficients of this model ($C_{\varepsilon 1}$ and $C_{\varepsilon 2}$). Recall that, for example, decreasing the constant $C_{\varepsilon 2}$ reduces the jet spreading rate close to the burner as well as intensifies the mixing process in the far-field. The correction proposed by Pope, on the other hand, gives much better representation of the flame. This is why all the results presented here are computed by using this correction instead of adjusting the model's constants. In addition, it is pointed out that the calculated results are not sensitive to the inlet profiles of the coflowing air. Contrary to the SLFM model, the fuel jet velocity profile and turbulence characteristics at the inlet have a noticeable effect on the predicted flame results in the near-field region with EDC model.

The Reynolds number of the flames was selected such that the flame is fully turbulent, but effects of buoyancy and local extinction are not present. The flames are attached and are in a fully burning regime and may therefore be considered to be a typical case which falls within the flamelet regime. The experimental data show deviations from chemical equilibrium near the fuel nozzle (The super-equilibrium values are about six times higher on the locations close to the burner) and the OH zone is much broader than at equilibrium. Also, there is a decay of the OH super-equilibrium values along the flame length approaching chemical equilibrium at the flame tip. First, the ability of both combustion models in capturing the deviation from equilibrium and the decay from super-equilibrium to equilibrium are verified by applying *Chemkin* code.

Both combustion models overpredicted the radial spreading profiles of the involved species and temperature in the near-field region. The stoichiometric contour (or the center of the reaction zone) occurs further away from the flame centreline (Figures 1 and 2). As a consequence, air entrainment and mixing are not well predicted. Contrary to k-ε, the RSM turbulence model predicts a better radial spreading because turbulence parameters are better modelled.

Increasing the turbulent Schmidt number in the transport equations for mixture fraction in the case of SLFM model and species mass fraction in the case of EDC model from standard values of 0.85 to 0.95 yields to a much

better agreement between the measured and predicted spreading of the jet close to the nozzle exit but less satisfactory in the far-field. Variable turbulent Schmidt numbers in the flow is suggested to overcome this problem.

The present predictions are sensitive to both turbulence and combustion modelling especially in (CH_4-H_2-N_2) / Air flame. The discrepancies between the prediction and measurement in the near-field region of the burner are attributed to differential diffusion in the case of (CH_4-H_2-N_2) / Air flame and the fact that turbulence is not fully developed in that region. Indeed, in this zone, the integral time scale is found to be higher than the turbulence time scale (τ_t) and the Kolmogorov time scale (τ_k) but far away, it is found to fall between τ_t and τ_k. Neither the SLFM nor the EDC are able to predict this feature. This is because the SLFM consider an infinite response of the flame (Steady flamelet), while the EDC model uses a residence time close to Kolmogorov time scale.

Figure 1 : Effect of turbulence modelling in : (a) : H_2 / Air flame, (b) : (CH_4-H_2-N_2) / Air flame

Conclusion

Numerical computations for two different diffusion flames are presented. The simulations include coupled models for turbulence, combustion and radiation. The turbulence models used are the k-ε model and the RSM model. Also flamelet library approach and EDC model have been applied to account for chemistry and turbulence interactions. The numerical approaches predicted with a reasonable accuracy the two flames characteristics which include flame shape, flame height and temperature distribution. Furthermore, in the near-field region of the jet exit which is characterized by high density ratio between the co-flowing air and the fuel jet with high injection velocity, it is found that the discrepancies between the prediction and measurement are mainly due to turbulence which is not fully developed in this region. Differential diffusion also plays a role in the case of (CH_4-H_2-N_2) / Air flame.

References

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