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Investigation of Modified EMST Micromixing Model Performance on Lagrangian PDF Transported in Lifted Hydrogen/Air Fames

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ABSTRACT

This article presents a numerical simulation of high hydrogen/air flames using the Lagrangian transported PDF method. This method enables the calculation of fluid composition changes resulting from convection and reaction without the need for modelling, while requiring modelling for molecular mixing. Consequently, the accuracy of calculations in this L-PDF method heavily relies on an accurate representation of the mixture model term. The Euclidean model, which provides a better description of physical mixing processes, is well-suited for modelling the molecular mixing term EMST. Additionally, the accuracy of this model depends on the value of the mixing constant, representing the ratio between the mechanical time scale and the scalar time scale. Two algebraic models for the mixing constant have been implemented in the computational code, employing a well-defined function to calculate this ratio for each cell. These models contribute to memory and CPU time savings. To account for turbulence and its interaction with physical phenomena, the RSM model is employed due to its ability to identify different areas of turbulent stresses. Hence, the primary objective of this study is to evaluate the capabilities of these algebraic models in predicting scalar fields within such flames. Overall, the predictions align well with experimental data, affirming the validity of these models.

1. Introduction

Combustion currently serves as the primary source of mechanical and electrical energy, and it will continue to play this crucial role in the foreseeable future. Turbulent combustion, commonly observed in a wide range of technologically relevant flows [1], holds significant importance.

To accurately predict turbulent combustion, precise knowledge of the concentration statistics of chemical species and temperature, along with a rigorous description of chemical reactions, is required. The most widely employed approach for simulating turbulent combustion is the

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composition probability density function (PDF) [2]. This method is based on the concept of flamelets [3], which are utilized to model turbulent premixed [4, 5] and diffusion [6, 7] flames. The underlying principle of this concept involves characterizing non-turbulent flames using small-scale structures. This parameterization is achieved by employing an ensemble average within the assumed PDF, providing an approximation of the statistical behavior of turbulent flames. By incorporating flamelets into the presumed PDF, a pre-calculated tabulation of these structures is obtained, serving as a practical modeling tool for turbulent flames.

The primary strength of the assumed PDF approach lies in its capability to fully account for the highly nonlinear reaction term, eliminating the need for additional modeling [8-10]. The micromixing term remains the only significant element to be modeled. Wang [11] employed LES/FDF simulations to investigate turbulent flames, considering the sub-grid reaction mixture. They proposed a novel hybrid-DD model that enhances combustion prediction in comparison to traditional models. In another study, an RIDM scalar mixing model for non-premixed turbulent flames [12] was presented, accounting for the disparities in molecular diffusion and the reaction-induced scalar gradient. The findings reveal a significant improvement in combustion prediction when compared to conventional models. Furthermore, a study identified 10 crucial species for differentiated mixing in non-premixed flames [13]. The results indicate that by exclusively considering the differentiated mixture of these species, effective replication of both average and conditional combustion quantities can be achieved. The Euclidean Minimum Spanning Tree (EMST) model, renowned for its effective representation of the mixing process [14, 15], is one of the commonly employed models, also utilized in this study. In this model, the mixing rate is determined by the mixing model constant, C_Φ, which represents the ratio of turbulent-to-scalar time scales. While the typical value for this constant is often set at 2, different values have been tested. Previous numerical investigations on turbulent diffusion flames have demonstrated the impact of varying this constant on PDF transport results [16-18]. It is important to note that this constant, which is usually not constant itself, also depends on its initial value and the dimensionless Reynolds number [19-21].

This study aims to enhance our comprehension of combustion processes within a lifted hydrogen/air flame by employing the Lagrangian PDF transport method. By evaluating the performance of algebraic models and comparing them to experimental measurements [22], we can determine their accuracy and suitability for predicting flame characteristics, thus contributing to the advancement of knowledge in the field of combustion.

