

Comparisons of LPDF and MEPDF for lifted H_2/N_2 jet flame in a vitiated coflow

Ahmed A. Larbi^{1,2*}, Abdelhamid Bounif³, Mohamed Bouzit¹

¹ Faculté de Génie Mécanique, Université des Sciences et de la Technologie Mohamed Boudiaf d'Oran, BP. 1505 Oran El M'naouar, 31000 Oran, Algeria

² Unité de Recherche en Energies renouvelables en Milieu Saharien, URERMS, Centre de Développement des Energies Renouvelables, CDER 01000, Adrar, Alegria

³ Institut des Sciences et de la Technologie, Centre Universitaire Ahemd Zabana -Relizane, Bourmadia, BP 48000, Relizane, Algeria

Corresponding Author Email: amine.larbi@univ-usto.dz

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ABSTRACT

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Transported probability density function (PDF) approach have been applied broadly and effectively for modelling turbulent reacting flows. The discretization of this approach is done with two methods, Multi-Environment Eulerian (MEPDF) and Lagrangian Monte-Carlo (LPDF) which each method has advantages and disadvantages. The aim of this work is to investigate the capabilities of each method in predicting hydrogen combustion in a turbulent flame. A comparative study has been adopted between the two methods by equivalent physical models and numerical parameters. The study was applied in the diffusion turbulent flame of hydrogen into a vitiated of hot coflow with modified K-epsilon model of turbulence. The chosen mixture model is the IEM (Interaction by Exchange with the Mean) with mixing constant (2.1). The number of environment in the first approach is (2.0). The model was solved in this work by the commercial CFD code, ANSYS fluent and the chemical reaction mechanism injected is GRI mech 2.1. The numerical results for temperature and species mass fractions are presented and compared with the experimental data. The comparison shows that the eulerian method gives better predictions than the lagrangian method. The advantages and disadvantages of both models are discussed in detail in relationship to the results.

1. INTRODUCTION

The study of reactive turbulent flows is governed by the characteristic equations resulting from fluid mechanics, thermodynamics and chemistry. In this investigation, we apply the hybrid method RANS-PDFT to solve these equations. After reynolds averaging (RANS) of the species equations, two unknown terms result that require closure. The first term is the turbulent scalar fluid which is modeled by the diffusion gradient. The second one is called the average reaction rate, one of the main sources of errors in the modeling of reactive turbulent flows since it is invariably very non-linear. Several models proposed as EDC and LFR to solve this problem. Due to the exact transformation and the closing of the rate of chemical reaction in the equation without the need for closure approximation; the PDF transported model (probability density function) [1] is the only model capable of accurately solving the problem of modeling the chemical source term. The focus of latter method takes precisely into account the chemistry and applicable to all combustion regimes. In particular, all terms defined at every point, such as the average chemical reaction rate. Pope [1] and fox [2] determine the modeling of this approach in a reactive turbulent flow. Haworth [3] discussed the progress and the advancement of this method in turbulent regime.

The literature on hybrid method RANS-PDFT shows two methods to solve the equation of PDFT, lagrangian monte-carlo method (LPDF) and multi-environment eulerian method (MEPDF).

For several years a great effort has been devoted to the study of lagrangian monte carlo method [4–11]. Cao et al [12] used the numerical analysis of lagrangian PDF for different flames and showed the influence of various mechanisms to represent the local extinction, reignition. Gordon et al. [13] studied the auto-ignition of methane flame to understand the mechanism and showed the dominant species that controlled auto-ignition. Several authors [14–16] have used this method by applying different mixing models (MC, EMI and EMST) to study the effect of the model and to make a comparative analysis.

The second one to solve this issue is the eulerian PDF method, some researchers has studied and proposed various ideas in the literature to explain the presumed shape multi-environment eulerian method (MEPDF) in turbulent reaction flow [17–22]. Tang et al studied the numerical investigation with direct quadrature method of moments (DQMOM) for tested the finite-rate chemistry by modeling a series of bluff-body stabilized flames and showed that the MEPDF model accurately take the trends exhibited among these flames [18]. Important study of sensitivity have been presented by Akroyd et al. [19] for new aspect of the method and discuss the

problems of boundedness and singularity by introduce a new DQMoM-IEM source terms.

