IJARSCT
ISSN (Online) 2581-9429
International Journal of Advanced Research in Science, Communication and Technology (IJARSCT)
Volume 2, Issue 7, June 2022
Impact Factor: 6.252

A Review of Non-Premixed Combustion Models: Study and Comparison

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Abstract:*The present work gives information about development in field of non-premixed combustion focusing on various models developed for non-premixed combustion. Key aspects of non-premixed combustion such as ignition, extinction and lift-off are first analysed and then summarised. The review also outlines the various CFD modelling approaches that have been carried out for validating the result that has been experimentally found out. This study will help in understanding the modelling of non-premixed combustion.*

Keywords: Fatigue Life, Resistance Spot Welding, Finite Element Analysis, etc.

I. INTRODUCTION

Combustion is important in many engineering applications; combustion of hydrocarbons is still by far the most common source of energy in the world. Computational fluid dynamics (CFD) is to predict the fluid behavior numerically such as the motion of fluids when they are mixed with each other. There has been a drastically increase in use of computation-based tools to model industrial processes within the chemical, metallurgical, and power generation industries. Combustion problems involve a series of coupled phenomena, such as fluid dynamics, heat transfer and chemical kinetics of gaseous species and soot. Chemical reactions directly affect the temperature and chemical species fields and, therefore, the heat transfer, which is interdependent with the temperature. Therefore, an accurate description of the chemical reactions and the heat transfer mechanisms is of great importance for simulations of combustion systems.

On the other hand, within the realm of Reynolds Average Navier–Stokes (RANS) models, modeling chemical kinetics is a difficult task due to the highly nonlinear dependence of average reaction rates on the fluctuating temperature and species fields. Eaton et al. (1999) provided a comprehensive revision of the commonly used Computational Fluid Dynamics (CFD) models for non-premixed combustion. The models are generally based on the conservation equations of mass, momentum, energy and chemical species, while the problem closure is achieved by turbulence models such as the k-ε (Launder and Sharma, 1974; Launder and Spalding, 1972) or the k-ω (Wilcox, 1988).

Several combustion models are available, such as the Arrhenius finite-rates, the Eddy Dissipation Concept (Magnussen and Hjertager, 1976), the Eddy Break-Up (EBU) (Spalding, 1971), or a combination of some of these models, such as the EBU/Arrhenius. The more recent flamelet-based models (Liew et al., 1981; Williams, 1975) are also very popular, such as the Steady Laminar Diffusion Flamelet (SLDF) (Peters, 1984, 1986) and the Flamelet-Generated Manifold (Gicquel et al., 2000; Pierce 2001; Pierce and Moin, 2004; Van Oijen and De Goey, 2000, 2004) models, among others.

II. MATHEMATICAL FORMULATION

[1] Mass Conservation

The Continuity equation can be written as

$$\nabla \cdot (\bar{\rho}\ \widetilde{\boldsymbol{u}}) = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where $\bar{\rho}$ means the density of mixture and $\tilde{u}$ is the mean velocity vector.

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Momentum Conservation

The equation of motion for fluid flow is given as

$$\nabla \cdot (\bar{\rho}\tilde{u}\,\tilde{u}) = -\nabla\tilde{p} + \nabla \cdot \left(\mu\left[\nabla\tilde{u} + (\nabla\tilde{u})^T - \frac{2}{3}\nabla\tilde{u}\,I\right] - \mu_t\left[\nabla\tilde{u} + (\nabla\tilde{u})^T\right] - \frac{2}{3}\bar{\rho}\,\tilde{k}I\right), \quad \text{……..(2)}$$

Where $\tilde{p}$ is the time-averaged total pressure, μ is the gaseous mixture dynamic viscosity, t is the eddy viscosity and I is the unity identity tensor?

[2] The $k-\varepsilon$ model

The equations for the mean turbulent kinetic energy, $\tilde{k}$, and its mean dissipation rate, $\tilde{\varepsilon}$, are

$$\nabla \cdot \left(\bar{\rho}\,\tilde{\boldsymbol{u}}\,\tilde{k}\right) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla\tilde{k}\right] + G_k - \bar{\rho}\,\tilde{\varepsilon}$$

and

$$\nabla \cdot (\bar{\rho}\,\tilde{u}\,\tilde{\varepsilon}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\tilde{\varepsilon}\right] + C_{\varepsilon 1}\frac{\tilde{\varepsilon}}{\tilde{k}}G_k - C_{\varepsilon 2}\,\bar{\rho}\,\frac{\tilde{\varepsilon}^2}{\tilde{k}} \quad \text{……..…(3)}$$

Where Gk is the term that controls the generation of the turbulent kinetic energy due to the average velocity gradients, Cε1 and Cε2 are the constants that control the production and destruction of the dissipation rate of the turbulent kinetic energy, respectively, and σk and σε correspond to the turbulent Prandtl numbers to $\tilde{k}$ and $\tilde{\varepsilon}$, respectively. The constants of the model are $C_{\varepsilon_1} = 1.44$ *and* $C_{\varepsilon_2} = 1.92$ found out by experiments.