The present paper introduces a Lagrangian PDF transport method for analyzing a lifted hydrogen/air flame. The Monte Carlo method is utilized to solve the PDF equation, while the finite volume method is employed to solve the dynamic field. The parameter CΦ is computed using two algebraic relations that have been implemented into our numerical code. The first relation is derived from an investigation of turbulent shear flows [23], while the second is based on Sanders' examination of scalar dissipation rate modeling [24], building upon the research conducted by Yoshizawa [25].

2. Modeling the Mean Flow Field

The equations governing turbulent reactive flows are of paramount importance, as they encompass the conservation of mass, momentum, and scalar quantities. These fundamental equations can be approached in a more practical manner by averaging and reformulating them in a new form, thereby enabling a deeper understanding and more efficient modeling of these intricate flows [26]. The significance of these equations resides in their capacity to accurately and comprehensively capture the interplay between various chemical species, turbulence, and chemical

reactions, thereby presenting promising prospects for the prediction and simulation of turbulent combustion. These equations can be written in the new form as follows:

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\,\tilde{u}_i\tilde{u}_j}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial(\bar{\tau}_{ij})_{eff}}{\partial x_j}+\frac{\partial}{\partial x_j}(-\bar{\rho}\,\widetilde{u_i''u_j''}) \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{\phi}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\tilde{\phi}}{\partial x_i}=-\frac{\partial J_i^{\phi}}{\partial x_i}-\frac{\partial}{\partial x_i}(-\bar{\rho}\,\widetilde{u_i''\phi''})-\bar{\rho}\,\tilde{S}_{\phi} \tag{3}$$

With $\widetilde{\tau_{ij}}$ viscous stress tensor, $-\bar{\rho}\widetilde{u_i''u_j''}$ the Reynolds stress, $-\bar{\rho}\widetilde{u_i''\emptyset''}$ is the turbulent scalar flux, $J_i^{\emptyset}$ the molecular scalar flux, $\emptyset$ the scalar (species mass fractions, $\widetilde{Y_\alpha}$ or enthalpy, $\tilde{h}$), and $\widetilde{S_\emptyset}$ the source term.

If the Reynolds number of turbulence is very high, the effects produced by turbulent agitation are important with neglect of the molecular effects. In this case, we are obliged to add an equation which describes the thermodynamic state or the ideal gas law for multicomponent fluids:

$$P=\rho R T\sum_{\alpha=1}^{n}\frac{Y_\alpha}{W_\alpha} \tag{4}$$

With R the perfect gas constant and Wα is the atomic weight of species α.

3. Turbulent Modeling

The utilization of the RSM (Reynolds Stress Model) is indispensable for addressing the closure issue of the Reynolds tensor in turbulent flows. In terms of species diffusion flux, Fick's law is employed, while the transport gradient hypothesis provides closure for the transport equation of the turbulent scalar [27]. Transport equations, encompassing Reynolds stress and dynamic dissipation, hold a pivotal significance in comprehending and modeling these intricate flow phenomena. Ensuring their precise and rigorous resolution is imperative to attain dependable outcomes and achieve an accurate prediction of turbulent and reactive behaviors.

$$\frac{\partial}{\partial x_k}(\bar{\rho}\,\tilde{u}_k\widetilde{u_i u_j})=\tilde{P}_{ij}+\tilde{D}_{ij}+\tilde{\phi}_{ij}-\frac{2}{3}\delta_{ij}\,\bar{\rho}\tilde{\varepsilon} \tag{5}$$

$$\frac{\partial}{\partial x_k}(\bar{\rho}\,\tilde{u}_k\tilde{\varepsilon})=\tilde{D}_{\varepsilon}+\bar{\rho}\frac{\tilde{\varepsilon}^2}{\tilde{k}}\tilde{\psi}(\varepsilon) \tag{6}$$

Modeling of different terms of Eq. (5) and Eq. (6) is detailed in our former work [12, 24]. The RSM is a complete model, considered the best classic model which is less expensive and gives good precision.