The theory of eulerian method (MEPDF) has been improved in recent years. However, several practical questions arise when dealing the ability of prediction compared with lagrangian monte carlo method (LPDF): 1) It is important to identify turbulent flame than LPDF. 2) It is crucial to predict the local extinction, reignition and lift-off height than LPDF. 3) It is a key to predict NOX. To answer all these questions, we present an original study which compares the capabilities of each method in predicting hydrogen combustion in a turbulent flame. Mobus et al.[23]used a flame of hydrogen for a comparative study between lagrangian and eulerian methods, insufficiently results due to the use of chemical mechanism of seven elements. In our study, we used a chemical mechanism of GRI mech 2.1 which helps us to predict precisely the phenomenon of extinction, reignition and lift-off height.

2 THEORETICAL FORMULATION OF PDF TRANSPORT APPROACH

The transport equation for a single point multi dimensional joint composition PDF in a reacting turbulent flow can be written as [1] :

$$\frac{\partial}{\partial t}(\rho p) + \frac{\partial}{\partial x_i}(\rho u_i p) + \frac{\partial}{\partial \psi_k}(\rho S_k p) = \frac{\partial}{\partial x_i}[\rho \langle u_i'' | \psi \rangle p] + \frac{\partial}{\partial \psi_k} \left[\rho \left\langle \frac{1}{\rho} \frac{\rho j_{i,k}}{\partial x_i} | \psi \right\rangle p \right] \quad (1)$$

Table 1. the main advantages and disadvantages between LPDF and MEPDF

	Advantages
LPDF	-Term chemical source is closed. -accurate transformation of the chemical source -Used successfully. -With good mechanism, good control of CO, NOX, extinction and ignition. -The molecular mixture is modeled by three models (IEM, EMST, MC) -In ANSYS FLUENT 15.0, a mechanism can be used that exceeds 50 species
	Disadvantages
	-Expensive in terms of calculation. -Requires a large number of particles to represent the PDF. - A large number of iteration to reduce statistical error.
	Advantages
MEPDF	-Term chemical source is closed. -accurate transformation of the chemical source. -Used successfully. -With good mechanism, good control of CO, NOX, extinction and ignition. -economical in terms of computationally. -Stochastic errors are eliminated.
	Disadvantages
	-The molecular mixture is modeled by the IEM model. -In ANSYS FLUENT 15.0, the number of species does not exceed 50 species.

There isn't any problems of closing in Equation (1) of left hand, this is the advantage and principal strength of the PDFT equation that the reaction term has closed[24] and require no modeling .The first term of the equation in right hand represents the turbulent scalar flux modeled by the gradient –diffusion.

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

Two methods of discretization for close the second term of right hand in PDF transport equation, lagrangian monte-carlo method (LPDF) and multi-environment eulerian (MEPDF) method. Table 1 shows the main advantages and disadvantages of the two methods of discretization of the PDF transport.

2.1 The lagrangian monte-carlo method

LPDF is the union between the methods of probability density function and the stochastic model of lagrange[24]. The particles in physical space and composition are monitored by the lagrangian method, monte carlo model is the stochastic model applied for the evolution of the properties following the particle as shown in Figure 1. Pope has defined that the particles from one moment to another evolve according to the equations of the stochastic model and that the theoretical particles contains the same information as the particles of the fluid, but at a fixed time does not contain any multiple of information. We can have the same position for two particle but with different velocity and compositions.

