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Study in the Approach Prediction Ability of the Euler PDF Transport by Different Models of Turbulence

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The main objective of this study is the evaluation of the numerical capacity of the RANS-EPDF hybrid method, by comparing different turbulence models, with numerical simulations in a turbulent jet flame (hydrogen / air), using the method of Eulerian multi-environment transport to model the turbulence-chemistry interaction. And predict take-off height, flame ignition and extinction, as well as kinetic control of NOX species. The study was applied with three turbulence models, the modified k-ε, k-ε and the RSM. Numerical results are compared and discussed with experimental data. It was concluded that predictions of the modified k-ε model are more credible than other turbulence models and favor more impact on the optimization of computational methods.

1. Introduction

For the numerical study of a turbulent diffusion flame of H_2 injected into a flow of air preheated to the temperature of 1045K; we used the RANS-PDFT hybrid method (Muradoglu et al., 2001). The approach presented is based on the use of reduced kinetic schemes in order to limit the cost of calculation by unnecessarily avoiding the transport of reaction intermediates and to improve the numerical stability during the integration of the transport equations of the species. Over the last decade, Haworth (2010) has attracted a lot of attention by developing the probability density function in turbulent reactive flows. The goal of RANS-PDFT Hybrid was to consider the appropriate chemistry for any burning regime. Specifically, all terms characterized in a variable were defined by the average rate of chemical reaction. According to research carried out on this RANS-PDFT approach, there are two methods to solve its equations: the Lagrangian method (LPDF) and the multi-environment method with the Eulerian method (MEPDF). Numerous studies on the Lagrangian method have been conducted (Cabra et al., 2005; Cao et al., 2005) use a configuration of hybrid RANS–LPDF for studying lifted flames as well as the problem of auto-ignition in a vitiated coflow. Cao (2005) performed a sensitivity study in a turbulent flame of lifted vitiated coflow on different mixing constant (1.5,2.0,2.5) and by applying the three mixing models (IEM, EMST, MC) using LPDF concluded that lift-off height is largely unaffected to the mixing parameters. On the other hand, OH production is influenced by the three mixing models as the EMI model is more accurate than EMST and MC. (Senouci et al., 2013) used this method by comparing different mixing models (MC, EMI and EMST) to highlight the effect of the mixing model. A few publications to study the resolution of equations of the PDFT have appeared in recent years on the MEPDF. Fox suggest the hypothesis of devlopper the method (MEPDF) presumed in a turbulent reaction flow. Tang et al. (2007) by a numerical study uses the method of the moments in direct quadrature (DQMOM) with finite rates of chemistry, tested on a modeling of stabilized bluff-body flames; found that the PDF model accurately predicted. this type of flames. Yadav et al. (2014) used this method of MEPDF in two lifted diffusion flames of H_2/N_2 and CH_4/air injected in vitiated coflow for numerical search introduced between different values of mixing constant and he found a good adequacy with experimental data. Another study by Yadav et al. (2013) uses the same approach for the non-gray radiation simulation with using WSGG method demonstrated that the prompt of a steady flame for lower estimations (C_{phi}=2). On the other side, LPDF approach found that an estimation of (C_{phi}=2) prompts global extinction, the estimation of (C_{phi}=3) prompts most precise outcomes

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(Yadav et al., 2013). Dongre et al. (2014) studied two different burners imitating Moderate and Intense Low Oxygen Dilution MILD by multi environment PDF and showed that the difference in the predictions for higher Re number is expanded and that is principally because of the errors in the turbulence model and wrong reaction of the micro-mixing term. Conduct a comparative study between the two Eulerian/Lagrangian methods in a hydrogen flame, and find insufficient results because of the weakness of the reaction mechanism of H_2 .Another comparative investigation by Jaishree et al. (2012) use The same comparison and demonstrated that the lagrangian model is much more accurate than eulerian. In this article, the hybrid RANS-EPDF approach is presented. The Eulerian method is otherwise called the multi-environment or just Eulerian method that is determined and developed. in a turbulent reactive flow. Although the accuracy of the Eulerian PDF approach model has been well developed during in recent years, there are nevertheless still areas of research to be developed in parallel improving the accuracy of prediction of the zones of the flames by the EPDF model with the evolution of the numerical performances of the various models of turbulence, in particular in the prediction of major phenomena such as that the detachment, extinction and ignition of the flame (Larbi et al., 2018). It is for this purpose that this work is devoted.

