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**Title**

# *Numerical study of $C_3H_8$ and $H_2$cmbustion*

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***Rabia Taghia***

*To…*

*My dear husband*

*And My mother & father*

*And My Family And My friends…*

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# *Nomenclature*

## *Latin letters*

| | |
|---|---|
| $A$ | Deformation tensor |
| $C$ | Specific heat |
| $c$ | Parameter progress |
| $C_W$ | WALE Constant |
| $D$ | Diameter tube |
| $E$ | Energy spectrum |
| e | Internal energy |
| $f_i$ | Body force per unit mass of species i |
| h | Enthalpy |
| $h$i | Enthalpy of species i |
| $\tilde{g}_{ij}^2$ | Velocity gradient resolved |
| $k$ | kinetic energy |
| $L$ | Large-scale Kolmogorov flow |
| $N$ | Number of chemical species |
| $n$ | Boundary-normal coordinate |
| $n_i$ | The number of moles of species $i$ |
| $n_s$ | Sum is the total number of moles |
| $p$ | Pressure |
| $Pr$ | Prandtl number |
| $q_R$ | Radiative heat flux vector |
| R | ideal gas constant |
| r | Radial coordinate |
| $Re$ | Reynolds number |
| $s$ | Source Term |
| $\tilde{S}_{ij}$ | Tensor velocity deformation |
| $t$ | Time |
| T | Temperature |

| | |
|---|---|
| $T_{ij}$ | Reynolds stress tensor |
| $u$ | Velocity |
| $u_{\alpha}$ | Velocity component |
| $Vi$ | Mass diffusion velocity of species i |
| $Wi$ | Chemical production rate of species i |
| x | Spatial coordinate |
| $X_i$ | The mole fraction of species $i$ |
| $y$ | The distance to the normalized wall |
| $y_{\mathrm{i}}$ | Mass fraction of species i |
| $Z$ | Mixture fraction |

## *Greek Symbol*

| | |
|---|---|
| $\rho$ | Mass density |
| $\lambda$ | Thermal conductivity |
| $\kappa$ | Thermal diffusivity |
| $\sigma$ | Stress tensor |
| $\mu$ | Dynamic viscosity |
| $\nu$ | kinematic viscosity |
| $\mu_T$ | Turbulent viscosity |
| $\eta$ | Small-scale Kolmogorov flow |
| $\omega_i$ | Chemical production rate of species i |
| $\tau_{ij}$ | Viscous stress tensor |
| $\delta_{ij}$ | Kronecker delta |
| $\phi$ | equivalence ratio |

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| | |
|---|---|
| $f$ | Chemical Species |
| i | Components along the axes x, y and z |
| r | Radial coordinate |
| x | Spatial coordinate |

***Abbreviations***

| | |
|---|---|
| CFD | Computational Fluid Dynamics |
| CRZ | Central Recirculation Zone |
| FPDF | Filtered Probability Density Function |
| HENG | Hydrogen-Enriched Natural Gas |
| LES | Large eddy simulation |
| PDF | Probability Density Function |
| RANS | Reynolds Averaged Navier Stokes |
| SGS | Subgrid scale |

# *Introduction*

In 1980 Tormod Forland et al have studied the entropy production by heat, mass, charge transfer and specific chemical reactions, It is emphasized that the number of variables used to describe the entropy production should be the minimum (basic) set of free variables that can describe the changes in the system [1] . J. Y. SAN et al (1987) studey Entropy generation in combined heat and mass transfer. For the case of laminar flow, the entropy generation is obtained as a function of velocity, the four sources of entropy generation are coupled through both the plate spacing and Reynolds number [2],and Adrian Bejan(1996) student Method of entropy generation minimization, or modeling and optimization based on combined heat transfer and thermodynamics Emphasis is placed on the engineering value of EGM models, was found that the tree network is the geometric-optimization result for minimal flow resistance between one point and a finite volume[3] .in 1999 Vasili Tatarin and et al calculated Entropy of Reversible Mixing of Ideal Gases is a classic thermodynamic problem Using a mathematical equation did not show of Gibbs Paradox [4].also dorin stanciu et al (2000) analyzed Second Law of the Turbulent Flat Plate Boundary Layer It found that the "volumetric mean motion irreversibilities" (generated by the mean velocity and mean temperature gradient) prevail in the viscous sublayer and reach their maximal values at the wall, while the "volumetric turbulent irreversibilities" (performed by the dissipation rate of turbulent kinetic energy and fluctuating temperature variance) rule the logarithmic sublayer but have the maximal values located in the buffer sublayer [5] .and in the same year too, Jerald A. Caton (2000) student The destruction exergy during combustion processes is examined for an adiabatic, constant volume system. This is an analytical examination and did not involve experimental measurements and described the implications of these findings to internal-combustion engines, An analysis based on the second law of thermodynamics, The analysis included the computation of entropy, availability, irreversibilities, and the related energy, entropy and availability balances[6] J.V.C. Vargas , et al (2000) have student of matching thermodynamically two one hot and the other cold , is determined by maximizing the power generation It is shown that the optimum is marked by an optimal ratio between the stream mass flow rates, they study documented numerically the position of the thermodynamic optimum and its sensitivity relative to all the parameters that govern the behavior of the two-stream system[7] .Dorin Stanciu et al (2001) investigated the irreversibility sources in both laminar and turbulent diffusion flames dependent on the local exergy transport equation and T. Shiba et al They shows that the internal geometric configuration of a component can be deduced by optimizing the global performance of the installation that uses the component. The objective is to show that all the dimensions of the counter flow heat

exchanger can be derived based on global thermodynamic optimization , shows that from the global optimization of the thermodynamic performance of an environmental control system (ECS) it is possible to derive the complete geometric structure of one of the major components and The general mechanism by which flow systems acquire geometric form (architecture) is the object of constructal theory and design[8] .Marc A. Rosen (2002) explains Clarifying thermodynamic efficiencies and losses via exergy he believe that we need to use exergy based efficiencies if we are to address energy problems effectively and to prioritize efficiency-improvement efforts appropriately[9] and in the same year Adrian Bejan(2002) have studied Fundamentals of exergy analysis, entropy generation minimization, and the generation of flow architecture ,he begins with a review of the concept of irreversibility, entropy generation And giving examples [10] ,and Huseyin Yapici et al (2004) have Numerical study of effect of oxygen fraction on local entropy generation in a methane–air burner, In order to investigate the effect of oxygen percentage on the combustion and entropy generation rate, the combustion of methane with air is examined at various oxygen percentages in the air by using Fluent CFD code The objectives of research work in the area of combustion are to improve the combustion process in order to achieve higher combustion efficiency, the results of this study Material resistant to high temperatures must be selected as the burner wall-material (especially in the cases of high $\varphi$ and $\gamma$ ), and in order to reduce the burner-wall temperature, the heat transfer coefficient at the burner wall should be increased [11] and Michel Pons (2004) has studied Irreversibility in energy processes , A non-dimensional irreversibility balance can be established for energy conversion cycles. Obtained from trivial derivations, the non-dimensional irreversibility balance appears as a robust, useful and unified framework for analysing complex processes, for instance involving several powering energies, irreversibilities attached to the process but taking place outside the process [12], A .Bejan et al (2004) have a formulation of the constructal principle in analytical and graphical terms that are analogous to terms employed in thermodynamics demonstrated this through examples from three wide classes of flow architectures low between two points, flow between a circle and its center and flow between one point and an area [13] and Ahmet Durmayaz and all (2004) have studied, optimization studies of thermal systems, that consider various objective functions, based on finite-time thermodynamics and thermo economics are reviewed, Found that it must rely on constructural and FTT theory[14] after 1 year Hüseyin Yapıcı et al (2005) have studied Numerical Study On Local Entropy Generation In Compressible Flow Through A Suddenly Expanding Pipe , Use the computer programs of research in this area several researchers The pray to several outcomes such as temperature and dimensions of the tube [15] and in same year too (2005) have studied Numerical student on transient local entropy generation in pulsating turbulent flow through an externally heated pipe

and use computational fluid dynamics (CFD) code , was analysed for three different flow cases The effect of the period of the pulsating flow on the entropy generation rate was also investigated, The results of this study indicate that flow pulsation has an adverse effect on the ratio of the useful energy transfer rate to the irreversibility rate. [16] V.D. Zimparov et al (2006) optimized the performance of several classes of simple flow systems consisting of T- and Y-shaped assemblies of ducts, channels and streams ,The fundamental study of the optimization of tree-shaped architectures also sheds light on the common design principles of engineered and natural flow systems, the objective was to identify the geometric configuration that maximized performance subject to several global constraints [17] and in same year too (2006) have studied optimize the performance of several classes of simple flow systems consisting of T- and Y-shaped assemblies of ducts, channels and streams, The objective is to determine flow architectures that reach two objectives: (1) minimal global entropy generated, and (2) maximum heat flow density [18], Huseyin Yapıcı et al (2006) studied numerical simulation of the combustion of hydrogen with air, The combustion is simulated for the fuel mass flow rate providing the same heat transfer rate to the combustion chamber in the each case , In order to investigate the effect of oxygen percentage on the combustion and entropy generation rate, the combustion of hydrogen with air is examined at various oxygen percentages in the air by using the Fluent CFD, the results of this study clearly demonstrate the numerical simulation of combustion of hydrogen with air and the numerical solution of local entropy generation rate in the combustion chamber for the various equivalence ratios and oxygen percentages in the air. Material resistant to high temperature must be selected as the burner wall material (especially in the cases of high / and c), and in order to reduce the burnerwall temperature, the heat transfer coefficient at the burner wall should be increased[19]. C.D. Rakopoulos et al (2006) studied the application and analyses of the second-law of thermodynamics to internal combustion engines, the main differences between the results of second- and first-law analyses are highlighted and discussed and Tabulation of energy and availability balances is given for many types of engines, accompanied by figures showing the effect of the most important parameters on the second-law performance of internal combustion engines[20] and C.Stuart Daw et al (2006) Minimizing destruction of thermodynamic availability in hydrogen combustion, First and second law analyses of an idealized hydrogen combustion process indicate that it is theoretically possible to eliminate the majority of combustion irreversibility from internal heat transfer by preheating the hydrogen and air in a counter-flow heat exchanger with recycled flue gas and Noam Lior[21] et al (2006) reviewed the exergy fields in transport processes, It presents the basic equations, the method for their use and three examples from the authors work flow desiccation[22] . Dorin Stanciu (2007) investigated the swirl angle influence on the turbulent diffusion flame

Irreversibilities, using the second law of thermodynamics relies on the local transport exergy equation, and The numerical simulations After able to propose two ways for reducing the combustion irreversibility [23.24] and Dorin Stanci(2008) is studied to analyze a digital way the influence of the undulation of a wall on the volume of the forced irreversibility inner turbulent convection. For the flow and transfer of turbulent heat the LRN models we chose two equations Abe, Kondoh and Nagano, The results showed that the distribution of all components of irreversibility volume along and normal directions of the wall are different [25] and S.K. Som et al (2008) have studied Thermodynamic irreversibilities and exergy balance in combustion processesb, the major source of irreversibilities is the internal thermal energy exchange associated with high temperature fossil fuels even today where combustion plays a key role in the energy utilization process , This information are furnished by the fundamental studies on the identification of irreversibilities and subsequent exergy analysis in a combustion process, which has been reviewed in the present study[26].

The main objective of this work is to present the thermochemistry 3D study of the non-premixed combustion fueled by $C_3H_8/H_2$ using the include FLUENT-CFD models. Whereas, the simulation is based on the modelling of the fundamental equations: fluid dynamic, heat transfer and chemical reactions.

The work organised in three chapters:

***Chapter I:*** We present theoretical models and we illustrate the mathematical formulation of the probability model.

***Chapter II:*** We illustrate the important steps for realise the non-premixed combustion in FLUENT_CFD.

- ***Chapter III:*** a numerical simulation using the Fluent-CFD to combustion Comparison between, $C_3H_8/H_2$ on one hand of field velocity, temperature and molar fraction of carbon monoxide.