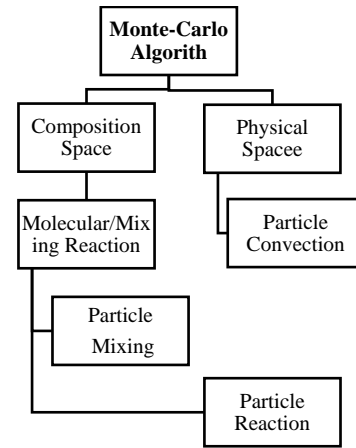


Figure 1. Monte-Carlo method

There is three methods for the treatment of particles, the first for the treatment of particle convection, the second for particle mixing and the last for particle reaction. The particle convection is solved by two steps, the first represented in equation (3) and the second in equation (5).

$$x_i^{1/2} = x_i^0 + \frac{1}{2} u_i^0 \Delta t \quad (3)$$

For steady-state flows, locale time are calculated as :

$$\Delta t = \min(\Delta t_{conv}, \Delta t_{diff}, \Delta t_{mix}) \quad (4)$$

$$x_i^1 = x_i^{1/2} + \Delta t \left(u_i^{\frac{1}{2}} - \frac{1}{2} u_i^0 + \frac{1}{\rho Sc_t} \frac{\partial \mu_{eff}}{\partial x_i} + \xi_i \sqrt{\frac{2\mu_{eff}}{\rho \Delta t Sc_t}} \right) \quad (5)$$

Particle mixing is modeled by IEM model (Interaction by Exchange with the Mean) in eq. (6) and the term chemical source integrated in eq. (7) for the last method of Particle reaction.

$$\phi^1 = \phi^0 - \left(1 - e^{-\frac{0.5c\phi}{\tau t}}\right) (\phi^0 - \tilde{\phi}) \quad (6)$$

$$\phi^1 = \phi^0 + \int_0^{\Delta t} S dt \quad (7)$$

2.2 The multi environment eulerian PDF transports (MEPDF) method

MEPDF has been defined in an associated probability between the composition space and the physical space. The composition space is defined by a smaller number of interactive environments by the coexisting in physical space[20].

$$p(\psi; \bar{x}, t) = \sum_{n=1}^{N_e} p_n(\bar{x}, t) \prod_{k=1}^{N_s} \delta[\psi_k - \langle \phi_k \rangle_n(\bar{x}, t)] \quad (8)$$

Since micro-mixing is modeled by IEM, the turbulent scalar modeled by diffusion gradient in the transport equation for a single point multi dimensional joint composition PDF, MEPDF was derived from this equation with these terms closed in eq.(8), the only problem is that we have two terms unknown[25].

$$\frac{\partial \rho p_n}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i p_n) = \nabla(\rho \Gamma \nabla p_n) \quad (9)$$

$$\frac{\partial \rho s_{k,n}}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i s_{k,n}) = \nabla(\rho \Gamma \nabla s_{k,n}) + \rho (M_{k,n} + S_{k,n} + C_{k,n}) \quad (10)$$

FOX[26] used as an alternative the DQMOM model (direct quadrature method of moments) to solve this problem and succeeded. His alternative for resolve the unknown terms, p_n and $\langle \phi_k \rangle_n$, in eq. (8) by using the DQMOM approach, the resulting equations for multi environment are presented in eq.(9) and eq.(10).

$$S_{k,n} = p_n S(\langle \phi_k \rangle_n)_k \quad (11)$$

$$M_{k,n} = \frac{C_{\phi}}{\tau} (\langle \phi_k \rangle_n - \psi_k) \quad (12)$$

$$\sum_{n=1}^{N_e} \phi_{k,n}^{m_k-1} C_{k,n} = \sum_{n=1}^{N_e} (m_k - 1) \langle \phi_k \rangle_n^{m_k-2} p_n C_{k,n} \quad (13)$$

were $S_{k,n}$ represent the reaction, $M_{k,n}$ represent the mixing and $C_{k,n}$ represent the correction terms.

3. FLAME OF VITIATED COFLOW

The flames of hydrogen considered in the current work have already been studied experimentally by Cabra et al[4]. (Fig.2). It has much higher lift off height compared to H₂ flame [27].

In this work, the vitiated co-flow burner consists of a fuel jet, which has an inner diameter $D = 4.57$ mm, located at the center of a perforated disk with a diameter of 210 mm to provide a hot co-flow which stabilize many premixed flames. The disk has 2200 holes of 1.58 mm diameter. The central fuel reaches out by 70mm downstream of the surface

of the punctured plate with the goal that the fuel mixture exits in a uniform composition for the coflow.