2. Theoretical Formulation of Eulerian PDF transport method (EPDF)

The complex phenomena of turbulent combustion are mainly governed by the Navier-Stokes equations and the transport equations of the majority chemical species, associated with a fast chemistry where the reaction rate is very high. all the variables are modeled by the diffusion gradient or by the average rate of reaction, with an invariable expression of its nonlinear function; For that, the modeling of the combustion must necessarily imply the resolution of the purely linear equations based on simplifying hypotheses.

$$\frac{\partial}{\partial t}(\rho p)+\frac{\partial}{\partial x_i}(\rho u_i p)+\frac{\partial}{\partial \psi_k}(\rho S_k p)=\frac{\partial}{\partial x_i}\left[\rho\langle u_i^{"}|\psi\rangle P\right]+\frac{\partial}{\partial \psi_k}\left[\rho\left\langle\frac{1}{\rho}\frac{\rho j_{i,k}}{\partial x_i}\middle|\psi\right\rangle P\right] \quad (1)$$

Equation (1) shows the equation of the transport PDF composition, it is not a closure problem, it is the main advantage of the PDFT equation that does not require modelling. The turbulent scalar flow in the first term of the equation is modeled by the term gradient - diffusion (2).

$$-\frac{\partial}{\partial x_i}\left[\rho\langle u_i^{"}|\psi\rangle p\right]=\frac{\partial}{\partial x_i}\left(\frac{\rho\mu_t}{Sc_t}\frac{\partial p}{\partial x_i}\right) \quad (2)$$

For the resolution there are two methods to close the second term of the PDF transport equation (1), multi-environment eulerian (MEPDF) method or lagrangian method (LPDF) based on the stochastic method of monte-carlo.(Larbi et al., 2018) shows in the table1 a comparison between the two methods LPDF and MEPDF.

EPDF it is an associated approach between the composition space and the physical space. The composition space is defined by a smaller number of interactive environments by coexistence in the physical space.

$$\mathrm{p}(\psi;\vec{\mathrm{x}},\mathrm{t})=\sum_{\mathrm{n}=1}^{\mathrm{N_e}}\mathrm{p_n}(\vec{\mathrm{x}},\mathrm{t})\prod_{\mathrm{k}=1}^{\mathrm{N_s}}\delta\left[\psi_{\mathrm{K}}-<\phi_{\mathrm{K}}>_{\mathrm{n}}(\vec{\mathrm{x}},\mathrm{t})\right] \quad (3)$$

So; The IEM will model the micro-mixture, and the diffusion gradient will model the turbulent scalar in the transport equation for a multi-dimensional associated composition space PDF, the MEPDF will take off from this equation with the closures of the terms in eq. (3), but there are still unknown terms.

$$\frac{\partial\rho p_n}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i p_n)=\nabla(\rho\Gamma\nabla p_n) \quad (4)$$

$$\frac{\partial\rho s_{k,n}}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho u_i s_{k,n}\right)=\nabla(\rho\Gamma\nabla s_{k,n})+\rho(M_{k,n}+S_{k,n}+C_{k,n}) \quad (5)$$

FOX (2005) proposes the DQMOM model (direct quadrature method of moments) as a method of effective resolution to this problem. This proposal will allow the resolution of unknown terms,p_n and $<\phi_K>_n$. in equation (3) the DQMOM approach, is used to present the resulting equations of MEDF in eq.(4) and (5), when $S_{k,n}$ describe the reaction, $M_{k,n}$ is the mixing and $C_{k,n}$ is terms of correction

$$S_{k,n}=p_n S(<\phi_{\mathrm{K}}>_{\mathrm{n}})_k \quad (6)$$

$$M_{k,n}=\frac{C_\Phi}{\tau}(<\phi_{\mathrm{K}}>_{\mathrm{n}}-\psi_{\mathrm{K}}) \quad (7)$$

$$\sum_{n=1}^{N_e}\phi_{\mathrm{K}_n}^{m_k-1}C_{k,n}=\sum_{n=1}^{N_e}(m_k-1)<\phi_{\mathrm{K}}>_n^{m_k-2}p_n c_{k,n} \quad (8)$$

3. Turbulence modeling

The approach used for numerical modeling of turbulent combustion is the Reynolds Means Techniques (RANS) for the purpose of predicting the behavior of the mean values of the reacting flow properties.