4. Combustion Modelling

There are various numerical methods available for modeling combustion, but the Lagrangian PDF transport method is widely regarded as the best and most popular approach. This method provides a comprehensive statistical description of turbulent reactive flows [28]. It relies on a unique Joint Probability Density Function (JPDF) that enables an accurate representation of chemical reactions without relying on overly simplistic assumptions [2]. However, modeling the molecular-level mixture still presents a challenge. The main limitation of PDF transport methods stems from the non-linearity of the different species, resulting in the treatment of all scalars independently and randomly. The transported PDF represents the spatial and temporal distribution function. Once the PDF is obtained, the average value of the scalars can be expressed as follows:

$$< Q(\phi) > = \int_{-\infty}^{\infty} Q(\psi)\, f(\psi; x, t).d\psi \tag{7}$$

where ϕ is the vector of physical scalars, x is the corresponding random variable vector, Q is a function of ϕ only and f is the JPDF, which represents the probability density of a compound event ϕ = ψ. in the case where we have a variable density including turbulent flows, we use the joint composition mass density function (JCMDF). $F_{\emptyset}(\Psi) = \rho(\Psi) f_{\emptyset}(\Psi)$.

Favre density means can be applied in this equation:

$$\tilde{Q}(x,t) = \frac{< \rho(x,t) Q(x,t) >}{< \rho(x,t) >} = \frac{\int_{\psi} < Q(x,t)/\psi >) F_{\phi}(\psi; x, t).d\psi}{\int_{\psi} F_{\phi}(\psi; x, t).d\psi} \tag{8}$$

4.1 Equation for the Transported PDF

When we use the JCMDF, we will have no problem solving the transport equations [22]:

$$\frac{\partial F_{\phi}}{\partial t} + \frac{\partial \tilde{U}_j F_{\phi}}{\partial x_j} + \frac{\partial}{\partial \psi_{\alpha}} (S_{\alpha}(\psi) F_{\phi}) = -\frac{\partial}{\partial x_i} [< u_i / \psi >) F_{\phi}] - \frac{\partial}{\partial \psi_{\alpha}} [\frac{1}{\rho(\psi)} < -\frac{\partial J_j^{\alpha}}{\partial x_j} / \psi > F_{\phi}] \tag{9}$$

Physical space and composition space are indicately by the summation indices α and i. <A/B> this is the conditional mean of event A when event B occurs. The terms LHS represent the evolution of the probability in time, in physical space represent the convection of the probability. His terms pose no closure problem. On the other hand, the terms RHS pose a problem of closure. The turbulent scalar flow in physical space modeled by the gradient diffusion hypothesis, the transport of probabilities in the molecular flow in the composition space is the weak link in this equation, it is the micromixing.

4.2 Hybrid Solution Method

To solve Eq. (9), we have to use a hybrid method which makes the Monte Carlo method consistent with the finite volumes [16]. Firstly, the turbulent dissipation rate, the kinetic energy of turbulence, the average pressure and the average velecity will be solved by the fine volumes and with a turbulent

timescale $\tau_t = \tilde{k}/\tilde{\varepsilon}$ we go directly to Monte Carlo methods. The spatial displacement of the particles in the Monte Corlo approach will be by a second order Lagrangian method. Evolution and movement of particles due to several reasons like diffusion, convection, mixing and reaction. The solution will be applied by several steps [12]. For the mixing step, the EMST mixing model is applied. Here, two algebraic models of C_Φ are used. The first model is given by [22]:

$$C_{\Phi} = \frac{3\alpha}{\lambda_T} \tag{10}$$

Where α is the thermal diffusivity and λT the length microscale of temperature.

