

Towards Sustainable Energy: Numerical Assessment of Hydrogen Combustion in Turbulent Environments

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ABSTRACT

In this study, we focus on the combustion of innovative fuels such as hydrogen, emphasizing its role as a promising alternative in the field of renewable energy. We examine turbulent diffusion flames (H₂/Air) using the second-order turbulence model and the flamelet model (FM), based on the assumed probability density function (PDF) approach as a combustion model. The main objective is to analyze the structure and behavior of these flames while evaluating the performance of models (RSM/PDF) in predicting hydrogen combustion within a turbulent diffusion flame. This approach is part of a broader perspective aimed at exploring the potential of hydrogen as a renewable energy source. The numerical results for dynamic and scalar fields are compared with experimental data from DLR Stuttgart. This comparison reveals a highly satisfactory agreement, with numerical results generally aligning with those from experiments, further reinforcing hydrogen's position as a promising alternative in the landscape of renewable energy.

I. Introduction

Hydrogen is one of the serious candidates to become the energy vector of tomorrow. It has the great advantage of having a total and clean combustion, since its oxidation produces neither CO₂ which generates a greenhouse effect, nor any other harmful polluting gas. Therefore, the study of hydrogen combustion is of great interest. Several different numerical simulation approaches are developed and used to describe turbulent combustion processes, depending on the needs and possibilities of the calculation means. Three main approaches have been proposed for the numerical simulation of turbulent flows[1]. Direct simulation calculations (or direct numerical simulation, DNS) consist of directly calculating all the turbulent scales present in the flow, from the largest to the smallest, without any modeling. Large-scale simulation (or large eddy simulation, LES) [2].consists of explicitly calculating only turbulent structures whose size is greater than a cut-off scale linked, in general, to the

calculation mesh[3].. The simulation of average flows (or RANS, for Reynolds Averaged Navier-Stokes equations) has been the subject of particular attention in the past few decades thanks to its wide scope of application and its reduced computational cost. This approach is based on a resolution of the average values of the physical quantities of turbulent combustion, using closure models for the conservation equations formulated as average values. Different closure models can be used, including the RSM (Reynolds Stress Model). The second order turbulence model (RSM) is considered, compared to other turbulence models, as a more sophisticated approach used for modeling turbulent flows[4].

The overall goal of this work is, on the one hand, to improve our knowledge of hydrogen/air combustion through a detailed study of the structure of a turbulent diffusion flame of diluted hydrogen (H₂/N₂/Air) using the flamelet model, based on the concept of probability density function (PDF), coupled with the RSM turbulence model and on the other hand, to examine the capabilities of such models (RSM/FM) in prediction of the combustion of hydrogen in a jet flame[5]....

II. Setting Average Conservation Equations

The system of equations, for reactive turbulent flow, defined by Favre mean and the boundary layer hypotheses[6]:

$$\text{Continuity equation: } \frac{\partial}{\partial x} (\bar{\rho} \tilde{U}) + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{V}) = 0 \quad (1)$$

Equations for conservation of momentum: axial and radial are:

$$\frac{\partial}{\partial x} (\bar{\rho} \tilde{U} \tilde{U}) + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{U} \tilde{V}) + \frac{\partial \bar{P}}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{u} \tilde{v}) - \text{Dif.Mol.} = 0 \quad (2)$$

$$\frac{\partial}{\partial x} (\bar{\rho} \tilde{U} \tilde{V}) + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{V} \tilde{V}) + \frac{\partial \bar{P}}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{v} \tilde{v}) - \bar{\rho} \frac{\tilde{w} \tilde{w}}{r} - \text{Dif.Mol.} = 0 \quad (3)$$