3.1 Standard K-ε model

Launder and splanding propose this model as a simpler and faster reference in the computation, based on the resolution of the turbulent length and the scalar time. This model is a first-order model based on the concept of turbulent viscosity introduced by Boussinesq.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k \quad (9)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_j}\right] + G_{1\varepsilon}\frac{\varepsilon}{k}(G_k + G_{3\varepsilon}G_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_k \quad (10)$$

This model is obtained by the derivation of a global equation of energies and transport, defined by the two terms turbulent kinetic energy k; and its dissipation rate called ε. Obtained from the two equations (9 and 10).

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (11)$$

The term G_b represents the turbulence production due to buoyancy. The term G_k represents the kinetic energy of turbulence generated by the average velocity gradients. The turbulence model kε has five constants to cite. For k on the nondimensional number called turbulent Schmidt number σ_k and σ_k. For the term ε there is $C\varepsilon_1$ (dissipation production), $C\varepsilon_2$ (dissipation of the energy dissipation) and C_μ in the expression of the turbulent viscosity which appears in equation 11.

3.2 RSM model

The Reynolds stress model is a second-order RANS turbulence model that has been designed for accurate predictions of complex flows. The closure of this model is performed by solving the Reynolds constraints and the dissipation rate equation. So here are the transport equations for the RSM model.

$$\frac{\partial}{\partial t}\left(\bar{\rho}\overline{u_i^{"}u_j^{"}}\right) + \frac{\partial}{\partial x_k}\left(\bar{\rho}\widetilde{u_k}\overline{u_i^{"}u_j^{"}}\right) = D_{ij}^T + D_{ij}^L - P_{ij} - G_{ij} + \varphi_{ij} - \varepsilon_{ij} \quad (12)$$

A simplified linear equation is used to model turbulent diffusion in the form of a scalar as follows:

$$D_{ij}^T = \frac{\partial}{\partial x_k}\left(\frac{\mu_t}{\sigma_k}\frac{\partial \overline{u_i^{"}u_j^{"}}}{\partial x_k}\right) \quad (13)$$

To model the term φ_{ij} we break down it as follows:

$$\varphi_{ij} = \varphi_{ij,1} + \varphi_{ij,2} \quad (14)$$

$\varphi_{ij,1}$ This term is known as: slow pressure-strain, and this term $\varphi_{ij,2}$ is known as rapid pressure constraint

$$\varphi_{ij,1} = -C_1\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\left[\overline{u_i^{"}u_j^{"}} - \frac{2}{3}\delta_{ij}\,\widetilde{k}\right] \quad (15)$$

$$\varphi_{ij,2} = -C_2\left[\left(P_{ij} + F_{ij} + G_{ij} - C_{ij}\right) - \frac{2}{3}\delta_{ij}(P + G - C)\right] \quad (16)$$

and the dissipation rate in (Ional et al. 1989).

$$\varepsilon_{ij} = \frac{2}{3}\delta_{ij}\bar{\rho}\tilde{\varepsilon} \quad (17)$$

4. Turbulent flame of (hydrogen/air)

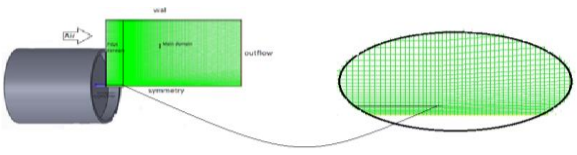

Figure1: Burner schematic and computational field of calculation of Flame

In this simulation Hydrogen flames chosen were experimentally studied by Cabra et al. (2005). The burner consists of a horizontal tube with an internal diameter of 4.57mm and an outside diameter of 6.35mm, centered in a cross-section with an internal diameter of 210 mm (Fig.1).
In computational domain shown above contains fuel flow, pilot co-flow, surrounding air; with a mesh grid of 25440 cells in fine-1. To validate our choice of mesh a study of independence is proposed with three different meshes: base with 18220 cells and fine-2 with 35320 cells (Cabra et al., 2005; Larbi et al., 2018).