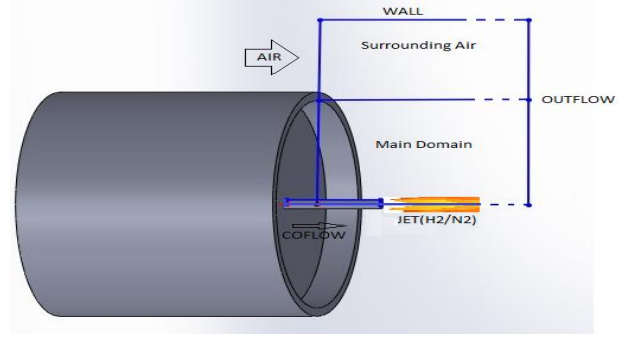


Figure 2. Burner schematic[4]

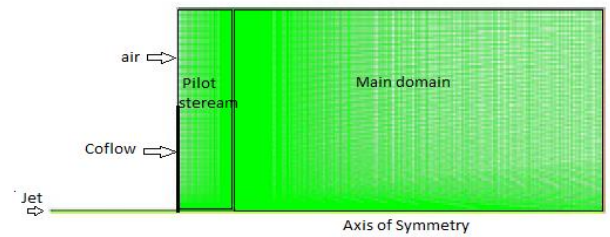


Figure 3. Computationally domain for the simulated lifted flame of hydrogen (MECH-2)

The figure shown above contain fuel jet, pilot stream and main domain with 9074 cells in mesh-2. The computational domain stretches out to $100 \times 50 D$ in the axial and radial directions, where D is the fuel jet diameter. In the radial direction, the grid reaches out up to $50D$ so as to consider about the impact of ambient cold air. three non-uniform distinct grids are formed to carry out the grid independence test. The following table shows the initial conditions:

The configuration of the geometry is axis of symmetric with a quadrilateral mesh shape. The ANSYS Fluent calculation code [28] uses a Cartesian coordinate system. A refining of the zones near the exit of the burner has been envisaged to take into account the large variations taking place in these zones, in particular the speed gradients. The definition of the geometry and the generation of the mesh were carried out using the Workbench15.0. The turbulence is modeled by modified $k-\epsilon$ model. A second order upwind scheme is used in all equations conservation for modeled the convective flux. The MEPDF and LPDF are used with the value of (2.1) in the mixing constant and combustion chemistry using in situ adaptive tabulation method ISAT [29]. The chemical reaction mechanism adopted is GRI-Mech2.1. Environment number equal two in the first approach ($N_e = 2$).

Table 2. Base-case conditions for the vitiated coflow burner

	Jet	Coflow
Re	23,600	18,600
D(mm)	4,57	210
V(m/s)	107	3.5
T(k)	305	1045
X _{H2}	0,2537	0,0005
X _{O2}	0,0021	0,15
X _{N2}	0,7427	0,75
X _{H2O}	0,0015	0,099

4. RESULTS AND DISCUSSION

The comparison between LPDF and MEPDF using turbulent lifted flame of H₂/N₂ in hot vitiated coflow are presented in the current section. A parametric study of the flame is performed with the same parameters for both approaches.

4.1. Grid-Independent study

In the study of grid independence test, we proposed three non-uniform distinct grids, in order to reduce the aspect ratio. The following table shows the various meshes used in the calculations.

Table 3. Information on the different meshes used in the calculations

		Jet	Pilot stream	Main domain	Total cells
X	From (mm)	-228.5	-70	0	
	To (mm)	0	0	457	
Y	From (mm)	0	2.285	0	
	To (mm)	2.285	228.5	228.5	
Mesh-1	Cells X	35	16	38	3065
	Cells Y	5	50	55	
Mesh-2	Cells X	58	32	140	9074
	Cells Y	5	47	52	
Mesh-3	Cells X	10	22	140	23426
	Cells Y	48	133	143	

The solution domain is subdivided into three regions that are then meshed as described in table 3. Some cells are made non-orthogonal.

