Simulation of opposed-jets configuration H₂/air, CH₄/air

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ABSTRACT The opposed-jets configuration is very used in industrial systems. The actual practical applications use clean fuels which in stead of classical hydrocarbons. The present work is a numerical simulation of opposed diffusion jets using FLUENT6.3.26. We have compared different turbulence models and combustion models and mechanisms to find which gives the best predictions for this type of flows. We have used methane and hydrogen fuels because they are considered as clean fuels. The comparison between k- ϵ , k- ω and RSM turbulent models shows that both of k- ϵ and RSM gives good results. The use of k- ϵ is more practical because it requires less long time to be implied. The comparison between the combustion models shows that EDC gives more realistic results than eddy dissipation and Finite rate models. In addition, the detailed chemical mechanisms are more adequate to this model. For both methane and hydrogen flames, the detailed mechanisms gives good results and temperatures.

1. INTRODUCTION

Turbulent combustion experienced in winning power and reliability, an important development in recent decades. Thus it occupies today a privileged place for the production of energy in the air, space, road transport, in electricity production. These two points are still valid, however, entirely for the development of future jet configurations. To these are added in recent years a reduction target of pollutants such as nitrogen oxides NO_x that destroy day to day ozone and CO₂ carbon dioxide that contributes to global warming. Progress towards these objectives requires better understanding of the physical and chemical phenomena at play during combustion. Knowing that the combustion in the industrial sector is closely linked to the turbulent nature of flows, it will study the interaction between the different physical phenomena. This coupling between the combustion and turbulence is studied since the last century and today gives many research subjects on the experimental aspects. The development, development models and computational techniques and computer power, show that the numerical calculation of turbulent combustion is playing an increasingly crucial in the optimization of energy processes. The numerical simulation of complex industrial configurations can be done today in modeling the physical phenomena involved.

The overall goal of this study was firstly, to improve our knowledge through a comprehensive study on the interaction between methane-air diffusion flame, hydrogen-air and turbulence and secondly, to define the different distributions where does this flame. This is performed on opposed jet injectors, which is the configuration of the injectors currently used in the combustion chamber of the gas turbine, the internal combustion engines, diesel engines, burners systems etc.

2. EQUATIONS GOVERNING THE ISSUE OF REACTIVE TURBULENT FLOWS

The description of flow and mixing between fuel and oxidizer field opposite jets was established by the conservation equations below

Equation of continuity or conservation of mass

$$\partial (\rho u_i) / \partial x_i = 0 \quad (1)$$

Equation of the conservation of momentum

$$\partial (\rho u_i u_j) / \partial x_i + \partial p / \partial x_j = \partial \tau_{ij} / \partial x_i + F_i \quad (2)$$

$$\partial \rho u_i Y_k / \partial x_j + \partial D_j^k / \partial x_j = \omega_k \quad (3)$$

Equation de conservation de la température

$$\partial \rho u_j T_t / \partial x_i + \partial (\rho u_j T''') + \rho \omega T \quad (4)$$

3. DEFINING THE PROBLEM

FIGURE 1 : DISPOSITIF DE JETS OPPOSÉS.

TABLE 1: TURBULENCE MODEL USED AND BURNING.

Modèles de turbulence	Modèles de combustion
k-epsilon	Finite-rate/Eddy Dissipation
k-omega	Eddy Dissipation
RSM	EDC

3-1. Maillage

FIGURE 2 : DOMAINE DE CALCUL MAILLÉ (VUE DE FACE)

TABLE 2: NUMBER OF KNOTS AND CELLS QUADRATIC

Nœuds	Nombre de cellules quadratiques
9061	8800

The first part of our work consists in varying turbulence models for simulating opposed jet methane / air to determine which model provides the best predictions. We compared the results we have obtained with experimental results conducted by Rolf Hoffmann [1].

FIGURE 3 : VITESSE AXIALE DU MODÈLE K- ϵ , K- ω , RSM ET DE L'EXPÉRIENCE DE ROLF HOFMANN [1].

FIGURE 4 : ENERGIE CINÉTIQUE DU MODÈLE K- ϵ , K- ω , RSM ET DE L'EXPÉRIENCE DE ROLF HOFMANN [1].

Figs 3, 4 and 5 show the evolution of the axial velocity, kinetic energy and mass fraction. For the evolution of the axial velocity: we can see that the results are very close to each other and the k- ϵ model is the closest experimental values.