Dif.Mol is the molecular diffusion term. At large Reynolds numbers[7]. Modeling the Reynolds tension equations:

$$\frac{\partial}{\partial x_k} (\bar{\rho} \tilde{U}_k \tilde{u}_i \tilde{u}_j) = \tilde{P}_{ij} + \tilde{D}_{ij} + \tilde{\phi}_{ij} - \frac{2}{3} \delta_{ij} \bar{\rho} \tilde{\epsilon} \quad (4) \quad \text{This}$$

last equation is solved for: $\tilde{u} \tilde{u}$, $\tilde{v} \tilde{v}$ et $\tilde{u} \tilde{v}$. Tangential fluctuations $\tilde{w} \tilde{w}$ are assumed equal to the radial [8].

$$\text{Production terms } \tilde{P}_{ij} = -\bar{\rho} \left(\tilde{u}_i \tilde{u}_k \frac{\partial \tilde{U}_j}{\partial x_k} + \tilde{u}_j \tilde{u}_k \frac{\partial \tilde{U}_i}{\partial x_k} \right) \quad (5)$$

They play an important role in creating turbulent stress mechanisms.

$$\text{Diffusion Term: } \tilde{D}_{ij} = C_S \frac{\partial}{\partial x_k} \left[\left(\bar{\rho} \frac{\tilde{k}}{\tilde{\epsilon}} \tilde{u}_k \tilde{u}_i + \bar{\rho} \nu \delta_{kl} \right) \frac{\partial}{\partial x_l} (\tilde{u}_i \tilde{u}_j) \right] \quad (6)$$

Pressure-strain correlation term its modeling is based on the Poisson equation relating to fluctuating pressure.

$$\tilde{\phi}_{ij} = \bar{p}'' \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) = \tilde{\phi}_{ij}^{(1)} + \tilde{\phi}_{ij}^{(2)} \quad (7)$$

The first term, called the Rotta term [3], was first modeled by this:

$$\tilde{\phi}_{ij}^{(1)} = -C_1 \bar{\rho} \tilde{\varepsilon} \left(\frac{\tilde{u}_i \tilde{u}_j}{\tilde{k}} - \frac{2}{3} \delta_{ij} \right) = -C_1 \bar{\rho} \tilde{\varepsilon} a_{ij} \quad (8)$$

The second term concerning the interaction between the mean motion and the turbulence[9]:

$$\tilde{\phi}_{ij}^{(2)} = -C_2 \left(\tilde{P}_{ij} - \frac{2}{3} \delta_{ij} \tilde{P}_k \right) \quad (9)$$

$\tilde{P}_k = \frac{1}{2} \tilde{P}_{kk} = -\bar{\rho} \tilde{u}_i \tilde{u}_k \frac{\partial \tilde{U}_i}{\partial x_k}$ is the average rate of production of turbulent kinetic energy.

The adjustment of the pair of constants (C1,C2) is based on certain research experiments [10] Table 1:

Table 1: Second-order turbulence model (RSM) constants.

Table 1					
C ₁	C ₂	C _s	C _{ε,1}	C _{ε,2}	C _ε
2.3	0.6	0.22	1.45	1.90	0.18

III. Modeling of Non-Premixed Combustion

III.1.Flamelet model

The principle of the flamelet model is to separate the problem of mixing from that of the structure of the flame.

Average mixing fraction and its variance

Obtained from both fields: the average mixing fraction, $\tilde{z}$, and its variance, $\tilde{z}''^2$.

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{z}) + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{z}) = \frac{\partial}{\partial x_i} (\bar{\rho} D_t \frac{\partial \tilde{z}}{\partial x_i}) \quad (14)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{z}''^2) + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{z}''^2) = \frac{\partial}{\partial x_i} (\bar{\rho} D_{t1} \frac{\partial \tilde{z}''^2}{\partial x_i}) + \bar{\rho} D_{t2} \frac{\partial \tilde{z}}{\partial x_i} \frac{\partial \tilde{z}}{\partial x_i} - c \bar{\rho} \frac{\varepsilon}{k} \tilde{z}''^2 \quad (15)$$

III.2. Flamelet equations

Under certain simplifying assumptions, the flamelet equations are written:

$$\rho \frac{\partial Y_k}{\partial t} = \frac{\rho \chi}{2Le_k} \frac{\partial^2 Y_k}{\partial z^2} \quad (16)$$

$$\rho \frac{\partial T}{\partial t} = \frac{\rho \chi}{2} \frac{\partial^2 T}{\partial z^2} \quad (17)$$