# *Chapter I*

# *Dynamic Model "LES" and Combustion Model "PDF"*

Turbulence is the state of fluid motion which is characterized by eddies and a random three-dimensional flow. Whereas, the turbulent flow is increasing the energy dissipation, mixture, heat transfer. So, the uses of the notions of the statistical physics deals with stochastic processes elementary of the fluid agitation, that wants to understand the behavior of the system in details on all scales. Indeed, the difficulty of the problem of turbulence lies mainly in the separation between large and small scales: cannot study the large-scale behavior without explicit consideration of the mechanisms involved at small scales, and vice versa. This is highlighting the universal statistical properties of turbulent fluctuations [27- 29].

## I. 1 Presentation of Approach "LES" Applied to Combustion

Large eddy simulation (LES) is a model used to resolve a very difficult theoretical problem of turbulent flows, related to the modeling of dynamic behavior on a small scale in the equations of motion on a large scale. LES is a valuable tool for filtering the vortex structure of the flow, because it captures a deterministic way the formation vortices structures. It also enables the prediction of many statistical parameters related to the induced turbulence and mixing. LES applies to turbulent flow for remedy the problem of closure [30- 32].

The objective of this section is to present some of the basics of the theory of turbulence and its statistical analysis. The focus is on the characteristics of the turbulent flow are of key interest for the prediction and modeling of flows: scales of turbulence, Kolmogorov scale, shearing structures flows (viscosity forces) and energy dissipation.

### I.1.1 Generalities on the turbulent flow

The majority of fluid flows in nature and in engineering applications are turbulent. Where, the turbulent flows can be easily observed but it is very difficult to give a precise definition. However, researchers and engineers are agreeing on certain characteristics of the turbulent flow, we briefly present it in the following [30,33]:

*Unpredictability*

Turbulent flows are characterized by their irregularity (Figure I.1). Variables such as velocity, pressure, density and the temperature fluctuate randomly which makes it impossible to determine parameters describing the movement of spatiotemporal function. For example, the

component considered speed fluctuates around an average value. The random nature of the flow leads to consider a statistical treatment of turbulence [34].

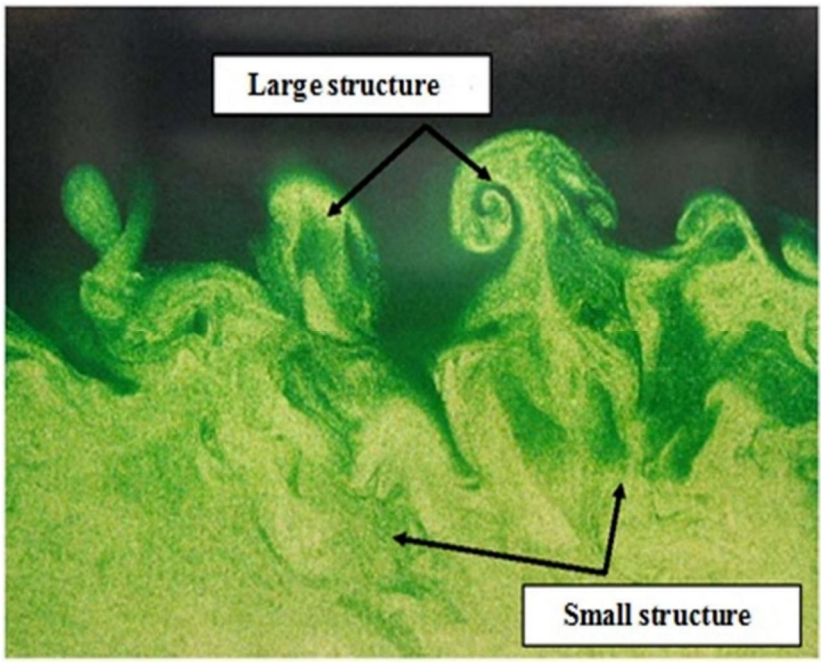



***Figure I.1:*** *Visualization of large-scale structures and small scales in the turbulent flows [34].*

*High Reynolds number*

Turbulence occurs in flows with Reynolds number is high ( $\mathrm{Re} = {uD}/{\nu}$ ). It has often caused the development of instability of a laminar flow. When the Reynolds number exceeds a critical value, small flow disturbances become unstable and rapid growth of the transition to turbulence. Thus the laminar boundary layer on a flat plate becomes turbulent when the Reynolds number ***Re*** exceeds $5.10^5$. Similarly, the transition occurs in a cylindrical pipe flow for a Reynolds number of 2500 [34].

*Turbulent flows are rotational*

For a large class of flows, turbulence arises due to the presence of boundaries or obstacles, which create vorticity inside a flow which was initially irrotational. Turbulence is thus associated with vorticity, and it is impossible to imagine a turbulent irrotational flow [27,35].

*Turbulent flows are dissipative*

Viscosity effects will result in the conversion of kinetic energy of the flow into heat. If there is no external source of energy to make up for this kinetic energy loss, the turbulent motion will decay [27,35].

*Turbulence is a characteristic of the flows, and not of fluids*

If the Reynolds number is high enough, most of the dynamics of turbulence is the same in all fluids (liquids or gases). The progress of the characteristics parameters is chaotic in the turbulent flows [27,35].

### I.1.2 Mathematical Description of Turbulence

#### I.1.2.1 Compressible Navier-Stokes Equations

The Navier–Stokes equations are non-linear equations that describe the movement of Newtonian fluid, resulting from the application of Newton's second law on the movement of fluid is considered one of the most important physical equations that describe a large number of phenomena[35]:

Continuity $$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_\alpha}(\rho u_\alpha)=0 \qquad \text{(I.1)}$$

Momentum $$\frac{\partial \rho u_\beta}{\partial t}+\frac{\partial}{\partial x_\alpha}(\rho u_\alpha u_\beta)=-\nabla p+\nabla \tau+\rho\sum_i y_i f_i \qquad \text{(I.2)}$$

Energy $$\frac{\partial(\rho e)}{\partial t}+\frac{\partial}{\partial x_\alpha}(\rho u_\alpha e)=-\nabla(pu)+\nabla(\tau.u)\ +\sum \rho V_i y_i h_i-k\nabla T+q_R \qquad \text{(I.3)}$$

Where: $\alpha=1,2,3$; $\beta=1,2,3$.

$q_R$ : Radiative heat flux vector.

zComponent $\sigma_{ij}$ the stress tensor presented can be written for a Newtonian fluid in the form [28,37]:

$$\sigma_{i1}=-p\delta_{ij}+2\mu A_{ij} \qquad \text{(I.4)}$$

and:

$$A_{ij} = \frac{1}{2}\left[\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3}(\nabla u)\delta_{ij}\right] \quad \text{(I.5)}$$

With $A_{ij}$ : Deformation tensor.

The total energy defined here for the ideal gas:

$$\rho e = \rho C_v T + \frac{1}{2}\rho(u_1^2 + u_2^2 + u_3^2) \quad \text{(I.6)}$$

In Cartesian coordinates, the equations of aerothermal balance can be expressed as the following flow [30,37,38]:

$$\frac{\partial Q}{\partial t} + \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} + \frac{\partial F_3}{\partial x_3} = s \quad \text{(I.7)}$$

with: $s$ : Source term.

$Q$ : Conserved variables.

$F$ : Field describes the rate of the conserved variables.

where

$$Q = \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho e \end{pmatrix} \quad \text{(I.8)}$$

If we neglect the effect of gravity, the flow $F_i$ is written $\forall i \in \{1,2,3\}$:

$$F_i = \begin{pmatrix} \rho u_i \\ \rho u_i u_1 - \sigma_{i1} \\ \rho u_i u_2 - \sigma_{i2} \\ \rho u_i u_3 - \sigma_{i3} \\ \rho e u_i - u_j \sigma_{i1} - \lambda \dfrac{\partial T}{\partial x_i} \end{pmatrix} \quad \text{(I.9)}$$

With:

$\lambda = \rho C_p \kappa$ : Thermal conductivity. And $\kappa$ : Thermal diffusivity.

The substitute of the means of deformation tensor of Eq, I.5 :

$$F_i = \begin{pmatrix} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} - 2\mu A_{i1} \\ \rho u_i u_2 + p\delta_{i2} - 2\mu A_{i2} \\ \rho u_i u_3 + p\delta_{i3} - 2\mu A_{i3} \\ (\rho e + p)u_i - 2\mu u_j A_{ij} - \lambda \dfrac{\partial T}{\partial x_i} \end{pmatrix} \quad \text{(I.10)}$$

To start using the empirical relationship of Sutherland to present the viscosity:

$$\mu(T) = \mu(273{,}15)\left(\frac{T}{273{,}15}\right)^{1/2} \frac{1 + T_0 / 273.15}{1 + T_0 / T} \quad \text{(I.11)}$$

With: $\mu(273{,}15) = 1{,}711.10^{-5}\,Pl$ and $T_0 = 110{,}4K$.

In the case $T<120K$ using an extension of the previous law:

$$\mu(T) = \mu(120)\left(\frac{T}{120}\right) \quad \text{(I.12)}$$

Viscosity and thermal conductivity are connected by the Prandtl number which characterizes the thermal properties of the fluids:

$$\mathrm{Pr} = \frac{\nu}{\kappa} = \frac{C_p \mu(T)}{\lambda} \quad \text{(I.13)}$$

The thermodynamic state equation is given by:

$$p = \rho R T \quad \text{(I.14)}$$

It recalled that $R = C_p - C_v = 287{,}06 J.kg^{-1}K^{-1}$ in air at room temperature, and $\gamma = C_p / C_v$

### I.1.2.2 Kolmogorov Scale

There exists a theory that has made a major contribution to the understanding of turbulence: the theory of Kolmogorov (1941). It is based on a vision "statistics" of turbulence [29,38].

According to this theory the vortices in the flow have a size between the two sizes following limits:

• The largest scale of the flow L (imposed by the geometry of the flow, for example typically the diameter of a cylinder),

• The smaller scale of the flow $\eta$: imposed by the viscosity of the fluid, this scale is called the Kolmogorov scale, or scale of viscous dissipation.

The ratios between L and $\eta$ is as follows:

$$\frac{L}{\eta} \approx \mathrm{Re}^{3/4} \tag{I.15}$$

Kolmogorov' s theory describes energy is transferred from larger to smaller eddies; these smaller eddies undergo break-up process and transfer their energy, and so on until the smallest scale existing in the flow, scale $\eta$. And molecular viscosity is effective in dissipating the kinetic energy. At these small scales, the kinetic energy of turbulence is converted into heat. When energy generation is equal to the energy dissipation, we speak of turbulence "in balance".

The basic idea of the theory of Kolmogorov turbulence shows that for a sufficiently large Reynolds number, the separation of scale between the energy of the flow structures and structures that dissipate this energy is considered [33,35,38]:

$$E(k) = \mathrm{Re}^{-5/3} \tag{I.16}$$

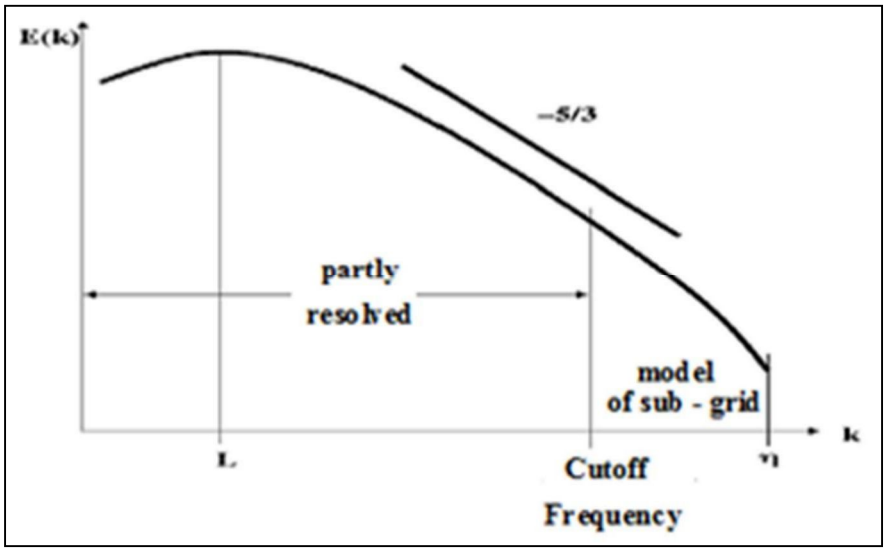



***Figure I.2**: Principle of LES model in the space of the energy spectrum [1].*

Between these two frequencies L and $\eta$, see figure I.2, the idea of LES model is to apply a filter to the equations in space. Structures that are larger than the cutoff frequency of the filter are explicitly represented by equations while smaller structures are modeled (figure I.2).