The term Gk is modeled according to the Boussinesq hypothesis

$G_k = \mu_t * \widetilde{S^2}$……..(4)

Where $\tilde{S}$ is the module of the tensor of the average strain rate, such that

$$\tilde{S} = \sqrt{2 * \widetilde{S_{ij}} * \widetilde{S_{ij}}}$$

$\widetilde{S_{ij}} = \frac{1}{2}[\nabla\tilde{u} + (\nabla\tilde{u})^T]$……(5)

The eddy viscosity, μt , in turn, is calculated by a secondary algebraic expression, combining ~k and ~ε, given by

$$\mu_t = \bar{\rho}\,C_\mu\frac{\tilde{k}^2}{\tilde{\varepsilon}} \quad \text{……(6)}$$

Where Cμ is a constant of the model.

[3] Energy Conservation

Assuming Lewis number to be unity i.e., the thermal diffusivity to be equal to mass diffusivity we obtain the following relation.

$$\nabla \cdot \left(\bar{\rho}\,\tilde{\boldsymbol{u}}\,\tilde{h}\right) = \nabla \cdot \left[\left(\frac{f}{c_p} + \frac{\mu_t}{Pr_t}\right)\nabla\tilde{h}\right] + \tilde{S}_{rad} \quad \text{……..(7)}$$

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Where mean total enthalpy of mixture is

$$\tilde{h} = \sum_{k} \tilde{Y}_k \tilde{h}_k$$

……(8)

The ~Yk and ~hk are the mean average mass fraction and mean total enthalpy of the kth chemical species, f is the thermal conductivity of the mixture, Prt is the turbulent Prandtl number,~Srad represents the source of thermal energy due to the radiative transfer . The term ~hk can be written

$$\tilde{h}_k = \sum_{k=1}^{N_k} \left[\frac{\overline{h_f^0}}{W_k} + \int_{T_{ref}}^{\tilde{T}} c_{p,k}\, d\tilde{T} \right]$$

……...(9)

Where ~T is the mean temperature of the mixture, h0f is the molar enthalpy of formation, Tref is the reference temperature and Wk is the molecular mass of kth chemical species.

[4] Chemical Species Conservation

Chemical Species conservation uses Arrhenius model with the two global chemical reactions involves six species: oxygen, methane, nitrogen, water vapor, carbon dioxide and carbon monoxide. A conservation equation is required for each species, with the exception of the nitrogen, which is computed taking into account that the mass fraction summation must be equal to 1. Thus, assuming unity Lewis number and no thermal diffusion, the conservation equation for the kth chemical species is given by

$$\nabla \cdot \left(\bar{\rho}\, \tilde{u}\, \tilde{Y}_k \right) = \nabla \cdot \left(\bar{\rho}\, \bar{D}_k\, \nabla \tilde{Y}_k + \frac{\mu_t}{Sc_t} \nabla \tilde{Y}_k \right) + \tilde{R}_k$$

……(10)

Where Sct is the turbulent Schmidt number which is defined as the ratio of momentum diffusivity and mass diffusivity and ~Dk and ~Yk are, respectively, the mass diffusivity and the mean mass fraction of the kth chemical species. The term ~Rk is the mean mass rate of formation or destruction of the kth chemical species.

The Non-Premixed Combustion Models

Any commercial simulation software package provides three options for description of the system chemistry when we use the non-premixed modeling approach. These options are:

1. **The Flame Sheet Approximation (Mixed-is-Burned)**

   The simplest reaction scheme is the flame sheet or “mixed-is-burned" approximation. This approach assumes that the chemistry is infinitely fast and irreversible, with fuel and oxidant species never coexisting in space and complete one-step conversion to final products. This description allows species mass fractions to be determined directly from the given reaction stoichiometry, with no reaction rate or chemical equilibrium information required. This simple system description yields straight line relationships between the species mass fractions and the mixture fraction, as shown in Figure1.

   Because no reaction rate or equilibrium calculations are required, the flame sheet approximation is easily computed and yields a rapid calculation. However, the flame sheet model is limited to the prediction of single-step reactions and cannot predict intermediate species formation or dissociation effects. This often results in a serious over prediction of peak flame temperature, especially in those systems that involve very high temperature (e.g., systems using pre-heat or oxygen-enrichment).