The length microscale of temperature λT is given by [29]:

$$\lambda_T = \frac{\alpha}{\tilde{k}^{1/2}} \tag{11}$$

$$C_{\Phi} = \frac{3\tilde{k}^2}{\alpha\tilde{\varepsilon}} \tag{12}$$

Thus;

The second model is an analytical solution of model equation of Yoshizawa [24] for the scalar dissipation rate which is investigated by sanders [23]. This model is given by:

$$C_{\Phi} = \frac{(\tilde{k}/\tilde{\varepsilon})}{(\Phi''^2/\tilde{\varepsilon}_{\Phi})} \tag{13}$$

With:

$$\varepsilon_{\Phi} = \Phi\Phi''^2\,\tilde{\varepsilon}^{(1/2)} \tag{14}$$

In which:

$$\Phi = \Phi_0(U_j D_{eq})^{-(1/2)} \tag{15}$$

With Φ_0 is a dimensionless constant determined by comparing predictions in a jet with experiments. In the present study the value of Φ_0 has been determined to be $\Phi_0 = 5$. The jet exit diameter Dj = 0.004 m, the jet exit velocity Uj = 296 m.s-1 and the effective diameter $D_{eq} = D_j\left(\rho_j/\rho\right)^{(1/2)}$

The use of Eq. (14) and Eq. (15) helps us to obtain the time scale relation C_Φ as a function of the turbulent kinetic energy, k its dissipation ε and

Its density ρ:

$$C_{\Phi} = 9.2\rho^{(1/4)}\varepsilon^{(1/2)}\left(\frac{\tilde{k}}{\tilde{\varepsilon}}\right) \tag{16}$$

Eq. (12) and Eq. (16) were implemented, in numerical ANSYS FLUENT by the UDF option.

An importance feature of these equations is that the mixing-model constant C_{Φ} depends only on the turbulent time scale.

5. Lifted Hydrogen Flame DOMAIN

In this study, we specifically focus on investigating the characteristics of turbulent and confined axisymmetric reactive jets, as they hold a crucial position in numerous industrial applications, including combustion in propulsion engines and industrial burners. Understanding and accurately modeling these jets bear significant importance in enhancing energy efficiency and reducing harmful emissions.

We have tailored our calculation code to a simplified yet representative configuration of these reactive jets. This configuration is commonly employed in theoretical and experimental studies due to its reproducibility and ease of implementation. Consequently, we can derive meaningful outcomes and compare them with other pertinent research in the field.

For our calculations, we utilize data obtained from our previous work [12], which has provided us with a well-established and coherent computational domain (see Figure 1). These data serve as a solid foundation for our study, enabling us to delve deeper into the properties and behaviors of turbulent and confined axisymmetric reactive jets.

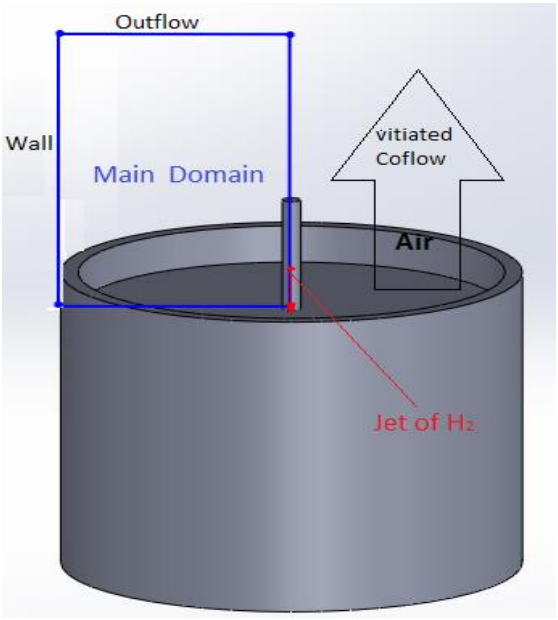

Fig. 1. The burner and the calculation domain

6. Results and Discussion

We will now present and discuss the results of the numerical simulation of the scalar field obtained using the two previously defined algebraic models, comparing them with the experimental data of R.S. Barlow [22]. As illustrated in Figure 2, the numerical results concerning the axial evolution of the average mixing fraction agree well with the experimental data.