### I.1.3 Simulation Description of Turbulence

#### I.1.3.1 Generality of the LES Model

The concept of LES model is now better known in the scientific community. The idea comes from the founder of the theory of Kolmogorov turbulence [39,41]. Requires that all structures solved on the mesh are properly calculated, while the contribution of small structures, sub-grid, is modeled. The use of numerical schemes centered high order to minimize the dissipation. Thus, the lack of robustness of low dissipative numerical methods is a central problem for the calculation of flows with high Reynolds number.

We consider a variable $f$ and $\overline{f}$ is there filtering used in LES. So in the model (LES), parameters are processed by using the decomposition Reynolds, $f' = f - \overline{f}$, to facilitate understanding of terms in sub-grid to model. In the case of Navier-Stokes compressible, to simplify the modeling terms filtered. However, in the case of a turbulent flow quantities per unit mass are best described by a Favre (density-weighted) called "average Favre" noted $\tilde{f}$, defined by[42,43]:

$$\overline{\rho}\,\tilde{f} = \overline{\rho f} \tag{I.17}$$

as well:

$$\tilde{f} = \frac{\overline{\rho f}}{\overline{\rho}} \tag{I.18}$$

The system of equations defined above (Eq.1-Eq.14) becomes:

$$\frac{\partial \overline{Q}}{\partial t} + \nabla \overline{F} = \overline{s} \tag{I.19}$$

$$\overline{Q} = (\overline{\rho}, \overline{\rho u_1}, \overline{\rho u_2}, \overline{\rho u_3}, \overline{\rho e})^T \tag{I.20}$$

The total energy filtered can be written as:

$$\overline{\rho e} = \overline{\rho \tilde{e}} = \overline{\rho} C_v \tilde{T} + \frac{1}{2}\overline{\rho (u_1^2 + u_2^2 + u_3^2)} \tag{I.21}$$

The filtered flow $\overline{F_i}$ therefore:

$$\overline{F}_i = \begin{pmatrix} \overline{\rho}\widetilde{u}_i \\ \overline{\rho u_i u_1} + \overline{p}\delta_{i1} - \overline{2\mu A_{i1}} \\ \overline{\rho u_i u_2} + \overline{p}\delta_{i2} - \overline{2\mu A_{i2}} \\ \overline{\rho u_i u_3} + \overline{p}\delta_{i3} - \overline{2\mu A_{i3}} \\ \overline{(\rho e + p)u_i} - \overline{2\mu u_j A_{ij}} - \lambda\overline{\frac{\partial T}{\partial x_i}} \end{pmatrix} \quad \text{(I.22)}$$

The LES governing equations are written as [33,44] :

Continuity $$\frac{\partial\overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0 \quad \text{(I.23)}$$

Momentum $$\frac{\partial\overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)] - \frac{\partial\overline{p}}{\partial x_j} + \frac{\partial\overline{\tau_{ij}}}{\partial x_i} \quad \text{(I.24)}$$

Energy $$\frac{\partial}{\partial t}\overline{\rho}\widetilde{h} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{h}) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i h} - \widetilde{u}_i\widetilde{h})] + \frac{\partial\overline{p}}{\partial t} + \frac{\partial}{\partial x_i}\overline{u_j\tau_{ij}} \quad \text{(I.25)}$$

Thermodynamic state $$\overline{p} = \overline{\rho}R\widetilde{T} \quad \text{(I.26)}$$

$(\overline{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)$ : Reynolds tensions of sub-grid.

$(\overline{u_i h} - \widetilde{u}_i\widetilde{h})$ : Heat flow sub-grid.

- The filtered viscous stress tensor is defined by [28, 39,45 and 46]:

$$\overline{\tau}_{ij} = 2\overline{\rho}\nu(\widetilde{S}_{ij} - \frac{1}{3}\delta_{ij}\widetilde{S}_{ll}) \qquad i,j=1,2,3 \quad \text{(I.27)}$$

Where: $\widetilde{S}_{ll}$ is the subgrid kinetic energy.

- The filtering is also applied on the tensor velocity of deformation as follows:

$$\widetilde{S}_{ij} = \frac{1}{2}(\frac{\partial\widetilde{u}_j}{\partial x_i} + \frac{\partial\widetilde{u}_i}{\partial xj}) \qquad i,j=1,2,3 \quad \text{(I.28)}$$

### I.1.3.2 Sub-grid Reynolds Stresses Models

The closure of subgrid model in the governing equations the system is presented in preview. The majority models of sub-grid is based on the Boussinesq hypothesis linking the unresolved stress tensor $\tau_{ij}$ (Eq I.27) to the tensor velocity deformation $\widetilde{S}_{ij}$ (Eq I.28) through a turbulent viscosity $\mu_T$ [32,41,48]:

$$\tau_{ij}=2\mu_T(\widetilde{S}_{ij}-\frac{1}{3}\delta_{ij}\widetilde{S}_{ll}) \quad \text{(I.29)}$$

The choice of model is therefore to explain the turbulent viscosity $\mu_T = \overline{\rho}\nu_T$ .

### I.1.3.3 Smagorinsky Model

The Reynolds stress tensor $T_{ij}$ is modeled by a turbulent viscosity [36] : $T_{ij}=\mu_T \tilde{S}_{ij}$ . $T_{ij}$ decomposed on an anisotropic term $T_{ij}^{ani}$ and an isotropic term $T_{ij}^{iso}$ is neglected, which gives[37,38] :

$$T_{ij}^{ani}=\mu_T \tilde{S}_{ij} \quad \text{(I.30)}$$

$\mu_T$ the turbulent viscosity is written in the form of an algebraic relation:

$$\mu_T = \overline{\rho}C_s \Delta_x^2 \left|\widetilde{S}_{ij}\right| = \overline{\rho}C_s \Delta^2 \sqrt{\widetilde{S}_{ij}\widetilde{S}_{ij}} \quad \text{(I.31)}$$

or:

$$\nu_T=C_s \Delta^2 \sqrt{\widetilde{S}_{ij}\widetilde{S}_{ij}} \quad \text{(I.32)}$$

$Cs$ is constant Smagorinsky $Cs$ =0.18.

This model was developed in 1963 by Smagorinsky[39,40], and it is classed in the sub grid models used for LES, where is tested in the academic and industrial configurations. However, we note some limitations to the use of Smagorinsky model[38,41]:

- It is the dissipative model, for example the transition to turbulence.
- Needs to an auxiliary model to predict the turbulent viscosity in viscous areas. For example, behavior nears the walls.
- This model is based on the assumption of isotropic turbulence, which is not always adapted to calculate complicate configurations.

### I.1.3.4 WALE Model

This model is an adaptation of the Smagorinsky model and provides a decrease in $\mu_T$ following the logarithmical law in $(y^+)^3$ , ( $y^+$ is the distance to the normalized wall). This model is used to correct a defect in the Smagorinsky model which over-estimates the turbulent viscosity in the near wall and this because the gradients due to the boundary layer[42].

This method takes into account the energy of the flow structures small to large transfer. But it requires the use of limiters to limit values $\mu_T$. In addition, this model is more complex to implement than those presented here, especially on unstructured meshes. The WALE model has been developed to improve [37,42]:

- The decrease $\nu_T$ of the wall,
- the transition to turbulence.

Eddy viscosity is defined as:

$$\nu_t = (C_w \Delta)^2 \frac{(s_{ij}^d s_{ij}^d)^{3/2}}{(\tilde{s}_{ij}^d \tilde{s}_{ij}^d)^{5/2} + (s_{ij}^d s_{ij}^d)^{5/4}} \tag{I.33}$$

With

$$s_{ij}^d = \frac{1}{2}(\tilde{g}_{ij}^2 + \tilde{g}_{ji}^2) - \frac{1}{3}\tilde{g}_{kk}^2 \delta_{ij} \tag{I.34}$$

and

$$\tilde{g}_{ij}^2 = \frac{\partial u_i}{\partial x_i} \tag{I.35}$$

$\tilde{g}_{ij}^2$ velocity gradient resolved.

According Nicoud and Ducros, constant *Cw* varies little according to the configuration (unlike *Cs* in the Smagorinsky model). The value of *Cw* = 0.49. $\nu_T$ = 0 if the flow is two-dimensional[37,42] .

## I.2 Presentation of the Model PDF combustion

The theoretical study of turbulence reactive flows is very complex, due to the coupling between random turbulent and non-linear reaction rates. For this problem we investigate in the auxiliary models and approach to resolve the transport equations which represents the evolution of mechanical quantities and thermodynamic characteristic of these flows. Moreover, the turbulent phenomenon leads us to use statistical approach to predict the average evolution of the reactive flow. The equations for the average quantities which result from this approach reveal additive terms which that must be modeled. We will use in this study the probability density function methods. Where, the PDF model have emerged as one of the most promising approaches for accommodating the effects of turbulent fluctuation in chemical reaction.

## I.2.1 Non-premixed Flames

In this type of combustion, both the fuel and the oxidizer are introduced separately, mixed and burned directly in the burner. The motion of chemical mixture composition are based on molecular diffusion [43].

### I.2.2 Governing Equation

Turbulence is a stochastic phenomenon, for this reason we will use a statistical description of turbulence. In this case all the characteristic parameters are write as a the average and fluctuating term [34],

$$U = \overline{U} + U' \qquad \text{(I.36)}$$

Where:

$\overline{U}$ : Average quantity

$U'$ : Fluctuation quantity

But in case of compressible turbulent flow, the average of quantities can be noted $U$ by using a density weighted average in the following [34,43,44]:

$$\widetilde{u}_i = \frac{\overline{\rho u}}{\overline{\rho}} \qquad \text{(I.37)}$$

Where $\widetilde{u}_i$ is the Favre average.

In order to study the combustion we use the following equations based on the aerothermochemical analysis:

Conservation of mass
$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0 \qquad \text{(I.38)}$$

Linear momentum
$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)] - \frac{\partial \overline{p}}{\partial x_j} + \frac{\partial \overline{\tau_{ij}}}{\partial x_i} \qquad \text{(I.39)}$$

Species
$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{Y}_f + \frac{\partial}{\partial x_i}(\overline{\rho}u_i\widetilde{Y}_f) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i Y_f} - \widetilde{u}_i\widetilde{Y}_f)] + \overline{\dot{\omega}}_f \qquad \text{(I. 40)}$$

Energy
$$\frac{\partial}{\partial t}\overline{\rho}\widetilde{h} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{h}) = -\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i h} - \widetilde{u}_i\widetilde{h})] + \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_i}\overline{u_j\tau_{ij}} \qquad \text{(I.41)}$$

With $i=1, 2, 3$ and $j=1, 2, 3$

Thermodynamic state
$$\overline{P} = \overline{\rho}RT \qquad \text{(I.42)}$$

## I.2.3 Progress Variable

Chemical reaction contain great number of elementary chemical reactions i.e. the flame case result from simplest hydrocarbon combustion and many intermediate species and chemical reactions are necessary. However, it should be noted that few reactions have influence on the general process. Consequently, chemical advance can be represented by progress variable of the reaction *"c"*. This variable must be standardized, it varies between zero for the fresh gases and one for the burned gases [34, 44 ,45].