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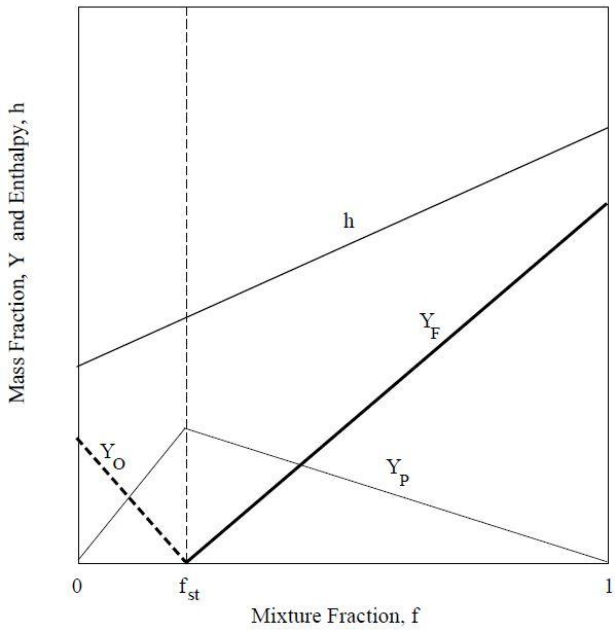

Figure 1: Species Mass Fractions and Enthalpy Derived Using the Flame Sheet Approximation

2. Equilibrium Assumption

The equilibrium model assumes that the chemistry is rapid enough for chemical equilibrium to always exist at the molecular level. An algorithm based on the minimization of Gibbs free energy is used to compute species mole fractions from mixture fraction *f*.

The equilibrium model is powerful since it can predict the formation of intermediate species and it does not require a knowledge of detailed chemical kinetic rate data. Instead of defining a species multi-step reaction mechanism, you simply define the important chemical species that will be present in the system. software then predicts the mole fraction of each species based on chemical equilibrium.

3. Non-Equilibrium Chemistry (Flamelet Model)

In combustion models where non-equilibrium effects are important, the assumption of local chemical equilibrium can lead to unrealistic results. Typical cases in which the equilibrium assumption breaks down are modeling the rich side of hydrocarbon flames, predicting the intermediate species that govern NOx formation, and modeling lift-off and blow-off phenomena in jet flames.

4. Probability Density Function Model

Any commercial simulation software applies the assumed shape probability density function (PDF) approach as its closure model when the non-premixed modeling approach is used. The probability density function, written as $p(f)$, can be thought of as the fraction of time that the fluid spends at the state f. Figure 2. illustrates this concept. The fluctuating value of f, plotted on the right side of the figure, spends some fraction of time in the range denoted as Δf. $p(f)$, plotted on the left side of the figure, takes on values such that the area under its curve in the band denoted, Δf, is equal to the fraction of time that f spends in this range. Mathematically it is written as,

$$p(f)\,\Delta f = \lim_{T\to\infty} \frac{1}{T} \sum_{i} \tau_i$$

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Where T is the time scale and Tis the amount of time that f spends in the Δfband. The shape of the function $p(f)$ depends on the nature of the turbulent fluctuations in f. In practice, $p(f)$ is expressed as a mathematical function that approximates the PDF shapes that have been observed experimentally.

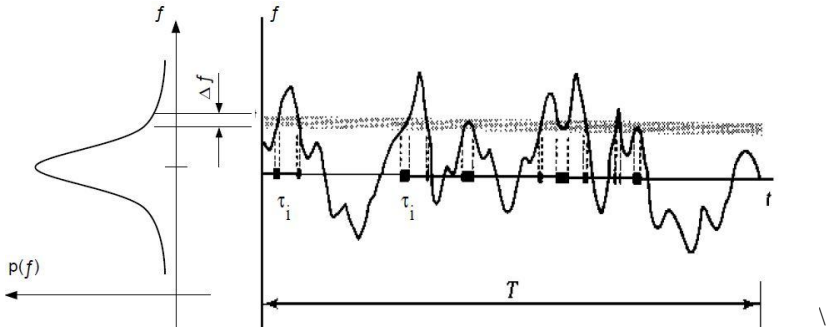

Figure 2: Graphical Representation of Probability Density Function

Researchers have made use of above discussed non-premixed combustion models, validating the results obtained byperforming the experimentscomputationally,with the results that have been obtainedexperimentally.

III. NUMERICAL ANALYSIS

Cristiano Vitorino da Silva et.al (2018) in their paper "Assessment of combustion models for numerical simulations of a turbulent non-premixed natural gas flame inside a cylindrical chamber", presented a Computational Fluid Dynamics (CFD) study of the non-premixed combustion of natural gas with air in an axisymmetric cylindrical chamber, focusing on the contribution of the chemical reaction modeling on the temperature and the chemical species concentration fields.