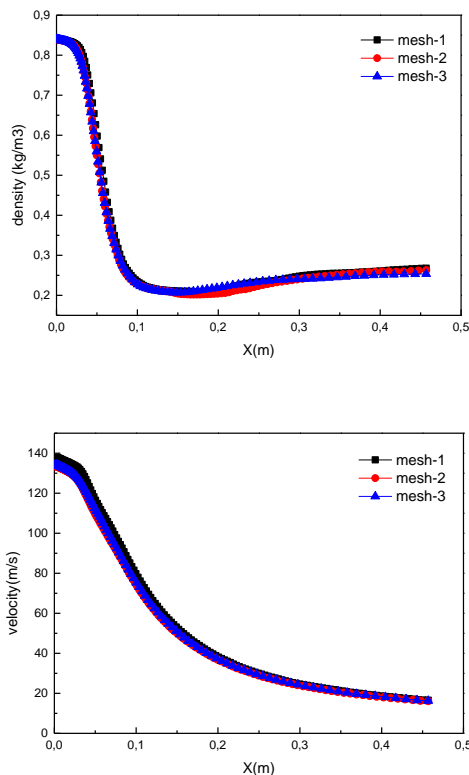


Figure 4. Axial profiles of density and velocity along centerline for approach of MEPDF

Figure 4 shows axial profiles of density and velocity along centerline for MEPDF method. Each plot shows three profiles for meshes 1, 2 and 3. Meshes 2 and 3 give very close results and either may be used to produce a grid independent solution. Mesh-1 shows only slight departures from meshes 2 and 3, especially for velocity. Figure 5 shows axial profiles of density and velocity along centerline for LPDF method. Each plot shows three profiles for meshes 1, 2 and 3. Mesh-1 give results far away than mesh-3. On the other hand Mesh-2 shows in both profiles only slight departures for mesh-3. Therefore, from figure 4 and 5 and for reasons of a comparative study. Meshes-2 and 3 give very close results and either may be used as grid independent solution. However, mesh-2 is selected here and is used in all further calculations.

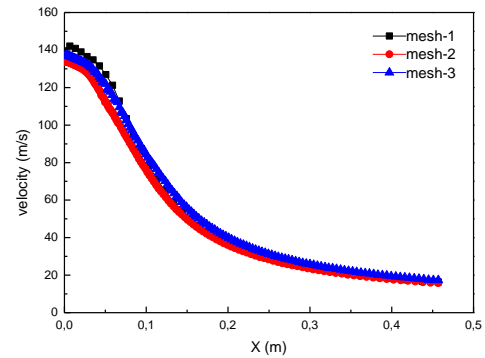


Figure 5. Axial profiles of density and velocity along centerline for approach of LPDF

4.2. Lifted H₂ flame in hot vitiated coflow

The figures below show the axial profiles of temperature, hydrogen and species mass fractions at centerline along for two different approaches (LPDF, MEPDF) with the experimental data [4].

In Figure 6, we can divide the domain in three zones. The first zone starts up from the jet exit until ($x/d=10$), this rise of temperature is primarily due to mixing and preheating. The second zone ($10 < X/D < 30$) which we have the maximum temperature due to the chemistry reactions, and thereafter the last zone.

The current predictions of MEPDF in profile of temperature are in good match with the experimental data. The temperature height difference of flattened peak between experiment and calculation does not exceed 9 k. But in LPDF, we have over-prediction and mainly in second zone of upstream ($10 < X/D < 30$) which we have an accelerated chemical kinetics, just after this point the temperature increase with lift-off height.

The temperature height difference of flattened peak between experiment and calculation does not exceed 9 k, but in another location of $X/D = 26$. The anomaly of LPDF is due to several reasons. The first reason is can be attributed to the constant of mixing [22]. The other possible reason is due to changing of the model of mixing. Changing the IEM model by the EMST model could give excellent results by LPDF model [13], but we cannot use this model with the MEPDF method in Ansys fluent 15.0. It is also impossible to use a reaction mechanism which exceeds 50 species in the second model but with LPDF, it can be usable and gives reliable results. We cannot make these changes for good results in LPDF because our aim is to make a comparison between two

methods of discretization in PDFT approach with the same mixture model and the same parameters. In order to understand what is happening in temperature curve for LPDF method at the point of ($X / D = 26$), we have plotted the radial curves in the last section.