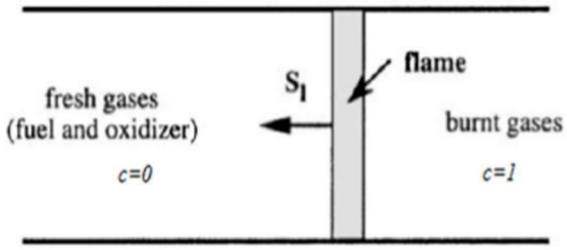



***Figure I.3 :*** *Definition of the progress variable.*

Usually, the premixed flames use the progress variable, and it can also replace the scalar rate of mixture fraction dissipation $\varepsilon_Z$ [34,46]:

$$\phi_i(Z,\varepsilon_Z) = \phi_i(Z,c) \tag{I.43}$$

In this case, the equation (I.43) is limited by the advance of reaction and the extinction of the diffusion flame. This transformation is arbitrary makes it possible to use the same control parameters of regime flow in premixed and non-premixed combustion, thus to facilitate the comparisons. There several definitions possible to describe the total advance of reaction. They can be defined according to the reactors and of the combustion products, or of the temperature. The definition of $c$ based on a homogeneous evolution in all the flame is necessary, which deviate the chemical species with chemical kinetics too fast or too slow. It can to know the concentration of the chemical species and the temperature of reactive mixture with only one variable?. If that is possible, the computing time in complex chemistry becomes piddling for 50 or more transport equations of the chemical species? [47.48].

In adiabatic systems closed, the temperature varies monotonically as a function of chemical process. In this case, temperature function normalized may define the progress variable of the reaction $c$ [34,44]:

$$c = \frac{T - T_0}{T_{eq} - T_0}. \tag{I.44}$$

The progress variable $c$ is defined as a normalized product mass fraction [34]:

$$c = \frac{Y_P}{Y_P^{eq}} \tag{I.45}$$

Where $Y_P$ is the mass fraction of productions.

It is possible to make combinations between the chemical species:

$$c = \frac{Y_{P1} + Y_{P2}}{Y_{P1}^{eq} + Y_{P2}^{eq}} \tag{I.46}$$

The transport equation gives the progress variable $c$ may be in the form [45,49]:

$$\frac{\partial}{\partial t}\rho c + \frac{\partial}{\partial x_i}(\rho u_i c) = \frac{\partial}{\partial x_i}(\rho \alpha_c \frac{\partial}{\partial x_i} c) + \rho \omega_c. \tag{I.47}$$

Where: $i=1, 2, 3$

### I.2.4 Probability Density Function (PDF) Methods

The non-premixed modeling approach involves to the solution transport equations for two conserved scalars (the mixture fractions and the progress variable). Equations for individual species are not solved. Instead, species concentrations and temperature are derived from the predicted mixture fraction and progress variable fields, where the uses approaches of the probability density function (PDF) [34].

If we denote that $y$ is the value of composition variable such as mass fraction at a point $x$ and moment $t$ in a turbulent reactive flow .For we give the nature of turbulence ,it is necessary that obtaining the values of $y$ in any point and any moment .But these values are in all probability different .In other words, $y$ is a random variable .It is not possible to predetermine the value of $y$ . However , it possible to ascribe probabilities to its value being in a give interval [43, 50].

The PDF of $y$ is defined by [43]

$$P(y) \equiv \frac{d}{dy} F(y) \tag{I.48}$$

Where $F(y)$ is the probability function and $P(y)$ probability density function. that is $P(y;x,t)dy$ is the possibility to obtain the values included between $y$ and $y + dy$ in point $x$ and moment $t$ [50].

### I.2.5 Fundamental Properties of PDF

In turbulence reactive flow contain N chemical species, we need to consider a set of N composition variables $y \equiv \{y_1, y_2, .....y_N\}$.

The three fundamental properties of PDF as follows:

- Since the probability is nonnegative, then [52,53,44]

$$P(y) \geq 0 \qquad \text{(I.49)}$$

- Since $\lim_{y \to -\infty} F(y) = 0$, and $\lim_{y \to +\infty} F(y) = 1$, then

$$\int_{-\infty}^{+\infty} P(y)dy = 1 \qquad \text{(I.50)}$$

Where, the integration $dy = dy_1 dy_2 .....dy_N$ is over the whole of composition space [46].

If $1 \geq y \geq 0$ then[35,53]

$$\int_0^1 P(y)dy = 1 \qquad \text{(I.51)}$$

- For any function $Q(y)$ the average is writes by the following relationship [51].

$$\overline{Q} = <Q> = \int_{-\infty}^{+\infty} P(y)Q(y)dy \qquad \text{(I.52)}$$

If the PDF is known, the mathematical expectation and the math central of any function of the random variable can be calculated. In particular the mean $\overline{y}$ and the math central $\overline{y^{"2}}$ can be determined.

If the composition variables are $y$, the density is given by the function $\rho_N(y)$ which can be determined by thermodynamic. The mean density by ( Eq I.49) is [52,44]:

$$\overline{\rho} = <\rho(x,t)> = \int P(y;x,t)\rho(y)dy \qquad \text{(I.53)}$$

Where the integration occurs on all values of the set $y$.

In variable density flow, the use of Favre average has advantages both theoretically and practically. Favre average for any function $Q(y)$ are defined by:

$$\tilde{Q} = \frac{\overline{\rho Q}}{\overline{\rho}} = \int_{-\infty}^{+\infty} Q(y)P(y)dy \qquad \text{(I.54)}$$

The Favre average for probability density function can be defined by:

$$\tilde{P}(y) = \rho(y)P(y)/\bar{\rho} \qquad \text{(I.55)}$$

One of the objectives of the models of turbulent combustion is to determine the average production rate generated by the chemical reactions. Because of strong not linearity of the rates production (or destruction) of the various species, the estimate of the average rate of chemical production is not direct and must be based on a phenomenological approach. We will use a progress variable of reaction *c* defined such that it is zero (*c*= 0) in gases fresh and equal to the unit (*c*= 1) in burnt gases. The fraction of mixture Z introduced here is zero (Z=0) in oxidant pure and equal to the unit (Z=1) in pure fuel [34,47,51].

Statistical properties of the scalar fields, in a point of the flow (averages, variances…), can be deduced from the probability density function (PDF). The utilization of PDF method makes it possible to obtain the statistical properties of intermediate states in other words in the forehead of flame[45,29].

$$\bar{y} = \int_0^1 yP(y;x,t)dy \quad \text{and} \quad \overline{y''^2} = \int_0^1 (y-\bar{y})^2 P(y;x,t)dy \; . \qquad \text{(I .56)}$$

It may be noted that Klimenko and Bilger proposed the use closings for these averages, this seems step suitable for the non-premixed flames since the chemical reaction occurs preferentially adjacent the stoechiometric conditions [45,53].

## Conclusion

The objective of this chapter is to treat the turbulent non-premixed combustion, by the LES-WALE turbulence model characterized by:

- This is the most suitable for complex geometries and 3D turbulent flow.
- Its good accuracy compared to other models when considering different lengths scales.
- Less number equations comparatively to other models.
- Independence of the semi-empirical constants.
- The ability to calculate the dynamic parameters far or close to solid walls.
- His performance in reactive flows and exothermic flows. In addition, this coupling with combustion models.

For evaluate the composition variable of combustion such as mass fraction of species or temperature in turbulence reactive flow, we use the probability density function approach because these parameters is random variable. The advantage of this method is the reduction of

the governing equations number which representing the evolution of aerothermochemistry phenomenon,

# *Chapter II*

# *Numerical Modeling for non-premixed combustion using FLUENT-CFD*

In this chapter, the numerical models described previously in chapter 1 are uses for a numerical simulation of cylindrical combustion chamber fueled by $C_3H_8$ -$H_2$/Air. This study is focused on non-premixed turbulent combustion in three dimensions numerical simulation this In order to predict the field of temperature , velocity and mass fraction of carbon monoxide (CO) in the all regions of the burner , we select the simulation using new coupling models LES/PDF in the FLUENT code. So, the FLUENT-CFD is a computational fluid dynamics commercial software program that is used in the research and industrial communities. Indeed, we use it to resolve the governing equations: heat transfer, chemical reaction and fluid dynamics. Moreover, the difficult of the analytic solution, we need to exploit the numerical model including in the software package FLUENT. Where, the ability to couple chemical kinetics and fluid dynamics .The objective of this chapter is to demonstrate the main steps to realize the non-premixed combustion using numerical simulations Fluent-CFD Software.

## II.1 Computational Fluid Dynamics (CFD)

The precise analysis of combustion phenomena by numerical simulation is now a reality. "The CFD" is a powerful and reliable tool for design and prediction of mean axial velocity, Fluid flow is mathematically described by differential equations representing the laws of physics and thermodynamics (conservation of mass, conservation of momentum, energy conservation ). This set of equations represents the exact behavior of the fluid whereas they are too complex[54].

## II.2 FLUENT_CFD Models

The study of 3D turbulent combustion (C3H8 or H2 /air) is difficult, because of many complex phenomenons , such as:

- Complex chemical reactions to the presence of different chemical elements.
- High temperature inside the combustion chamber.
- Stochastic processes, heat transfer, high viscosity in the boundary layers, dissipate energy,……
- Complex geometry of the combustion chamber in many industries.

All these problems lead to the difficulty of the mathematical solution to the Navi-Stokes equations previously mentioned for the gaseous phase (conservation of mass equation ,momentum, energy), which describes this flow burning, for these reasons we chose numerical simulation using fluent software to overcome these difficulties.

A combustor simulation is modeled using the Probability Density Function model. The reaction can be modeled using either the species transport model or the non-premixed combustion model. In this work we will solve a natural gas and hydrogen combustion problem using the non-premixed combustion model for the reaction chemistry.

The non-premixed combustion model uses a modeling approach that solves transport equations for conserved scalars (the mixture fractions and progress variable). Multiple chemical species, including intermediate species, may be included in the problem definition. Their concentrations and temperature will be derived from the predicted progress variable and mixture fraction distribution [55].

## II.3 Setups and Solution

### Step 1 : starting FLUENT

1.Start the version of FLUENT three-dimension double precision (3ddp).


***Figure II.1 :*** *Window starting FLUENT version.*

### Step 2 : Meshing

1. Read the mesh ( Name.msh)

**File → Read → Case**

2. Check the grid

**Grid → Check**

3.Scal the grid

**Grid → scale**

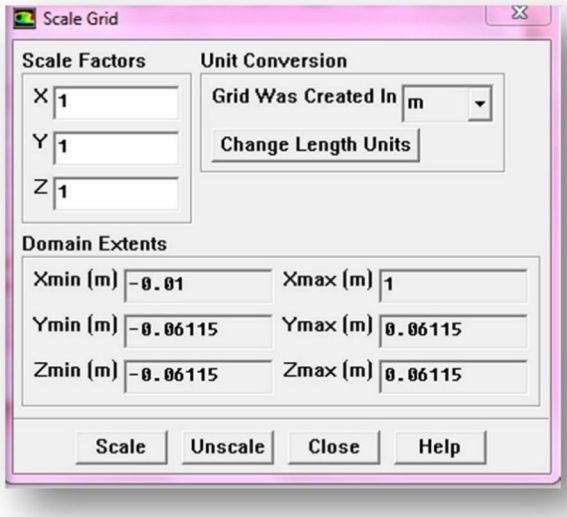



***Figure II.2 :****Scaling the grid.*

* Select m (meters) from the Grid Was Created in drop-down list in the Unit Conversion group box.
* Click Change Length Units.
* Click Scale to scale the grid.
* Close the Scale Grid panel

4. Display of grid

**Display → Grid**

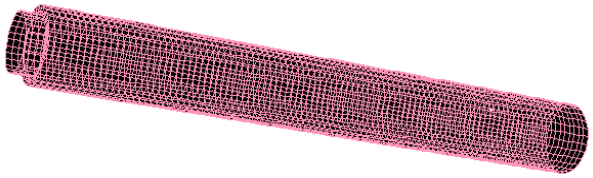


***Figure II.3 :****Grid display.*

**Step 3: Definition of models**

1. Change the spatial definition to 3D.

**Define → Models → Solver**

*Retain the default selection of Pressure Based in the Solver list (The non-premixed combustion model is available only with the pressure-based solver).

* Select 3D in the Space list.

* Click OK to close the Solver panel.

2. Enable the Energy Equation.

**Define → Models→ Energy**

Since heat transfer occurs in the system considered here, we will have to solve the energy equation.

3.Select the standard LES turbulence model.

**Define → Models→ Viscous**

* Select Large Eddy Simulation from the Model list.

* Retain all other default settings.

* Click OK to close the Viscous Model panel.

4. Select the P1 radiation model.

**Define → Models→ Radiation**

*Select P1 from the Model list.

* Click OK to close the Radiation Model panel.