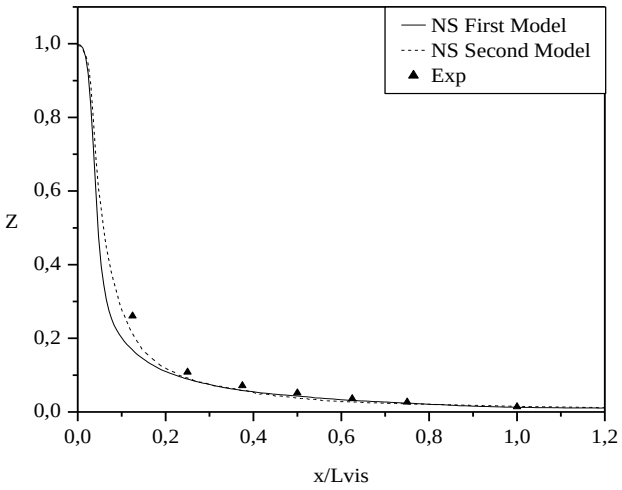

Fig. 2. Axial profile of the predicted and experimental mean mixture fraction

The radial evolution of the average mixing fraction at x/Lvis = 1/8 and 3/4 of the axial locations (Figures 3 and 4) qualitatively demonstrates the same behavior as observed in the experiment. Researchers Meier [31] and Sanders [32] have also corroborated this trend at the center of the axis. The second model, based on these observations, provides an accurate prediction that aligns well with experimental values, particularly in remote regions (at x/Lvis = 3/4). Conversely, despite its limitations, the first model manages to make satisfactory predictions in these same regions. These findings validate the proposed models and their ability to elucidate the behaviors observed in this study.

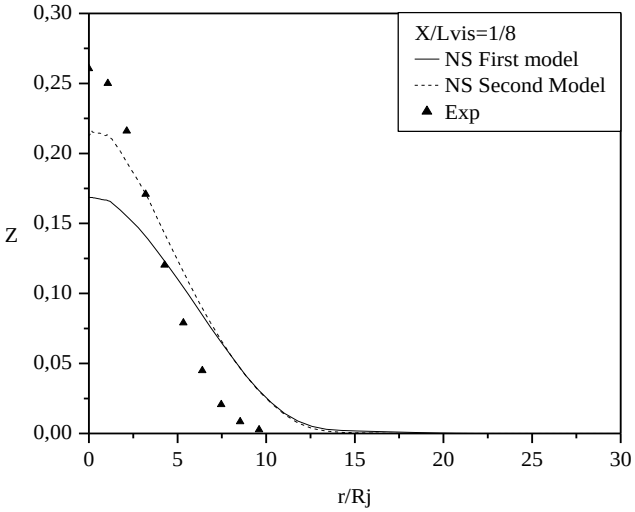

Fig. 3. Radial profile of the predicted and experimental mean mixture fraction at the axial location of x/Lvis = 1/8