Table 2: The different entry conditions of H2 /Air

Parameters	Re	D(mm)	V(m/s)	T(k)	X_{H2}	X_{O2}	X_{N2}
H2 (Jet)	23,600	4,57	107	305	0,2537	0,0021	0,7427
Air(Co-flow)	18,600	210	3.5	1045	0.0005	0,15	0,75

This configuration has an axisymmetric geometry, using ANSYS Fluent 15.0 as the calculation code. The refinement of the mesh in the areas close to the outlet of the ejection nozzle was considered to take into account the various phenomena due to the premixing and contact of the reagents. The mesh has been realized with the software Gambit 15.0. the method used in this calculation is the EPDF with a mixing constant of 1.8 using the ISAT approach as a tabulation method (Larbi et al., 2018). The reaction mechanism chosen is GRI-Mech2.1. Table 2 gives us the different entry conditions.

5. Results and discussion

The study of the turbulent (H_2/Air) flame; using the Eulerian Transport PDF approach, with a hot coflow that is nessaisaire for the stabilization of this flame. It should be noted that the quality of numerical simulation of turbulent diffusion flames depends essentially on the performance of the selected turbulence model. For it, three different turbulence models were used for this study. The first is the standard k-ε model; the RSM is the second model. The last is the modified k-ε that we modify in these constants and parameters.

5.1. GRID-Independent study

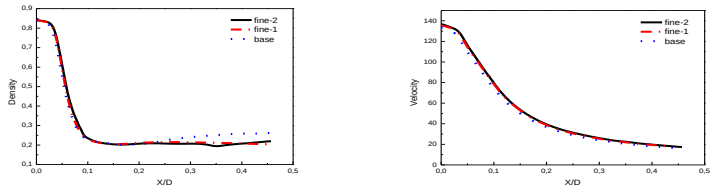

Figure 2: Axial evolution of density and velocity for approach of MEPDF

We show here the effect of the mesh, with a comparison of the axial evolution of density and velocity along the central axis of the flame for the EPDF approach. The two graphs compare the evolution of the velocity and density profiles for each mesh which are in refinement level difference for more precision (Base, Fine, Fine). Each plot shows three profiles for meshes 1, 2 and 3. Mesh 2 shows in both profiles slight differences from

5.2. Flame of hydrogen in a hot vitiated Co-flow

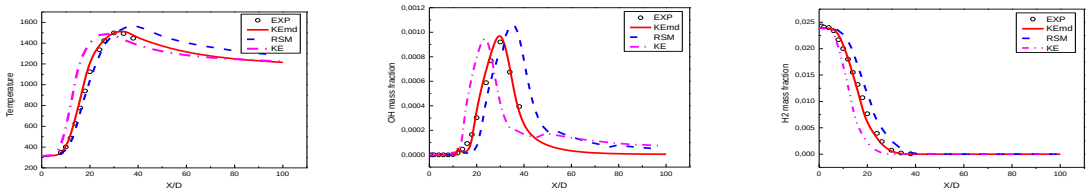

Figure 5: Axial profiles of temperature, and species mass fractions for different turbulence models

Figure 5 shows the axial evolution of the temperature profiles and the mass fractions of the species (OH, H_2) along the flame jet. According to the figure, the area of calculation is divided into three zones, the first one where (X/D<10) is the mixing and preheating zone and the point of (X/D=10) represents the beginning of the production of 'chemical species. Subsequently (10<X/D<30) is the zone of chemical reactions where the reaction rate is maximal, until reaching the temperature PIC, and the last zone where (30<X/D≥100) where the flame is reduced and cooled. For the temperature profile, we can see that the models k-ε and RSM are both late in the experiment and this is very visible in the reaction zone where the temperature is maximal from the axial positions with a sub-phase. estimation of the k-ε model and overestimation of the RSM model, while a very good estimate is identified by the modified k-ε model. The predictions from the EPDF approach using modified k-ε for temperature are in good agreement with experience in all flame zones. The height difference of the temperature pic does not exceed 10k. but there is a visible disagreement in the curve of the k-ε. RSM model with experimental in the mixing and reaction zone which is the most important area of the flame.