5.Select the Non-Premixed Combustion model.

**Define → Models → Species → Transport & Reaction**

* Select Non-Premixed Combustion from the Model list.

When we use the non-premixed combustion model, we need to create a PDF table. This table contains information on the thermo-chemistry and its interaction with turbulence.

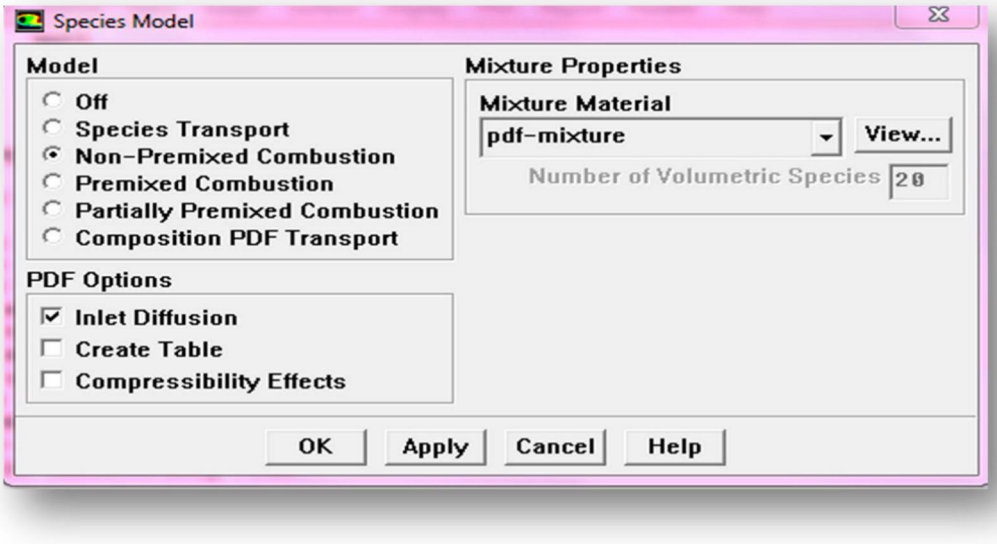



***Figure II.4 :*** *Definition of Transport & Reaction model.*

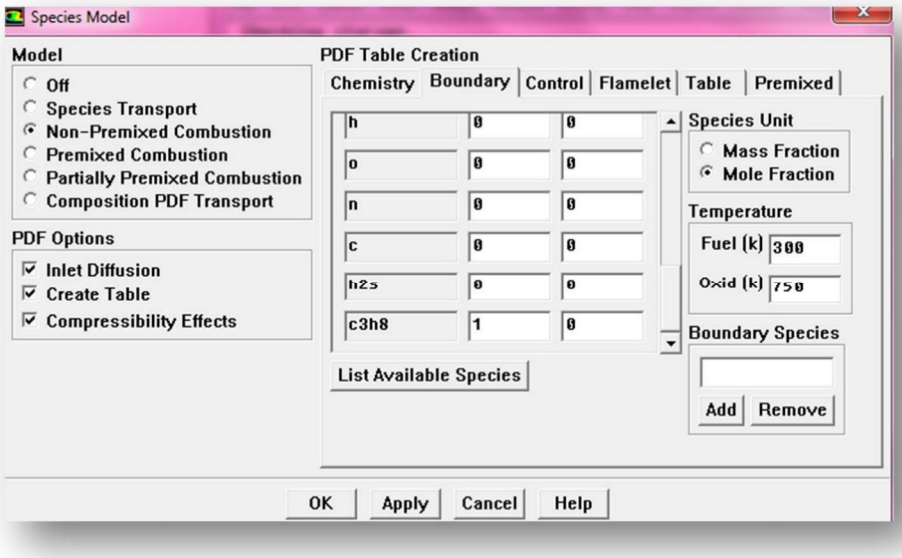
**Step 4: Non Adiabatic PDF Table**

1. Enable the Create Table option, in the PDF Options group box of the Species Model panel.
2. Click the Chemistry tab to define chemistry models.

3. Click the Boundary tab to add and define the boundary species.

* Select Mole Fraction from the Species Units list.

* Enter the rate of $c_3H_8$




***FigureII.5:****Creating the PDF table.*

* Click apply.

5. Click the Table tab to specify the table parameters and calculate the PDF table.

* Click Apply.

* Click Calculate PDF Table to compute the non-adiabatic PDF table.

* Click the Display PDF Table button to open the PDF Table panel.

* Click the Display button.

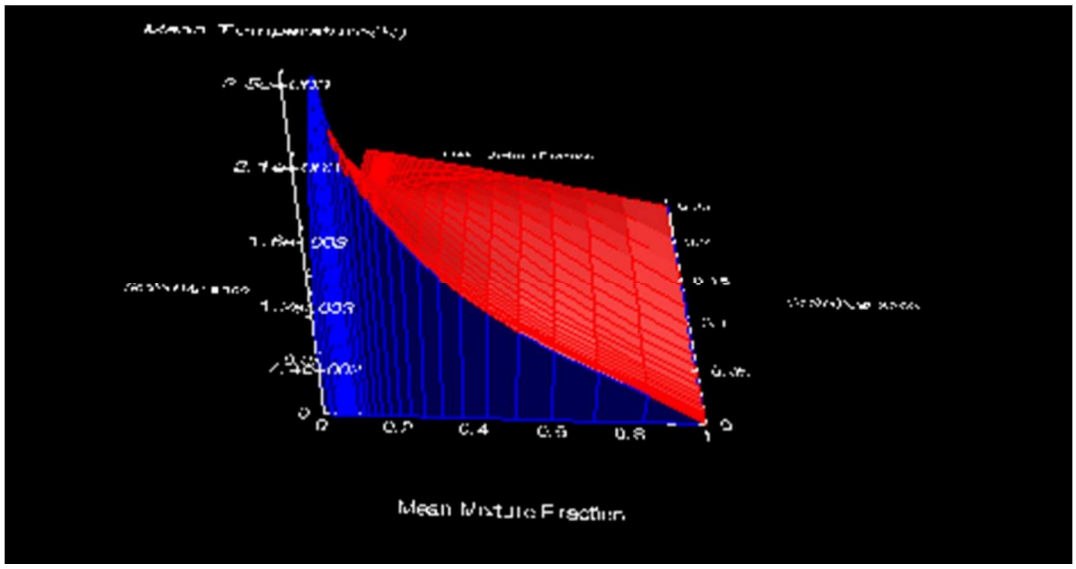



***Figure II.6 :*** *Mean temperature as function for average mixture fraction.*

6. Save the PDF output file (Name.pdf).

**File → Write → PDF.**

7. Click OK to close the Species Model panel.

**Step 5: Materials**

All thermodynamic data including density, specific heat, and the formation enthalpies are extracted from the chemical database when the non-premixed combustion model is used. These properties are transferred as the pdf-mixture material, for which only transport properties, such as viscosity and thermal conductivity, need to be defined.

**Define → Materials**

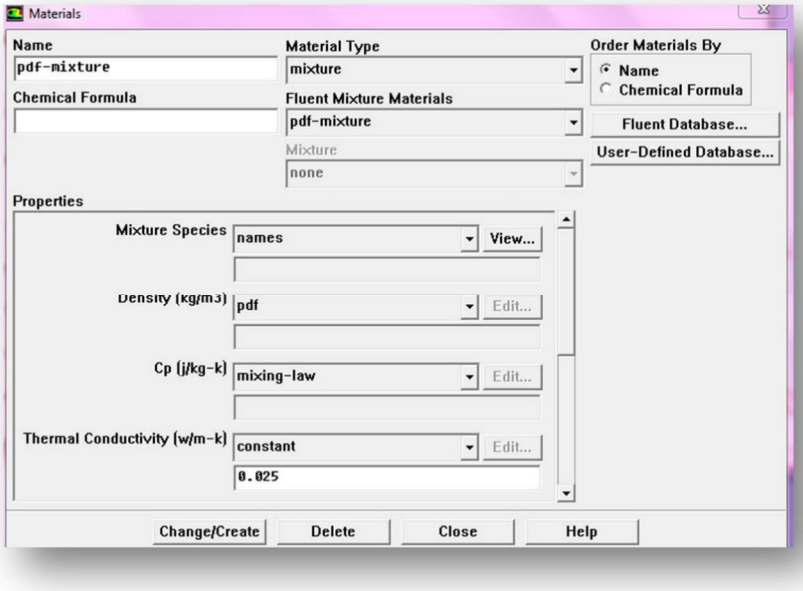



***Figure II.7 :*** *Materials definition.*

**Step 5: The boundary conditions**

1.Define the boundary conditions for the zones.

**Define → Boundary Conditions**

2. Set the boundary conditions for velocity inlet ( velocity-$c_3H_8$).

* Enter 0.9287 m/s for the Magnitude Velocity of $C_3H_8$.

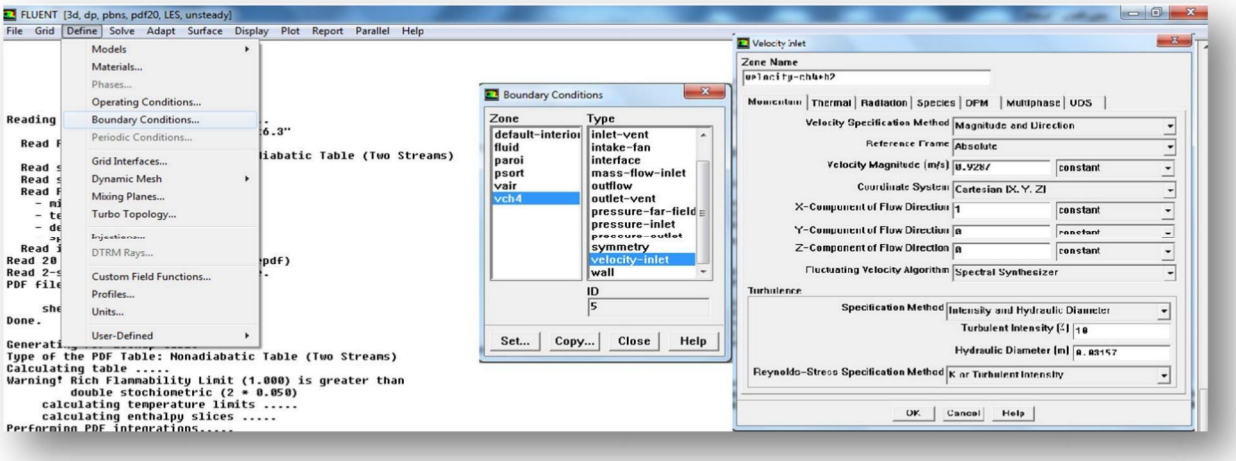



***Figure II.8 :*** *Definition of boundary condition.*

2. Set the boundary conditions for the velocity inlet (air-velocity).

* Enter 20.63 m/s for the Magnitude Velocity of air.

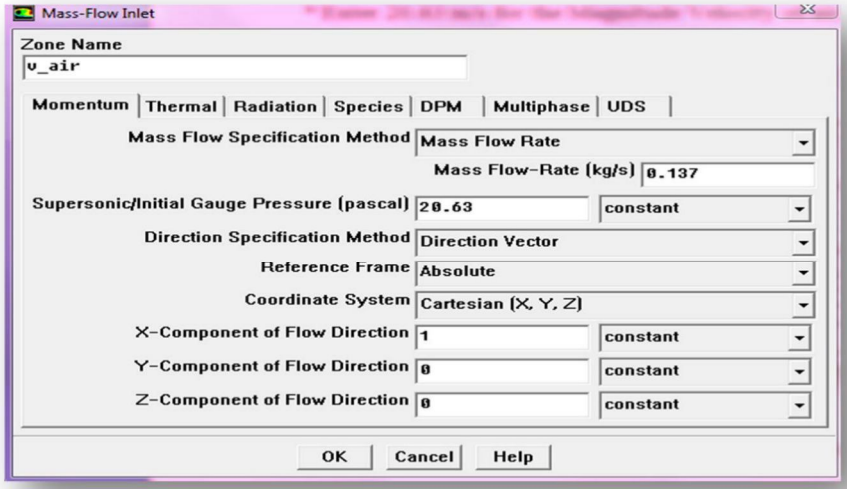



***Figure II.9 :*** *Boundary conditions of the velocity inlet.*

3. Set the boundary conditions for walls.

* Click the Thermal tab.