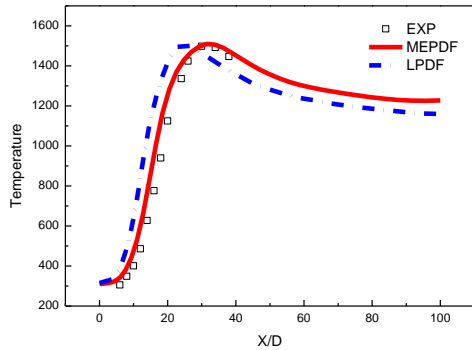


Figure 6. Axial profile of temperature along centerline for both approaches (LPDF, MEPDF)

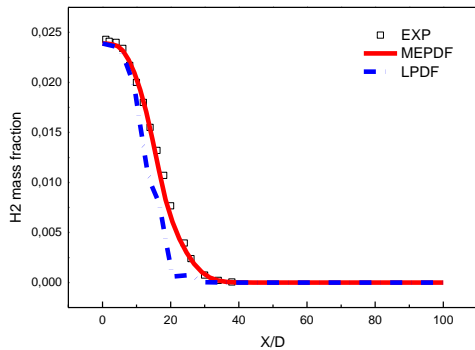


Figure 7. Axial profile of H₂ mass fractions along centerline for both approaches (LPDF, MEPDF)

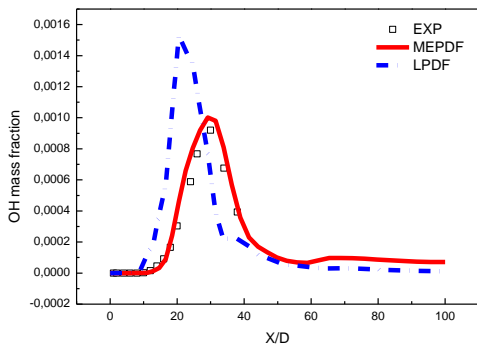


Figure 8. Axial profiles of OH mass fractions along centerline for both approaches (LPDF, MEPDF)

In the figure 7 which represents the H₂ mass fraction, we can see from the jet exit that the faster decay of mass fraction is due to the consumption of hydrogen. The current predictions of MEPDF method are in good match with the experimental data, but in LPDF method under-prediction. The computed values of LPDF method after location of ($X/D=10$) are lower than the experimental data, the faster consumption of hydrogen is signified by the high temperature in the same point in the temperature curve.

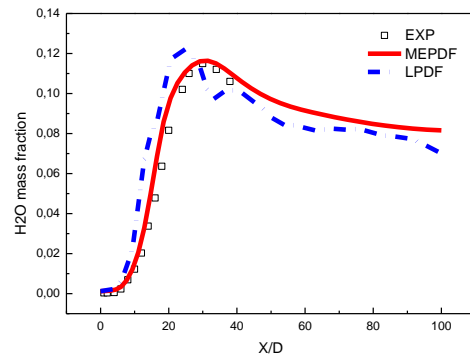


Figure 9. Axial profiles of H₂O mass fractions along centerline for both approaches (LPDF, MEPDF)

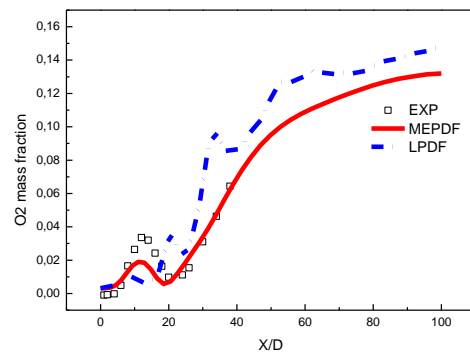


Figure 10. Axial profiles of O₂ mass fractions along centerline for both approaches (LPDF, MEPDF)