The solutions for average sizes are written:

$$\tilde{Y}_k = \int_0^{+\infty} \int_0^1 Y_k(z, \chi) P(z, \chi) dz d\chi \quad (18)$$

$$\tilde{T} = \int_0^{+\infty} \int_0^1 T(z, \chi) P(z, \chi) dz d\chi \quad (19)$$

Their calculations require knowledge of the probability density function $P(z, \chi)$. [5]. We can therefore write the relation:

$$P(z, \chi) = P(z) \cdot P(\chi) \quad (20)$$

$P(z)$ is determined using the assumed PDF. In this method, the functional form of the probability density function

IV. Simulation and Discussions

IV.1 Configuration studied

We have adapted our calculation code to a less complex configuration and the most widely used in studies, whether theoretical or experimental, this configuration is the one shown in Figure 1.

The combustion is carried out with a mixture within a jet of diluted hydrogen (75% H₂ and 25% N₂) coming from an injector located between two parallel air flows with a velocity $U_j = 42.3$ m/s. The ejection Reynolds number $Re_j = 10500$, which corresponds to fully turbulent flow. The secondary jet of air, the co-current, has a speed $U_{air} = 0.3$ m/s

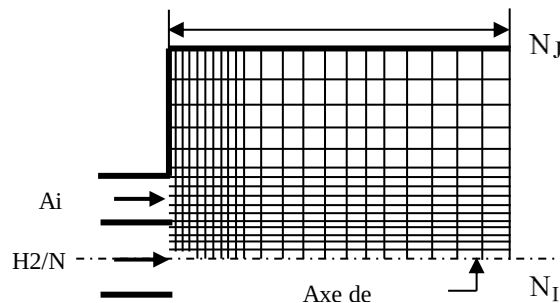


Fig 1: Configuration of confined axisymmetric je

IV.2 Results and discussion

We will now present and discuss the results obtained by the model used in this study (RSM/FM), in comparison with those from the DLR Stuttgart experiments [1][2]

Velocity field

Figure 2 shows the axial profiles obtained for the average longitudinal velocity. The numerical results are, in general, in good agreement, compared to those of the experiment [1], more particularly in the regions with a long axial distance from the ejection nozzle.

The radial profiles of the average longitudinal velocity, for the two cross sections, $x/D_j = 5$ and 20 , are represented in Figure 3. Compared to the experimental results, the radial evolution of the velocity longitudinal average of the reactive jet is slightly overestimated by the simulation results (RSM/FM) in the cross sections very close to the ejection nozzle, $x/D_j = 5$. For cross sections relatively far from the ejection nozzle, $x/D_j = 20$, the model (RSM/FM) underestimates the experimental results in the region with very small radial distance from the jet axis, $x/D_j \leq 1$, and overestimate them in the relatively small radial distance region, between 2 and $3 r/D_j$ [5]. This overestimation is, as can be seen, less significant compared to the underestimation in the region with low radial distance. This effect may be due to upstream conditions which greatly influence the initial area of the jet and/or to the significant density gradient. The region near $x/D_j = 20$ is characterized by significant turbulence.

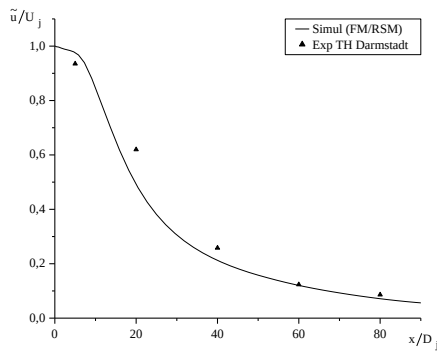


Fig 2: Axial evolution of the average velocity.