For the evolution of the kinetic energy: We see that the paces are pretty much the same with a larger or smaller peak in the stagnation plan. The turbulence reaches its maximum at the impact of the two jets. These peaks correspond to a large increase in the turbulence associated with the jet entry velocity and the chemical reaction.

For the evolution of the mass fraction: the impact of turbulence models on combustion was drawn by the curves of the mass fraction of CH₄ (Fig 5). The general appearance is the same for all three models. The comparison with the experiment shown, however, shows that the k- ϵ model is the most realistic.

So we can learn from past results that the k- ϵ and RSM models give the best predictions for the dynamic field. The k- ϵ model is however the most accurate. Moreover, this model is the most used because it requires a calculation time smaller than that of RSM.

FIGURE 5: MASS FRACTION OF CH₄ MODEL K- ϵ , K- ω , RSM AND ROLFHOFFMANN [1]

4. STUDY OF COMBUSTION MODELS AND FLAME STRUCTURE

The k- ϵ model having proved most suitable for turbulence, we conducted several case simulation using this model and varying combustion models. The models for diffusion flames are: eddy dissipation, EDC and Finite spleen. The results are shown in the following.

FIGURE 6 : DISTRIBUTION DE LA TEMPÉRATURE TOTALE K- ϵ FIGURE 7 : DISTRIBUTION DE LA TEMPÉRATURE TOTALE K- ϵ
EDDY-DISSIPATION. FIGURE 8 : DISTRIBUTION DE LA TEMPÉRATURE TOTALE K- ϵ
FINITE-RATE.

FIGURE 9 : FRACTION MASSIQUE DU CH₄ DU MODÈLE EDC ,EDDY-DISSIPATION, FINITE-RATE/EDDY-DISSIPATION ET DE L'EXPÉRIENCE DE ROLF HOFFMANN[1]

Figs 6, 7 and 8 show the temperature distribution for the three combustion patterns. We can see the flame represented in the computational domain. The EDC model is more realistic because it provides the flame in the stagnation plan reflecting reality. Fig 9 which compares the results of three models with the experience shows that the EDC model is the most effective. This model takes into account the chemical reaction.

We retain the previous study that the EDC model provides the best predictions for this type of flame.

5. COMPARISON OF THE MECHANISMS

We were interested in that part of the flame chemistry by varying the chemical mechanisms. The calculations were made with the turbulence and combustion models that are previously selected the k- ϵ model and EDC. We did the simulation using a simple one-step process and the detailed mechanism reduced25.

FIGURE 10 : DISTRIBUTION DE LA TEMPÉRATURE TOTALE
AVEC UN MÉCANISME À UNE SEULE ÉTAPE.

FIGURE 11 : DISTRIBUTION DE LA TEMPÉRATURE
TOTALE AVEC UN MÉCANISME DÉTAILLÉ.

FIGURE 12: MASS FRACTION OF CH₄ MECHANISM WITH ONE STEP WITH DETAILED MECHANISM AND EXPERIENCE OF HOFFMANN ROLF [1]

Figs 10 and 11 show the temperature distribution in the computational domain. The detailed mechanism gives more realistic temperatures. In fact, methane flames produce intermediate chemical species such as CO, NO ... these species are ignored when the mechanism is one step which increases the resulting temperatures.

The mass fractions of methane (Fig 12) show that the methane exists in both mechanisms. The flame area predicted by the detailed mechanism is more realistic. We can therefore hold that the use of a detailed mechanism is important for some flame parameters such as temperature and pollutants. It better represents reality.

We conducted the simulation of a hydrogen / air flame in opposed jet. Following the previous results in which we retained the turbulence models and combustion k- ϵ and EDC, we decided to make a further application on the flames by testing two mechanisms: a single and the other detailed hydrogen37.

FIGURE 13: SPEED AXIAL MECHANISM WITH ONE STEP WITH DETAILED MECHANISM AND EXPERIENCE OF JOHANNES Eckstein [12].

FIGURE 14: MASS FRACTION OF H2 MECHANISM WITH ONE STEP WITH DETAILED MECHANISM AND EXPERIENCE OF JOHANNES Eckstein [12].

FIGURE 15: DISTRIBUTION OF TEMPERATURE WITH THE MECHANISM SINGLE STEP.

FIGURE 16: DISTRIBUTION OF TEMPERATURE WITH THE MECHANISM DETAILED.