The exact forecast of OH is one of prime significance and essential criteria to judge the model exactness [22]. In Figure 8, we can see from the jet exit that there is no production in mass fraction of OH until ($x/d=10$), after this point the OH production startup until ($x/d=30$), and finally the production of OH will be stopped but the consumption continues for the production of H₂O. The predictions of MEPDF are in good adequacy with the experimental data and also it's better than the computed results of Yadav[22]. Concerning LPDF, the anomaly always starts from point of take-off bridge ($X / D = 10$). Mobus et al[23] show that in order to establish a good spatial precision it is necessary to have a good prediction of the ignition. The application of this model LPDF has practical problems and requires an increase in the numerical cost, increase of node number and finally a huge computing time, which is contrary that the second model of MEPDF. It is the same thing for H₂O.

In O₂ profile, we can see that the prediction of MEPDF has the same form with experimental data but with some deviations. The phenomena that directly influence and give remarkable deviations on the results are many, among them the turbulent viscosity and the turbulent mixture [21].

The following figures show the radial profiles of temperature, hydrogen and species mass fractions at axial location of $X/D=26$ for two different approaches (LPDF, MEPDF) with the experimental values [4].

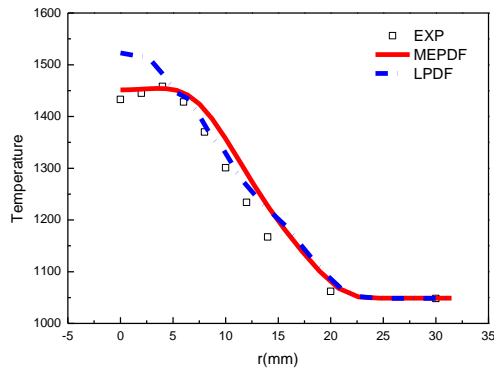


Figure 11. Radial profiles of temperature along centerline for both approaches (LPDF, MEPDF)

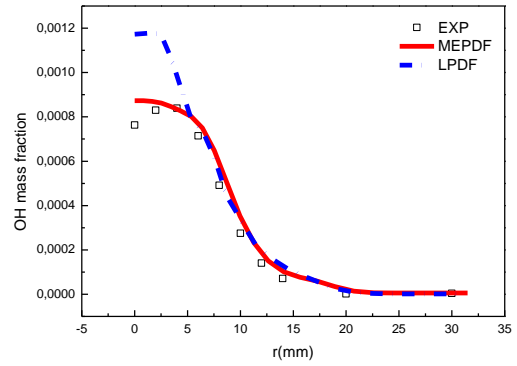


Figure 15. Radial profiles of OH mass fractions along centerline for both approaches (LPDF, MEPDF)

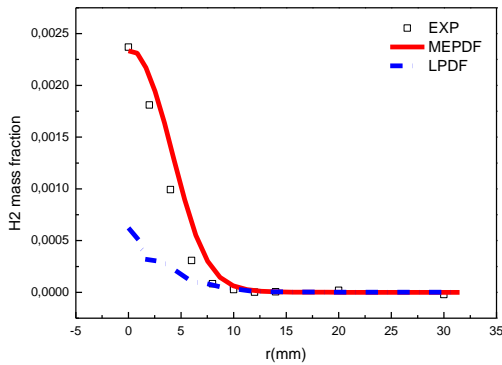


Figure 12. Radial profiles of H₂ mass fractions along centerline for both approaches (LPDF, MEPDF)

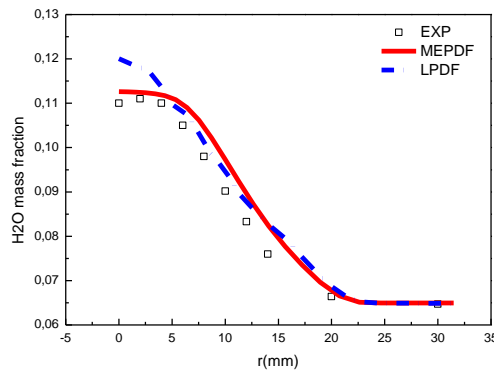


Figure 13. Radial profiles of H₂O mass fractions along centerline for both approaches (LPDF, MEPDF)