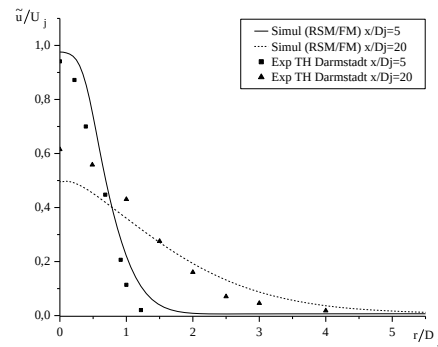


Fig 3: Radial evolution of the average velocity.

Average mixing fraction

The axial evolution of the average mixing fraction is shown in Figure 4. The results obtained by the simulation (RSM/FM) are in very good agreement with those of the experiment [1].

The radial evolution of the average mixing fraction is represented, for the two cross sections $x/D_j = 5$ and 20 , in Figure 5. Compared to the experimental results [1] [3], the model (RSM/FM) underestimates slightly the maximum value reached by the experiment on the jet axis and overestimates the results in the radial distance regions relatively far from the jet axis, between $2 \times (r/D_j)$ and $4 \times (r/D_j)$. By getting closer and closer to the axis of the jet, we can notice that the model (RSM/FM) and the experimental results are in good agreement and more particularly in the regions with short radial distances [4].

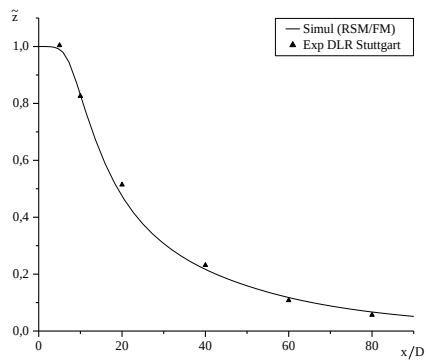


Fig4: Axial evolution of the mixing fraction.

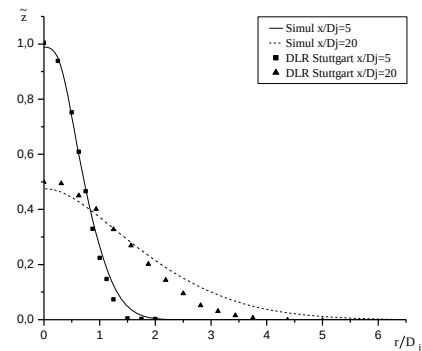


Fig 5: Radial evolution of the mixing fraction.

Evolution of the average temperature

The axial evolution of the average temperature is shown in Figure 6. This evolution presents the same behavior as that of the experiment. The maximum value reached, for the reactive jets of diluted hydrogen, is almost the same in amplitude and axial position. The simulation results are very close to those of the experiment [1], particularly in the initial zone of the jet. The effect of differential diffusion in such flames is particularly important, as indicated by [3], near the ejection nozzle.

Figure 7 shows the radial evolution of the average temperature. Compared to the experimental results [1][2], the maximum values are reached at the same axial position as that of the experiment with a significant difference in amplitude for the cross sections very close to the ejection nozzle ($x/D_j \approx 5$). This discrepancy, as mentioned previously, is probably due to the differential diffusion effect which becomes important near the ejection nozzle. Non-equilibrium chemistry can also play an important role in this region.

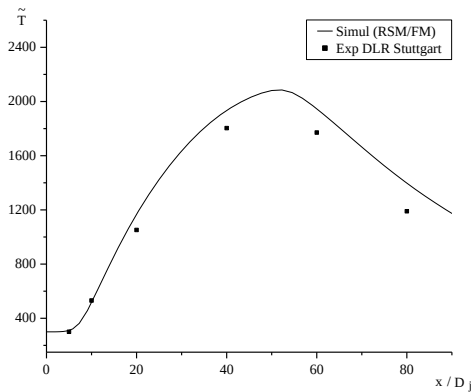


Fig 6: Axial evolution of temperature.