* Select Temperature from the Thermal Conditions list.

* Enter 500 K for Temperature.

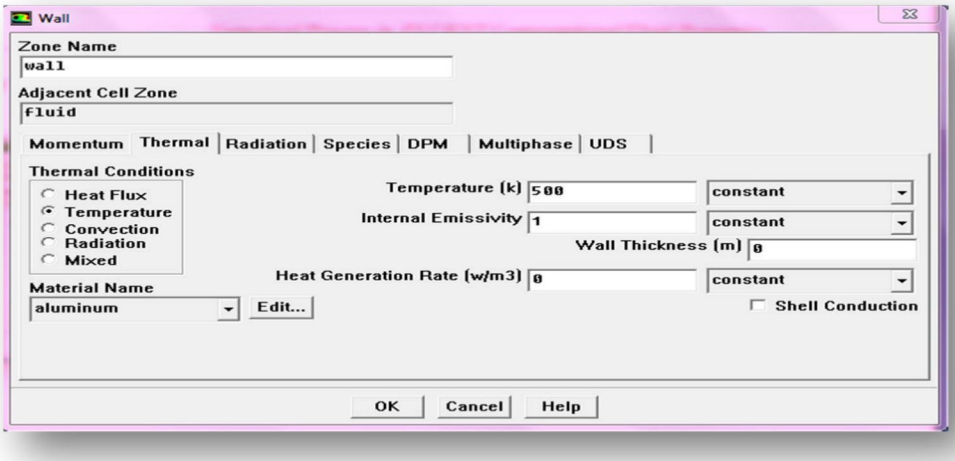



***Figure II.10 :*** *Boundary conditions of wall temperature.*

## Step 6: Solution

1. Set the solution control parameters.

**Solve →Controls→ Solution**

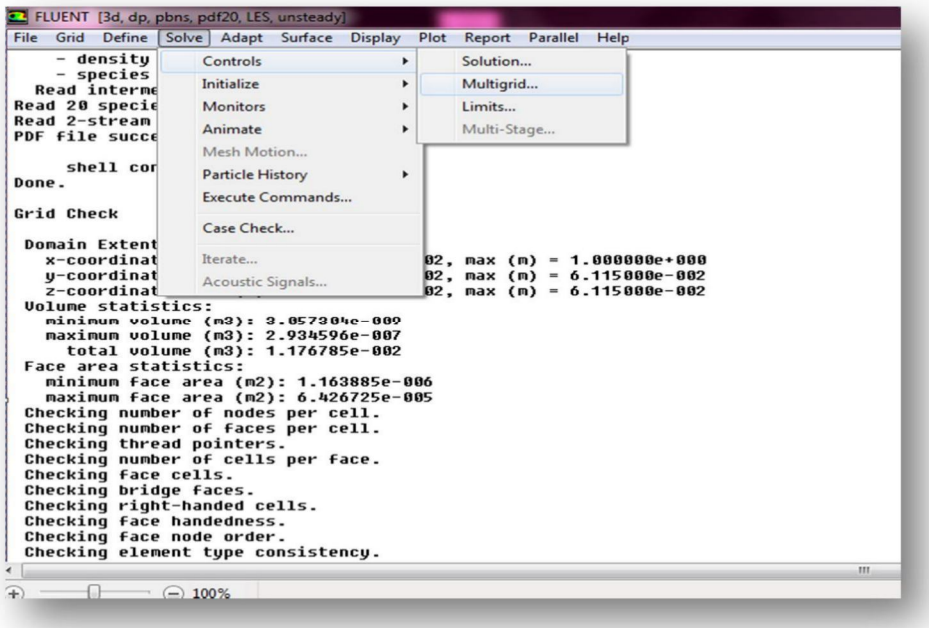



***Figure II.11 :*** *Solution.*

2. Initialize the calculations use the condition at **velocity air**.

**Solve → Initialize → Initialize**

* Select **vair** from the Compute From drop-down list.

* Enter 20.63 m/s for the X Velocity.

* Enter 750 K for the Temperature.

* Click **Init** and close the Solution Initialization panel.

3. Enable the display of residuals during the solution process.

**Solve → Monitors→ Residual**

4. Save the case file (Name .cas)

**File →Write →Case**

5.Start calculations after choosing the number of iterance (in our case we choose 2000 iterations) .

**Solve → Iterate**

**6.** Save the data file (Name.dat).

**File → Write → Data**

## Step 7: processing the results

1.Display the predicted temperature or concentration of CO field

**Display → contours**

**a)Temperature**

* Select Temperature and Total Temperature from the Contours of drop-down lists.

* Click Display.

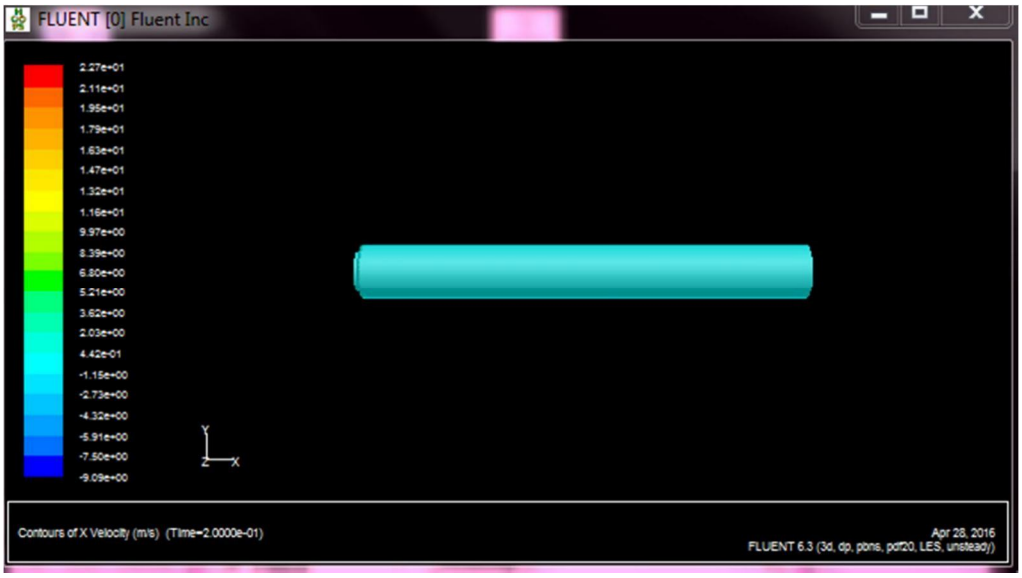



***Figure II.12 :*** *Total temperature contours.*

**b) CO Mass fraction**

*Select Species... and Mass fraction of CO from the Contours of drop-down lists in the Contours panel.

*Click Display.


***Figure II.13 :*** *CO Mass Fraction Contours.*

1.Drawing the graphs

**a)Temperature**

* Select Temperature and Total Temperature from the Solution XY plot of drop-down lists.

* Click plot.

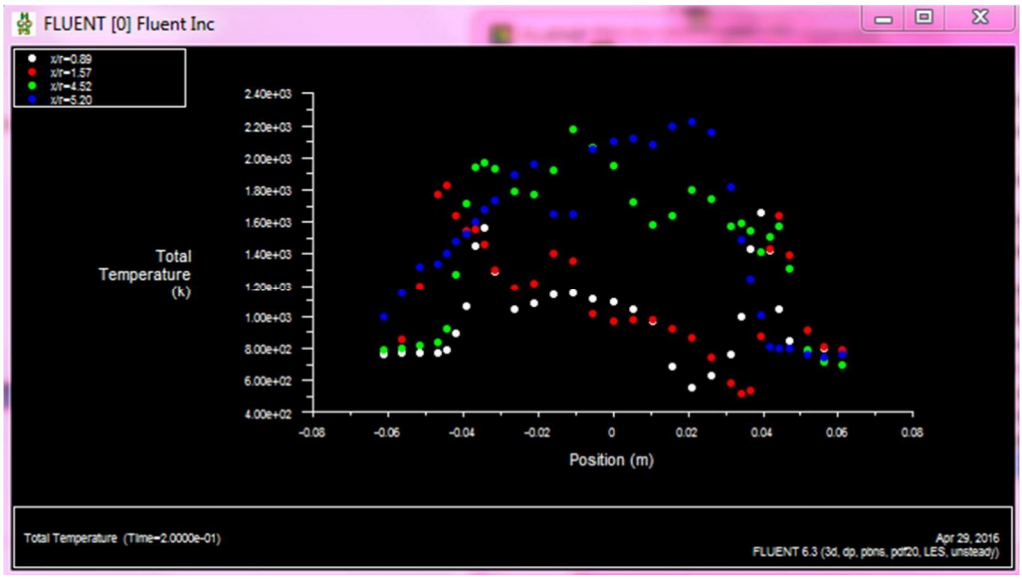



***Figure II.14 :****Radial distribution of total temperature in position X/R=0.89, X/R=1.57, X/R=4.52 and X/R=5.20.*

**b) CO Mass fraction**

* Select Species... and Mass fraction of CO from the Solution XY plot of drop-down lists.

* Click plot.

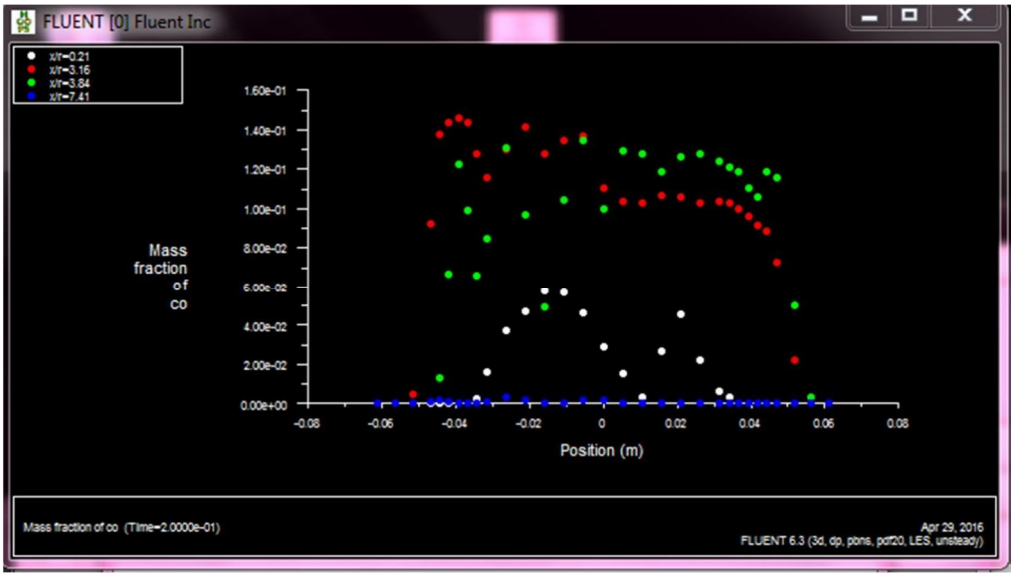



***Figure II.15 :*** *Radial distribution of CO mass fraction in position x/R=0.21, x/R=3.16 , x/R=3.84 and x/R−7.41*

## Conclusion

In order to know the influence of hydrogen addition for non-premixed combustion ; on temperature and formation of carbon monoxide in the combustion chamber have a cylindrical form we used the FLUENT 6.3 code. Because this later treat the combustion problem in three dimension and have two models LES and PDF, which use for solution the governing equation of combustion. Also we explained in this chapter the main steps that must be followed in FLUENT6.3 code in order to find the temperature field and mass fraction of carbon monoxide in the burner.

After illustrate the main steps to realise the computation in FLUENT-CFD program, the results obtained will be discussed in the next chapter

*chapter III*

# *Application of Non-Premixed Combustion of Propane and Hydrogen*

In this chapter we illustrate and discuss the temperature and carbon mass fraction, results obtained by the simulation Combustion is not mixed hydrogen and propane in cylindrical burner The simulation was performed using the LES dynamic model based on PDF thermochemical approach by FLUENT-CFD code.