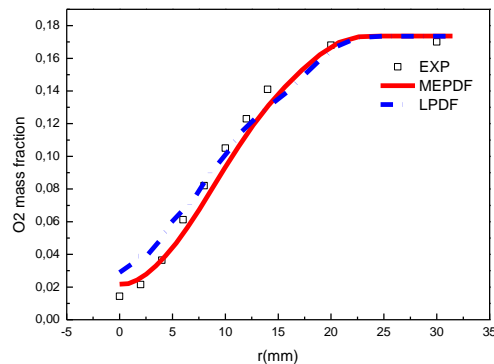


Figure 14. Radial profiles of O₂ mass fractions along centerline for both approaches (LPDF, MEPDF)

We can see that the current prediction of MEPDF is in good adequacy with the experimental data except for a little over-prediction in the OH and the H₂O curve, which means delay starting of reaction, lesser oxidation of OH and the same thing in production of H₂O which gives a lesser of the temperature. But in LPDF may be different and mainly in axial location. We can see in the temperature profile that the maximum temperature of the MEPDF model is in the first point of the profile, which means that the flame is stable. In H₂ profile, we can see a drop in H₂ because of the very high consumption of H₂ in the prediction of MEPDF. This consumption is due early start of reaction[22]. In the OH curve, one also notices in the same point a high in oxidation of oh with the experimental values. The same thing for the H₂O curve, the produced is due to oxidation of OH.

5. CONCLUSIONS

The applications of the PDF transport model to study a turbulent diffusion flame. The flame studied is a flame of Hydrogen (H₂). The comparison was studied between Lagrangian (LPDF) and Eulerian (MEPDF) approaches by equivalent numerical parameters in the CFD fluent solver. The selected turbulence model is Kε modified and IEM mixing model. it can be concluded that the the approach Eulerien (MEPDF) is very promising. It is very important to identify turbulent flame and crucial to predict the local extinction, reignition and lift-off height. The predictions of temperature and all mass fractions with EPDF approach are compatible with the experimental results. The temperature height difference of flattened peak between experiment and calculation does not exceed 9 k. The good prevision of OH in the current study is one of prime essential criteria to judge the EPDF model exactness and capability. Regarding to Lagrangian approach (LPDF), we did not found a good results with this approach; we found the early starting of reaction in the downstream, which given the bad prediction of the ignition in this model. Due to the previous explanations we can say that the Lagragian approach has a real practical problem which the improving of the approach behavior to computationally expensive. In conclusion, it is evident that this study has shown the value of the MEPDF model, the ease of having good results with minimal cost. On the basis of the promising findings presented in this paper,

work on the remaining issues is continuing and will be presented in the future papers.

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NOMENCLATURE

Symbols

P	Probability
u	velocity [m.s ⁻¹]
S	Reaction rate
J	Molecular diffusion flux
μ	Viscosity [m ² .s ⁻¹]
Sc	Schmidt number
x	Particle position [m]
C _φ	Mixing constant
X	Mole fraction
Re	Reynolds number
D	Diameter[m]
T	Temperature [K]
S	The net reaction rate
V	velocity [m.s ⁻¹]

Greek letters

ρ	Density [kg/m ³]
ψ	Composition space vector
ζ	Standardized normal random
τ _t	Turbulent time scale
∅	Mean composition vector
δ	Delta function

Γ Diffusion coefficient

Subscripts

t	Turbulent
k	Species index
i	Species index

Abbreviation

PDF	Probability density function
CFD	Computational Fluid Dynamics
LPDF	Lagrangian PDF
MEPDF	Multi-environment PDF
EDC	Eddy Dissipation Concept
LFR	Laminar Finite Rate
DQMOM	Direct Quadrature Method of Moments
RANS	Reynolds-Averaged Navier-Stokes
EMST	Euclidean Minimum Spanning Tree
IEM	Interaction by Exchange with the Mean.
MC	Modified Curl

Other symbols

<>	Expectations
<A/B>	Condition probability of A, for a given B