By analyzing the curves of the two models of turbulence (modified k-ε and RSM). Bounif et al. (2007) shows that the RSM model is better suited in the case of the combustion process, especially in the high reaction zone where combustion is at high efficiency; because it calculates the equations of the constraints of velocity whereas the computation of the model k-ε is more simplifying since it rests only on the hypothesis of Boussinesq. But in this case, we can say that this model is more appropriate since we have a simple configuration with small turbulent vortices. This is what we see with the results of the model k-ε modified especially with the profiles of the mixing fractions, the prediction disagreement of this model is probably due to the choice of the reaction mechanism or the turbulent viscosity effect.

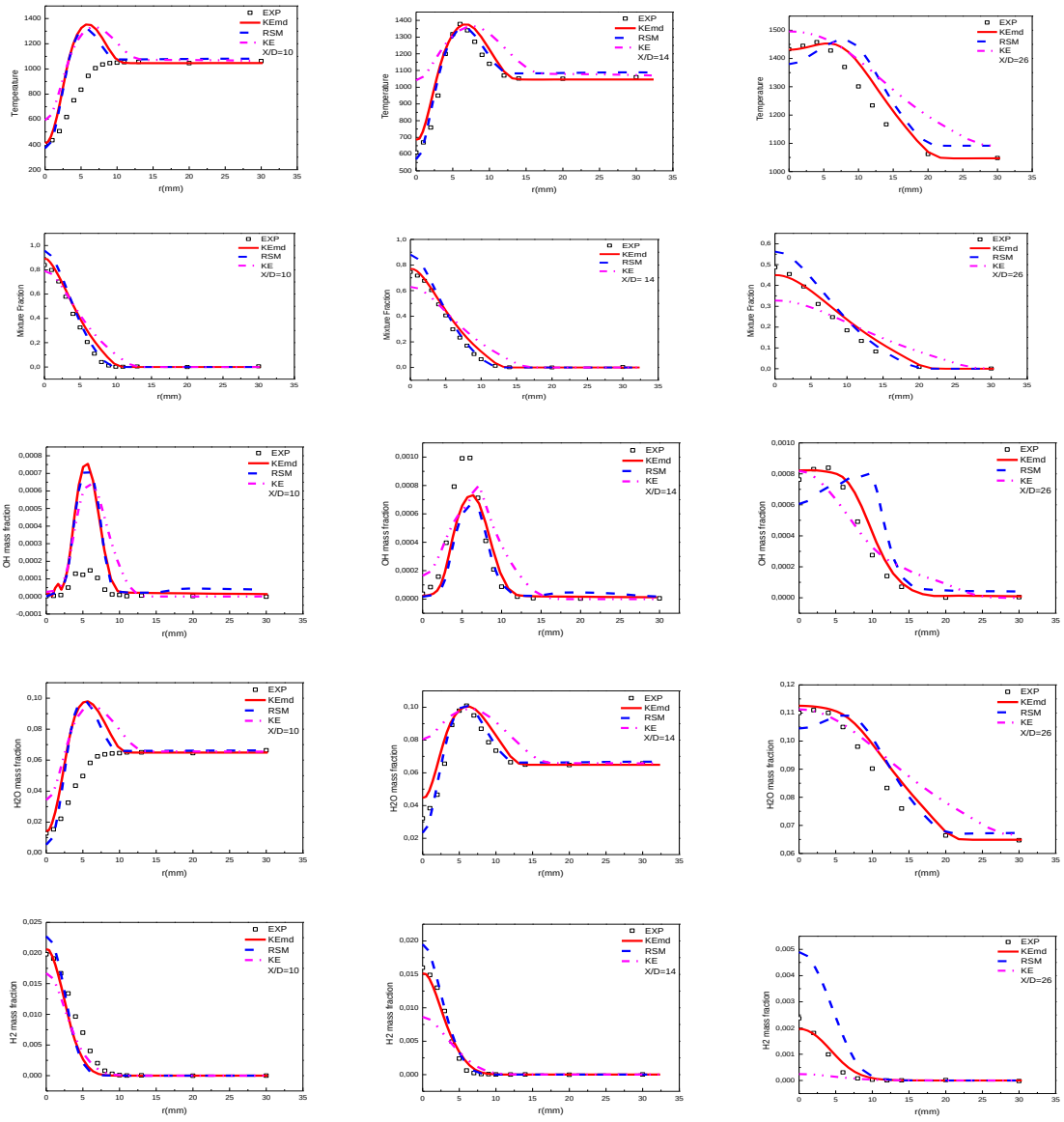

Figure 6: Radial evolutions of the temperature, the fraction of mixture, the mass fraction at stations=10,14,26

For the profile of the OH mass fractions, the predictions of the EPDF approach with the modified k-ε model are in total adequacy with those of the experimental since the difference is less than 4%. The exact results of production species such as OH are one of the essential criteria to prove the ability of the EPDF model to predict this type of flame; and this confirms the results published by Yadav (Tang et al., 2007). By observing the and H_2 curves, there is also a very good agreement between the calculated values of modified k-ε and the experimental values, contrary to the curves of the other turbulence models which are out of step with the experimental results. we can see it in the figures. Figure 6 shows the radial changes in temperature, the mixing fraction and the mass fractions of the majority species on three axial stations (X/D=10,14,26) using the

EPDF approach to compare the three turbulence models. For the radial profiles of temperature, one notes that for all the models of turbulence one has a good concordance with the experiment especially downstream, except on two points. The first is at station X / D = 10, a difference in height on the temperature PIC is observed in all three models, which means an over-prediction compared to experience. This ecard is also found in the radial profiles of the mass fraction of OH and H_2O in the same place just after the exit of the nozzle. the combustion of H_2 goes through a very fast chemistry. This explains the high temperature peak in this flame zone. From the beginning, there is an important production of the majority species, observed by the high rate of production of the mass fractions of OH and by chain reaction of the H_2O species in this reaction zone. A good prediction is