## III .1 Description of the combustion chamber

The configuration of the two coaxial jets that confine the combustor is given in figure III .1Where it was the focus of numerous experimental investigations because of its relatively simple geometry and its similarity to gas turbine burner [57,58]. Thereby, we investigated the numerical validation of the LES/PDF coupled models with the experimental data, to study the behavior of the non-premixed combustion fueled by mixture of $C_3H_8$ and $H_2$. Whereas, the study consists of three main parameters: mean axial velocity, mean temperature and mean mass fraction of Carbone monoxide. The cylindrical combustion chamber is of ray $R_4$=0.06115m and L=1m in length supplied by two coaxial jets, the central one has an internal ray $R_1$=0.03157 m and an external $R_2$=0.03175 m, which injects the methane with inlet mass flow rate and temperature respectively $Q_1$=0.0072 kg/s and $T_1$=300K. The annular one has an internal ray $R_3$= 0.04685m, that injects the air with an inlet mass flow rate $Q_2$=0.137 kg/s and preheated at a temperature $T_2$=750K. The combustion chamber is pressurized to 3.8atm and has a constant temperature wall of $T_{wall}$=500K [57,58].

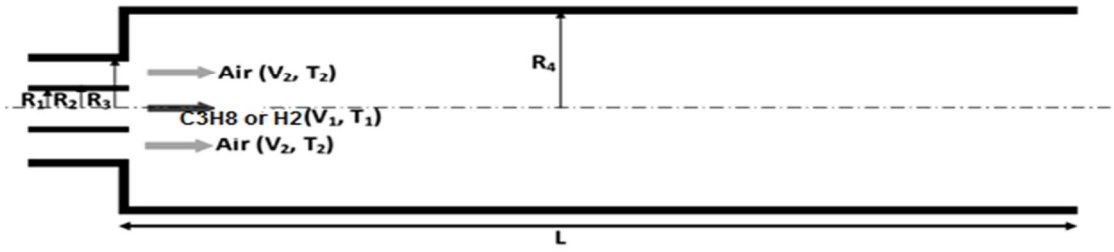



***Figure III.1:*** *Schematic of the burner.*

The present numerical study investigates Three dimension (3D) cylindrical burner. Where, the grid used for all the simulations is performed by Gambit. Therefore, the selected meshes are of parallelepipeds type; the grid is smooth and refined for both nearly solid boundaries of the burner and in the longitudinal direction in the level of interaction of air and fuel, to accommodate more information in

the solid boundary and the flame zone. The volume contains approximately 40.000 cells, the size of a cell ranges from 3.62e-07 $m^2$ to 7.57e-05 $m^2$.

## III.2 The Governing Equations

The turbulent combustion can be written in Cartesian coordinates as [43-56]:

Mass: $$\frac{\partial \overline{\rho}}{\partial t}+\frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i)=0 \qquad \text{(III.1)}$$

Momentum: $$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t}+\frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j)=-\frac{\partial}{\partial x_i}[\overline{\rho}(\overline{u_i u_j}-\widetilde{u}_i\widetilde{u}_j)]-\frac{\partial \overline{p}}{\partial x_j}+\frac{\partial \overline{\tau_{ij}}}{\partial x_i} \qquad \text{(III.2)}$$

Mixture fraction: $$\frac{\partial}{\partial t}\overline{\rho}\widetilde{Z}+\frac{\partial}{\partial x_i}(\overline{\rho u_i}\widetilde{Z})=\frac{\partial}{\partial x_i}(\overline{\rho\alpha_c}\frac{\partial}{\partial x_i}\widetilde{Z}) \qquad \text{(III.3)}$$

Progress variable: $$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t}+\frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{c})=-\frac{\partial}{\partial x_i}\tau_c+\frac{\partial}{\partial x_i}.(\overline{\rho}\alpha_c\frac{\partial}{\partial x_i}\widetilde{c})+\overline{\rho\dot{\omega}_c} \qquad \text{(III.4)}$$

Thermodynamic state: $$\overline{p}=\overline{\rho}R\widetilde{T} \qquad \text{(III.5)}$$

Where:

*i=1, 2, 3* and *j=1, 2, 3*

- Unresolved Reynolds stresses $(\overline{u_i u_j}-\widetilde{u}_i\widetilde{u}_j)$, requiring a subgrid scale turbulence model.
- Unresolved species fluxes $(\overline{u_i Y_f}-\widetilde{u}_i\widetilde{Y}_f)$ and enthalpy fluxes $(\overline{u_i h}-\widetilde{u}_i\widetilde{h})$ requiring a probability density function (PDF) approach.
- Filtered chemical reaction rate $\overline{\dot{\omega}}_f$.

## III.3 Experimental Configuration and Application Domain

The configuration of the two coaxial jets confined within the combustor is given in figure III .1. It was the focus of numerous investigations because of its relatively simple geometry and its similarity to power plant burner [57,58]. The cylindrical combustion chamber is of ray $R_4$=0.06115m and L=1m in length supplied by two coaxial jets, the central one has an internal ray $R_1$=0.03157 m and an external $R_2$=0.03175 m, which injects the methane with inlet mass flow rate and temperature respectively $Q_1$=0.0072 kg/s and $T_1$=300K. The annular one has an internal ray $R_3$= 0.04685m, that injects the air with an inlet mass flow rate $Q_2$=0.137 kg/s and preheated at a temperature $T_2$=750K. The combustion chamber is pressurized to 3.8atm and has a constant temperature wall of $T_{wall}$=500K [57,58].

## III .4 Results and Discussion

We begin with the validation of the coupled models described previously with the experimental data [58]. After that, the same parameters used for the validation are used also to control the flame behavior supplied by the $H_2$ or $c_3H_8$ fuels. Moreover, the presentation and comparison of results are based on normalizing length and velocity by using, respectively, the injector radius ($R \equiv R_3$) and the inlet bulk velocity of the air ($U \equiv V_2$).

### III .4 .1 Mass Fraction of Carbon monoxide CO

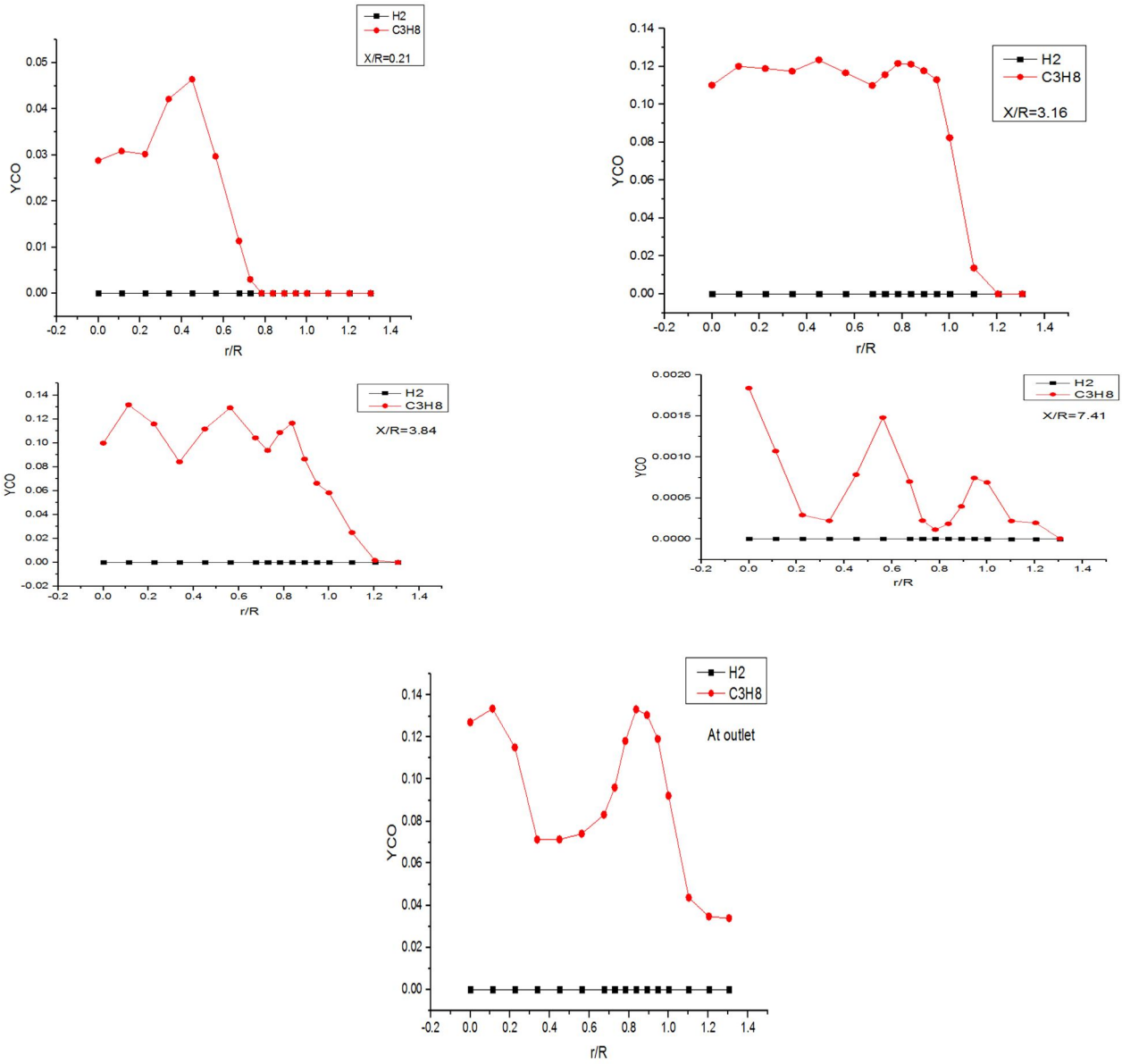



***Figure III.2:*** curves comparison between quantity of CO from burning fuel Propane and hydrogen fuel.

the data turned out that the value of CO hydrogen fuel is much less (almost non-existent) of its value for the fuel propane, where the distance between the two curves in the range of 92%, when the first leg ( at the beginning of the combustion chamber) have low CO value and is highest peak for CO for propane fuel when Yco=0.13 then decreases to be absent in the mid the radius of the combustion chamber