FIG 13 shows the profiles of the axial speed. The trends are the same at a speed which cancels the torch stagnation plan. The comparison with experiment shows that the mechanisms predict

fairly well with the tendency to overestimate the detailed mechanism and underestimation for the simple mechanism.

FIG 14 shows the mass fractions of hydrogen and their comparison with experiment. We note as for methane that trends are the same with a slight difference with experience. However, the values are acceptable and the detailed mechanism illustrates the flame zone in which hydrogen is consumed quickly.

The temperature distributions are shown in Fig 15, 16. We note that the flame predicted by the detailed mechanism corresponds better to the reality as it is in the stagnation plane between the two jets. This zone corresponds to meet the fuel and oxidant. On the other hand, the temperature data by the detailed mechanism reflect intermediate species are formed and thus approach more reality.

We can remember that the detailed mechanism provides more realistic results because it takes into account most importantly species that actually form during combustion and can therefore give better results concerning the formation of pollutants.

6. CONCLUSION

The numerical simulation we have performed by the FLUENT software has covered some very important aspects

- The turbulence model k-omega has little effect while the RSM model gives good predictions.

- The k- ϵ model is very effective and easy to implement despite its simplicity. It can therefore be accepted for opposite-jets.

- Combustion Models Eddy dissipation and give finite rate rather good predictions but they are poorly adapted to the detailed mechanisms.

- The EDC model is closest to the experimental results. This is a very malleable model that meets all the mechanisms.

- The use of a detailed mechanism reveals important if one wants to predict the emissions of pollutants and temperature distribution. The dynamic range is not influenced by this type of mechanism unlike the scalar field.

The work we have done is a very important step in simulating opposed jet: it is a database for future work in this area.

References

- [1] Rolf Hoffmann., 1999. A numerical study of turbulent jet flow, Technische Universitat Darmstadt, p. 73
- [2] R. P. LINSTEDT, D. S. LUFF, J. H. WHITELOW, Proc. Combust. Inst., 31, 1459-1466, 2007.
- [3] E. MASTORAKOS, A. M. K. P. TAYLOR, J. H. WHITELOW, Combust. Flame 91, 40-52, 1992.
- [4] L. W. KOSTIUK, K. N. C. BRAY, R. K. CHENG, Combustion and flames, 92 (1993), 396-409.
- [5] L. W. KOSTIUK, K. N. C. BRAY, T. C. CHEW, Combustion Science and technology, 64(1989), 233-241.
- [6] Williams F.A., (1985) "Combustion theory", Benjamin/Cummings, 2nd edition.
- [7] Moss J. B., Bray K. N. C., (1977), "a unified statistical model of the premixed turbulent flames, Acta Astronautica, 4: 291-319

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- [8] Bray K. N. C., "Turbulence flows with premixed reacting", dans turbulent reacting Flows, p. 115-183. Libby P. A. et Williams S. A.. (1980), "topics in applied physics", Springer-verlage, Heidelberg Vol.44
- [9] Wilcox., (1998), $k-\omega$ turbulence model to a jet co-flow, second international conference in CFD in the minerals and process industries, CSIRO, Melbourne, Australia, 6-8 December, p. 479-484
- [10] Spalding D.B., (1971), "Mixing and chemical reaction in steady confined turbulent flames", 13th Symp. (Int.) on Combust., 649-657, The Combustion Institute, Pittsburgh
- [11] Launder, B. E. and Spalding, D. B. 1972, Lectures in mathematical models of turbulence. Academic press, London
- [12] Johannes Eckstein., 1999. A one dimensional joint scalar pdf modeling of turbulent opposed jet flames, University of California at Berkeley, p. 99
- [13] Boussinesq J., (1877), "Essai sur la théorie des eaux courantes", Mémoire, Académie des Sciences, Paris, 23 (1) : 252-260
- [14] G.MONNOT.1978, La combustion dans les fours et les chaudières.292 PAGES
- [15] Andrea Ciani., 2006, Hydrogen and Methane Edge and Diffusion Flames in Opposed Jet Configurations: Structure and Stability, Ancona University, Italy, p 126
- [16] D.Geyer, A.Kempf, A.Dreizler, J.Janicka., 2005, Turbulent opposed-jet flames: A critical benchmark experiment for combustion LES, Germany; Department of Mechanical Engineering, Imperial College London, SW7 2AZ London, UK