observed with the model k-ε modified practically on the three stations. For the profile of the mixing fraction, the three turbulence models predict a good H_2 / Air mixture up to station X/D=14 but for station X/D=26, only the modified model k-ε is just. The predictions of the OH and H_2O species are almost identical. Except with the first note mentioned above for the three models, it can be said that the modified k-ε model gives good results in all the zones, which confirms the probability of calling into question the choice of the reaction mechanism. It should be noted that only this model reasonably predicts the consumption of H_2 throughout the flame can be seen on (X/D=10). since the beginning of the mixing, the differences in calculation for the other two models with the experiment are clearly observed with the RSM model, in particular at the last station X/D=26, an overestimation of H_2. Unlike the model k-ε, which underestimates more and more the consumption of H_2.

6. Conclusions

We have studied numerically a turbulent diffusion flame of H_2 / air by the RANS-EPDF hybrid method with the use of different turbulence models (k-ε, modified-k-ε-RSM), the calculation results are compared with experimental data. We can say that given the good prediction of the OH species, which is one of the essential tests to evaluate the accuracy and capacity of the EPDF approach it can be said that the EPDF approach coupled to the modified turbulence model k-ε is more suitable for predicting this type of flame; because it is very important also to identify the areas of turbulence and recirculation to correctly detect the local extinction and return flames as well as the height of detachment. D'autre part, les résultats obtenus avec les modèles k-ε et RSM sont relativement crédibles avec des zones de décalage très visibles avec l'expérience. . Mathématiquement, le modèle RSM donnerait de meilleures prédictions que le modèle k-ε parce qu'il résoudrait les équations du tenseur de Reynolds et pourrait mieux capturer les phénomènes d'anisotropie alors que k-ε est basé sur l'hypothèse de Boussinesq.But in our case, we have a simple configuration that makes it easier to control the performance of the turbulence models and to make some modifications of improvement, which allowed us to obtain good results with the k-ε modified its method is more optimized than other methods. The discrepancy between predictions and experience can be explained by the effect of other parameters; such as the influence of differential scattering or the interaction of chemistry phenomena. In the end, it is certain that this study also shows the advantage of the RANS-EPDF hybrid method.

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