### III .4 .2 Temperature

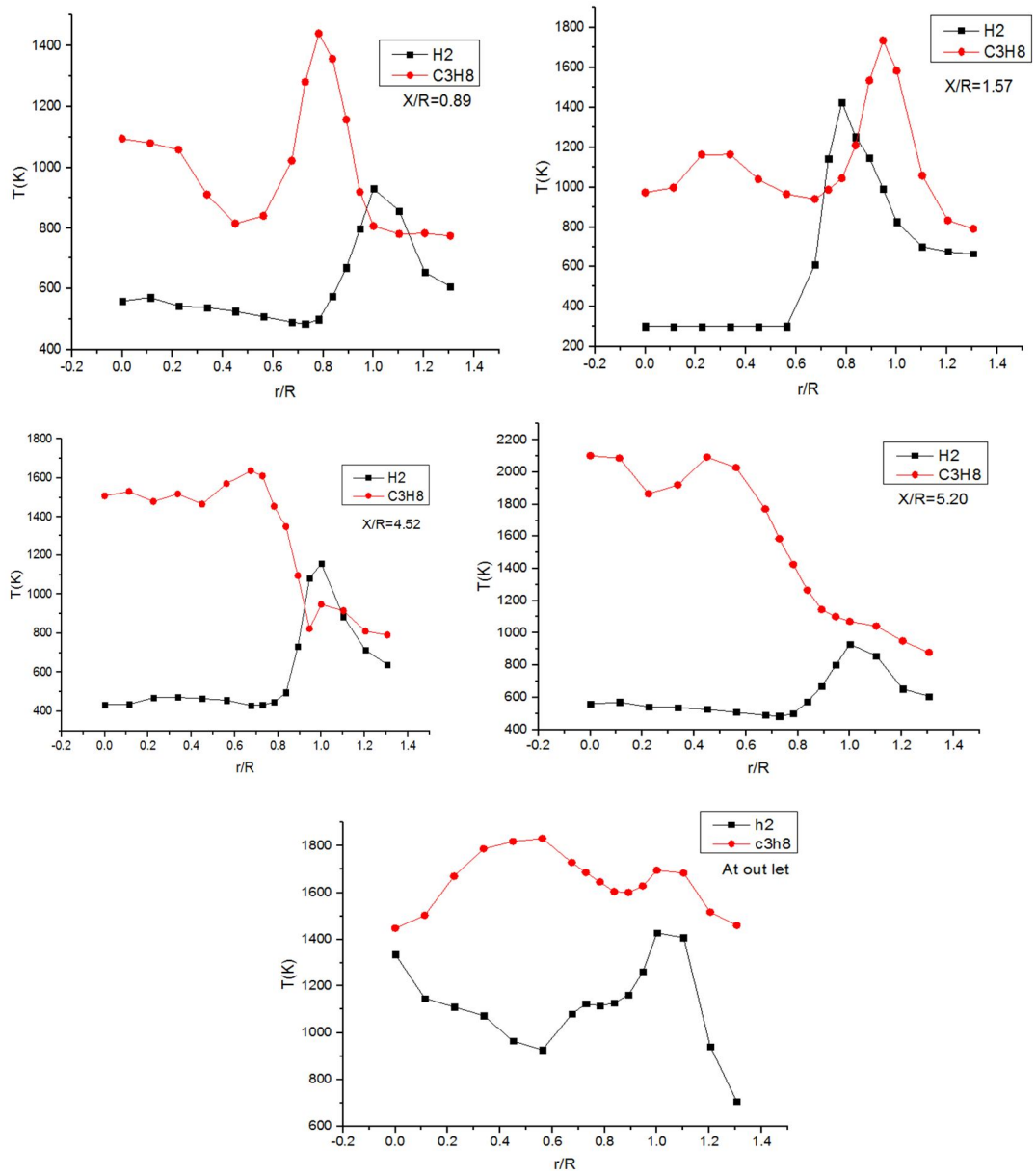



***Figure III.3:***a comparison between the temperatures of fuel $C_3H_8$ and hydrogen fuel

Curves showing a comparison between the temperatures $C_3H_8$and hydrogen where the highest value in the fourth leg of the temperature amounting 2100K, All curves peak in the flame districts decreasing when the wall of the combustion chamber, Because the flame zone is the chemical reaction of fuel with air districts is also considered these interactions publisher of heat, to disappear this summit and diminish their value. This is due to move away from the combustion zone When Which move away from the flame zone, the temperature stabilizes at close values lower than the previous stations to the values of this region and containing the

combustion gases . Explain the high degree of fuel propane heat in the various stations, compared with hydrogen fuel

### III .4 .3 Velocity Field

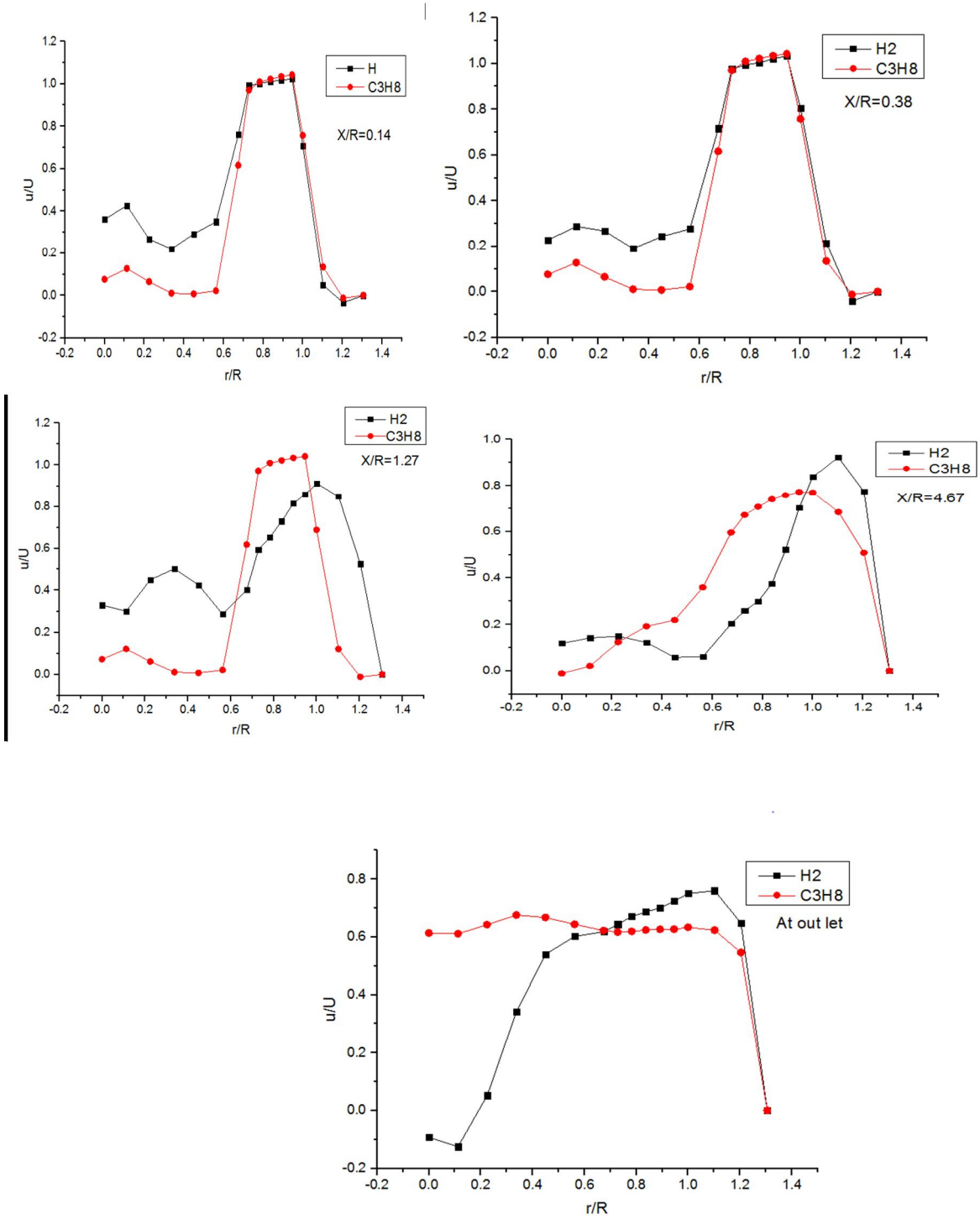



***Figure III.4:***Shown comparison between the velocities of propane and hydrogen at different stations inside the chamber

We can see in this figure the comparison between the speeds of the propane and hydrogen in different steps inside the combustion chamber. We can observe that the curves of the two combustibles have almost the same shape. The curves shows too that they have a peak in the flame zone. This peak equal one (U=1). We can also see negative values for this two curves in the upper and lower turbulence zones and the alimentation combustible zone of the combustion chamber. Then, this values cancel in the fourth and the fifth station; this is due to the distance of the flame zone. We observe that the speed of the Hydrogen is greater in percentage than the speed of the Propane; because the mass of the Hydrogen is lower than that Propane. The consequence is that the gas speeds are greater in the same quantities of flow for the two combustibles.

## Conclusion

After comparing the combustion of propane and hydrogen we found that the:

- The emission of carbon monoxide Non-existent for hydrogen combustion in the combustion chamber of all stations , but exists for Propane .
- High degree of fuel propane temperature in different stations, compared with hydrogen fuel .
- Hydrogen is faster than propane.

Through these results we conclude that the hydrogen fuel is better than propane, which is clean and is not harmful for Environment

# *General Conclusion*

# Conclusion

Hydrogen is the simplest element. An atom of hydrogen consists of only one proton and one electron. It's also the most plentiful element in the universe. Despite its simplicity and abundance, hydrogen doesn't occur naturally as a gas on the Earth it's always combined with other elements. Water, for example, is a combination of hydrogen and oxygen ($H_2O$). Hydrogen is also found in many organic compounds, notably the *hydrocarbons* that make up many of our fuels, such as gasoline, natural gas, methanol, and propane. Hydrogen can be separated from hydrocarbons through the application of heat - a process known asreforming. Currently, most hydrogen is made this way from natural gas. An electrical current can also be used to separate water into its components of oxygen and hydrogen. This process is known as *electrolysis*. Some algae and bacteria, using sunlight as their energy source, even give off hydrogen under certain conditions. Hydrogen is high in energy, yet an engine that burns pure hydrogen produces almost no pollution.. Hydrogen fuel cells power the shuttle's electrical systems, producing a clean byproduct - pure water, which the crew drinks. A fuel cell combines hydrogen and oxygen to produce electricity, heat, and water. Fuel cells are often compared to batteries. Both convert the energy produced by a chemical reaction into usable electric power. However, the fuel cell will produce electricity as long as fuel (hydrogen) is supplied, never losing its charge.

In the present work, a study simulation Hydrogen and propane combustion both separately into the combustion chamber So, We have used FLUENT-CFD in numerical computation based on aerothermochemical equations for the control of the velocity field, temperature field and the carbon mass fraction distribution, where the calculations are carried out by FLUENT-CFD coude. Moreover, we used for these objective mathematical models, especially LES for dynamic parameters and PDF for thermochemical in order to reduce the number of equations. Finely, we conclude with main results obtained in this study:

- The emission of carbon monoxide Non-existent for hydrogen combustion in the combustion chamber of all stations , but exists for Propane .
- High degree of fuel propane temperature in different stations, compared with hydrogen fuel .
- Hydrogen is faster than propane.

Through these results we conclude that the hydrogen fuel is better than propane, which is clean and is not harmful for Environment

In the future, this study can interest in evaluating the rate of entropy generation produced by combustion in ORACLES burner supplied by C3H8 / H2. This configuration is similar to the combustion chamber of a gas turbine. For, the simulation we can based on the dynamic model (LES) coupled with themochemical model (PDF), using FLUENT-CFD. Then, we exploit those parameters for estimate generation of entropy by friction and by heat transfer.

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**ملخص**

**في هذا العمل قمنا بمحاكاة عددية لاحتراق غاز الهيدروجين وغاز البروبان داخل غرف الاحتراق باستخدام برنامج FLUENT-CFD, وذلك بهدف إيجاد الخصائص الكيميوحرارية والديناميكية أثناء الاحتراق. نستخدم لهذا الغرض عدة نماذج رياضية خاصة لمعالجة هذه المسالة وقد اخترنا في هذه الدراسة نموذجي LES و PDF. اللذان أثبتت كفاءتهما في دراسة الاحتراق من خلال دراسات سابقة وبعد مقارنة احتراق الهيدروجين و البروبان وجدنا أن الهيدروجين هو أفضل غاز للاحتراق لأنه غير مضر للبيئة.**

***كلمات مفتاحية: الاضطراب, نموذجي LES و PDF, الاحتراق غير الممزوج, محاكاة CFD.***

## Abstract

In this work, we simulated numerical combustion of hydrogen gas and propane gas inside the combustion chambers using FLUENT-CFD program. The aim is finding thermochemical and dynamic characteristics which occur during combustion. We use for this several special mathematical models intended to address this issue, we have chosen in this study two models: LES and PDF. They proved their efficiency in the previous studies of combustion through, after comparing hydrogen and propane combustion we have found that hydrogen is the best gas for combustion because it is not harmful to the environment.

***Keywords:*** *Turbulence, LES and PDF Model s, Non Premixed combustion, CFD.*

## Résumé

Dans ce travail, nous avons simulé la combustion numérique de gaz d'hydrogène et de gaz de propane à l'intérieur des chambres de combustion à l'aide de programme CFD-FLUENT. L'objectif est de trouver des caractéristiques thermochimiques et dynamiques qui se produisent lors de la combustion. Nous utilisons pour cela plusieurs modèles mathématiques spéciales destinées à résoudre ce problème, nous avons choisi dans cette étude deux modèles: LES et PDF. Ils ont prouvé leur efficacité dans les études précédentes de combustion à travers, après avoir comparé l'hydrogène et le propane combustion, nous avons constaté que l'hydrogène est le meilleur gaz pour la combustion, car il ne nuit pas à l'environnement.

***Mots-clés:*** *Turbulence, Couplage LES/PDF, Combustion no prémélangée, Simulation numérique.*