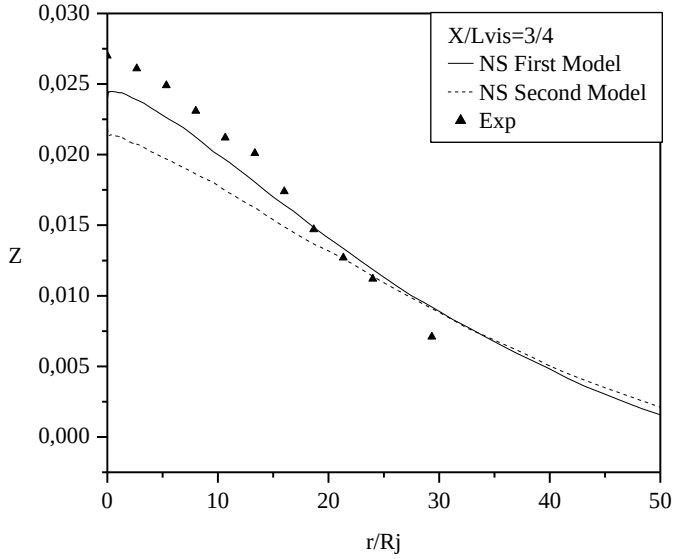

Fig. 4. Radial profile of the predicted and experimental mean mixture fraction at the axial location of x/Lvis =3/4

Figure 5 illustrates the axial profiles of the mean temperature. Both models exhibit the same behavior as observed in the experiment. The disparity between the predicted peak temperature values from the two models and the experimental results is negligible. Furthermore, their axial positions are approximately identical. Consequently, both models effectively predict the experimental data. These findings highlight the accuracy and reliability of the proposed models in capturing the observed outcomes in this study.

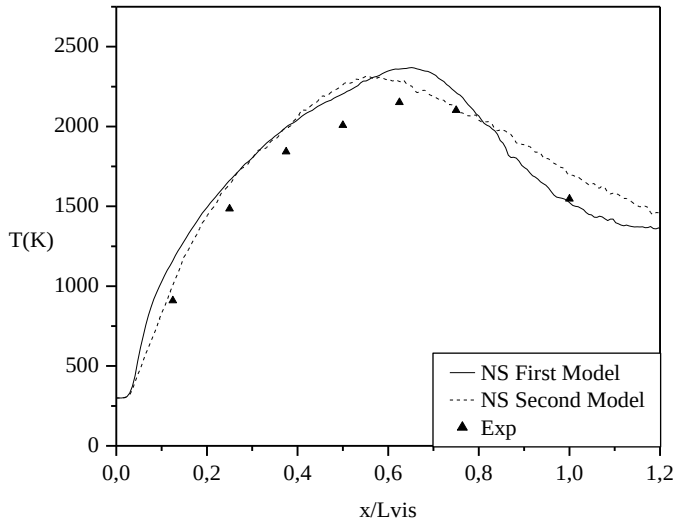

Fig. 5. Axial profile of the predicted and experimental mean temperature along centerline

Figure 6 and Figure 7 respectively present a comparison between the evolution of the radial profiles of the mean temperature and the experimental results. The second model provides a more accurate prediction of the experimental results at the center of the axis compared to the first model. Additionally, the temperature peak value and its radial position closely match those observed in the experiment. At the distant axial stations (x/Lvis=3/4), the results show a high level of precision, particularly for the second model. These findings demonstrate the second model's ability to faithfully

replicate the observed behaviors in this study, encompassing both the radial profile and the accurate prediction of temperature values.

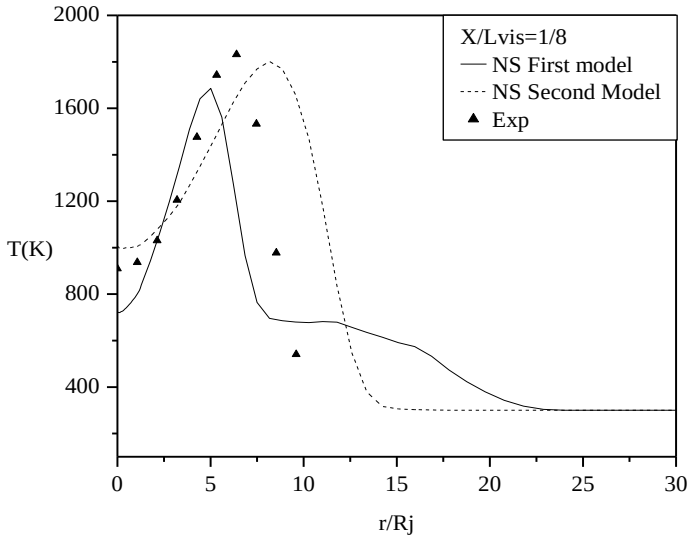

Fig. 6. Radial profile of the predicted and experimental mean temperature at the axial location of x/Lvis = 1/8