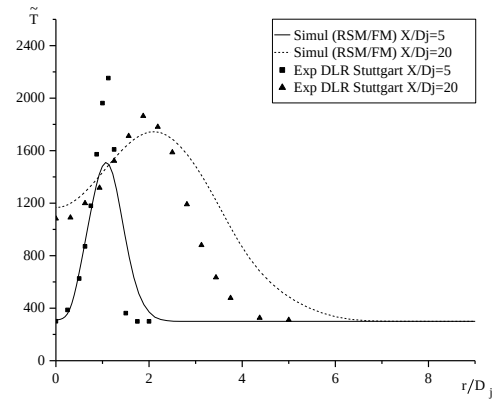
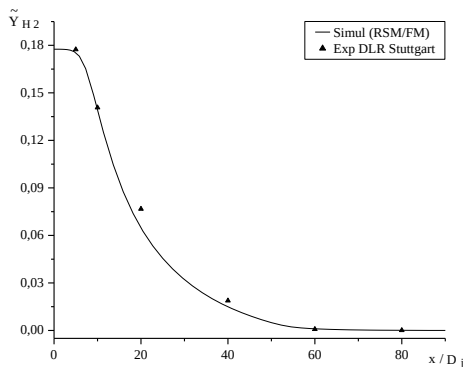
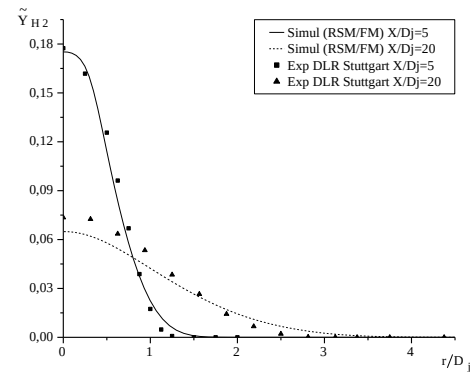


Fig 7: Radial evolution of temperature.

Average mass fraction of hydrogen

The axial evolution of the average mass fraction of hydrogen, Figure 8, shows a very good agreement between the simulation results (RSM/FM) and those of the experiment [1].

The radial evolution of the average mass fraction of hydrogen, for the two cross sections, is shown in Figure 9. It can be observed that the model (FM/RSM) slightly underestimates the experimental results on the axis of the jet (the maximum) and the regions very close to this axis, ($r/D_j \leq 1$), and this in the cross sections relatively far from the ejection nozzle ($x/D_j \approx 20$). For cross sections very close to the ejection nozzle, the results are in very good agreement with those of the experiment.


Fig 8: Axial evolution of the mass fraction of H₂

Fig 9: Radial evolution of the mass fraction of H₂

Average mass fraction of water

Figure 10 shows the axial evolution of the average mass fraction of H₂O. The simulation results are in very good agreement with those of the experiment [1].

In Figure 11, we can notice a behavior similar to that of the average temperature, of the radial evolution of the average mass fraction of water. The maximums are also reached on the co-current side (air), close to the flame wall ($1 \leq r/D_j \leq 1.6$). The effect of differential diffusion, which is very important near the ejection nozzle, can be the cause of the relatively large difference between the maximum values reached at the same radial position by simulation and experiment, for the distances axial very close to the axis of the jet. non-equilibrium chemistry and upstream conditions, which have a significant influence in this region, can also favor this gap.