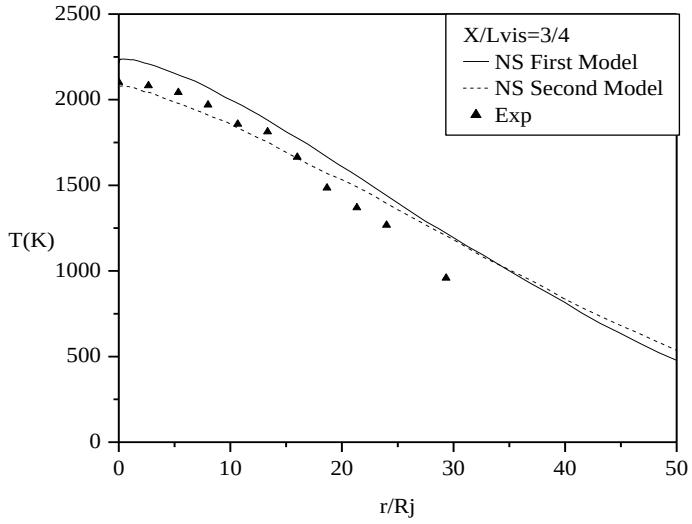

Fig. 7. Radial profile of the predicted and experimental mean temperature at location of x/Lvis = 3/4

Figures 8, 9, and 10 display the predicted axial evolution of the average mass fraction of hydrogen, oxygen, and water, respectively. In general, both models exhibit excellent agreement with the experimental data. However, the models underestimate the experimental values of the average mass fraction of O2 in the regions near the nozzle outlet. This discrepancy between the simulations and experimental results can be attributed to various factors. For instance, upstream conditions significantly influence the regions near the injection point, and the preferential diffusion effect [30-32] characterizes stagnant hydrogen flames. Additionally, non-equilibrium chemical effects [33] and turbulence modeling may also contribute to this observed difference. Despite these limitations, the numerical results from both algebraic models provide a reasonably accurate prediction of the experimental data. These findings underscore the validity and efficacy of the proposed models in capturing the observed behaviors in this study.

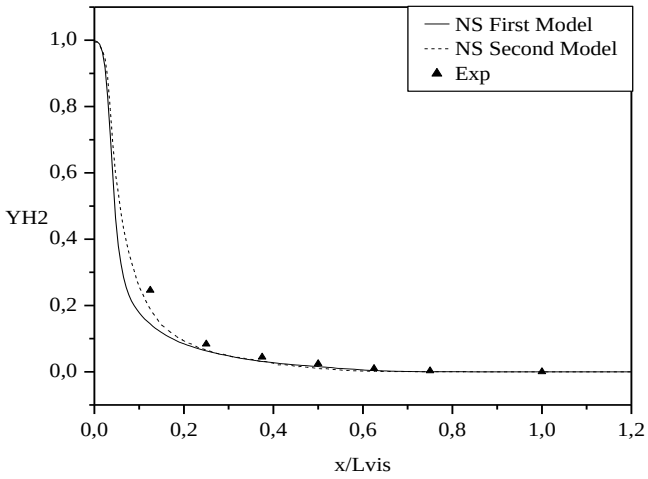

Fig. 8. Axial profile of the predicted and experimental mean mass fraction of H2 along centerline

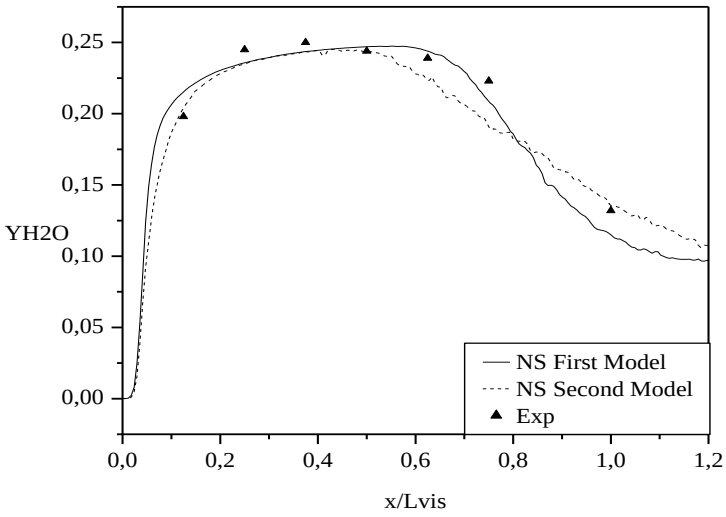

Fig. 9. Axial profile of the predicted and experimental mean mass fraction of H2O along centerline

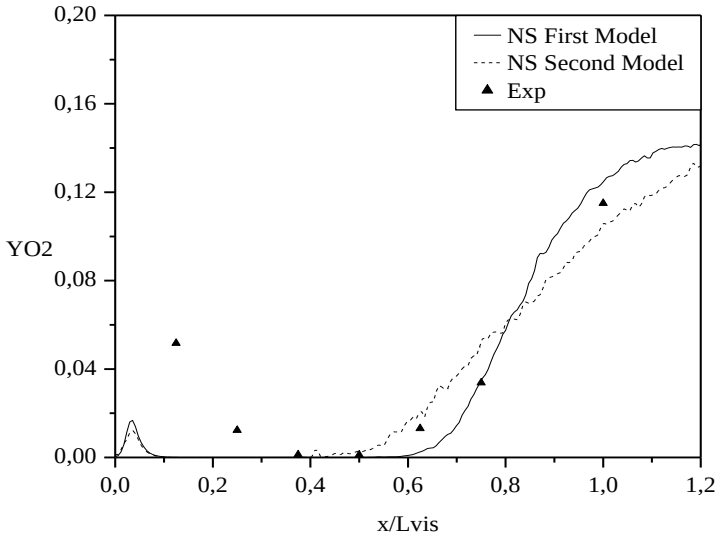

Fig. 10. Axial profile of the predicted and experimental mean mass fraction of O2 along centerline

7. Conclusions

We have investigated a coherent approach utilizing the Lagrangian transported PDF method to analyze a high hydrogen/air flame, with turbulence effects incorporated through RSM models. By employing the Monte Carlo method, we achieved a detailed modeling and solution of the Lagrangian PDF equation, effectively capturing the interaction between chemistry and turbulence. However, the mixing term remains a limitation in this methodology, prompting us to employ the EMST model for its representation in our study. The algebraic functions integrated within the ANSYS-Fluent code play a critical role in determining the mixing constant CΦ. Opting for an algebraic expression to evaluate this constant, rather than solving the scalar time scale transport equations, offers notable computational time and memory savings. The numerical results demonstrate a high level of satisfaction, particularly with the second model. To further enhance the precision of these outcomes, it would be prudent to consider the influence of various parameters, such as preferential diffusion, which characterizes turbulent flames and manifests in proximity to the jet nozzle. Additionally, refining turbulence modeling and gaining a better understanding of upstream jet conditions could significantly impact nozzle exit dynamics and the resulting lift-off height.

Author Contributions

Author 1 planned the scheme, initiated the project and distributes the tasks; Authors 2 and 3 conducted the simulations and analyzed the results obtained; Authors 3 and 4 developed the mathematical modeling and examine the validation of the theory. The manuscript was written thanks to the contribution of all the authors. All authors discussed the results, reviewed and approved the final version of the manuscript.

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