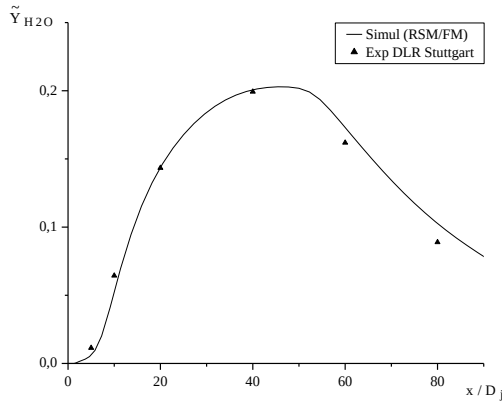
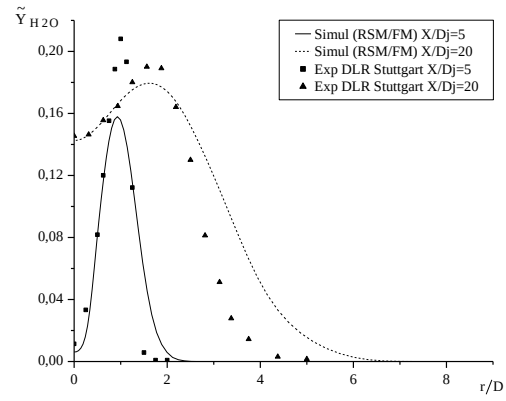
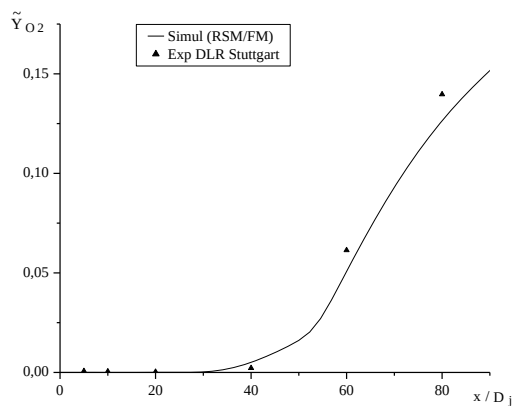
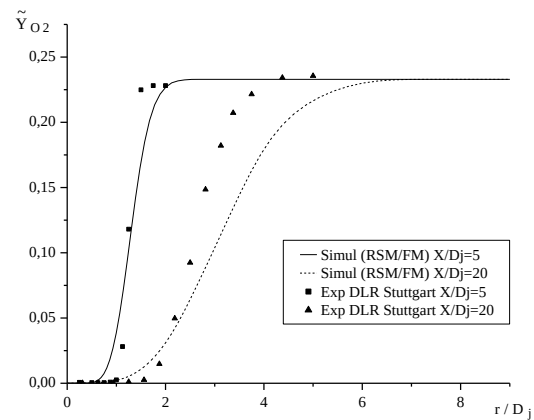

Fig10: Axial evolution of the mass fraction of H₂O.


Fig 11: Radial evolution of the mass fraction of water.

5.6. Fraction massiquemoyenne de l'oxygène

In Figure 12, which represents the axial evolution of the average mass fraction of oxygen, we notice a very good agreement between the simulation results and those of the experiment [1].

The radial evolution of the average mass fraction of oxygen is shown in Figure 13. The experimental measurements show the same behavior for cross sections very close to the ejection bus with a slight underestimation of the simulation. This underestimation becomes relatively important between $2.5 \leq r/D_j \leq 5$ for cross sections relatively far from the ejection nozzle. This discrepancy can be attributed to the effect of differential diffusion or non-equilibrium chemistry that is present in these regions.


Fig 12: Axial evolution of the mass fraction of O₂ .

Fig 13: Radial evolution of the mass fraction of O₂

Conclusion

This innovative study on reactive turbulent jets relies on the use of the second-order model (RSM) for turbulence and the flamelet model for combustion, with a specific focus on diluted hydrogen (75% H₂ and 25% N₂). The results, validated by experimental measurements from [1] and [2], reveal significant convergences and divergences. The evolution of velocity and mixture fraction, in accordance with the RSM model, aligns well with experimental observations. However, disparities emerge near the ejection nozzle, involving effects of differential diffusion and non-equilibrium chemistry.

Despite observed discrepancies near $x/D_j=20$, attributed to turbulence, the results (RSM/FM) generally converge with experiments in Stuttgart [1] and Darmstadt [2]. These divergences are primarily attributed to the inherent

differential diffusion in hydrogen flames. It is crucial to emphasize that hydrogen, as a renewable energy source, presents promising prospects. Its unique properties and potential as a clean fuel make it a strategic alternative in the renewable energy landscape. Nevertheless, nuances related to non-equilibrium chemistry and turbulence modeling must be considered. This study highlights the crucial role of hydrogen in the renewable energy landscape, justifying the need for further research to maximize its potential in the energy transition.

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