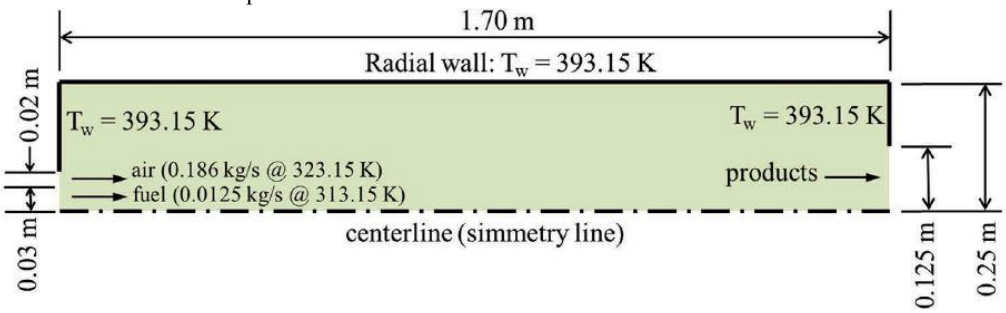

Figure 3: Combustion Chamber Geometry

The problem under consideration was a cylindrical combustion chamber, as shown in figure 3, operating with natural gas at approximately 600 kW with a fuel excess of 5%. Natural gas is injected into the chamber by a duct aligned with the chamber centerline. The fuel mass flow rate is 0.0125 kg/s at a temperature of 313.15 K, while the air mass flow rate is 0.186 kg/s, at a temperature of 323.15 K.

The fuel enters the chamber through a cylindrical duct having a diameter of 6 cm, while the air enters the chamber through a centered annular duct having diameter of 10 cm. For such mass flow rates, the fuel and air velocities are 7.76 and 36.29 m/s, respectively. The inlet air is composed of oxygen (23% in mass basis), nitrogen (76%) and water vapor (1%), while the fuel is composed of 90% of methane and 10% of nitrogen. The Reynolds number at the fuel inlet is approximately 18,000, characterizing a turbulent flow. Buoyancy effects are neglected due to the high velocities.

Boundary condition assumed were that the combustion chamber walls were kept at the constant temperature of 393.15 K. In addition, impermeability and no-slip conditions were assumed on the walls. In the symmetry line, it was assumed that both the radial velocity and the velocity gradient were null. In the outlet, null diffusive fluxes were assumed for all variables, the axial velocity component was corrected by a factor to satisfy mass conservation and the radial velocity was imposed to be null. The walls were assumed gray, diffusive emitters with an emissivity of 0.6. The inlet and the outlet were modeled as black surfaces at the respective temperatures.

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While the first one has a prescribed temperature, the outlet temperature was equal to the outlet flow bulk temperature which is a function of the combustion and heat transfer processes.
Mesh used consisted of 50 divisions in radial direction and 340 division in axial direction as shown in following figure:

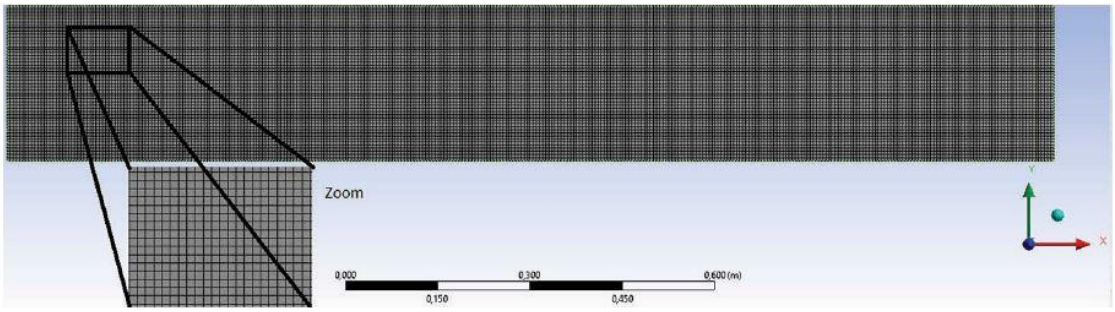

Figure 4: Mesh with 50 × 340 radial and axial equally spaced control volumes

The main goal of this investigation was the analysis of the effect of the combustion model on the numerical simulation of a non-premixed combustion of natural gas in a cylindrical chamber. Temperature and chemical species concentration profiles obtained with the EBU/Arrhenius and SLDF models were then presented and discussed. All results were compared with experimental measurements of Garréton and Simonin (1994) presented in Magel et al. (1996).

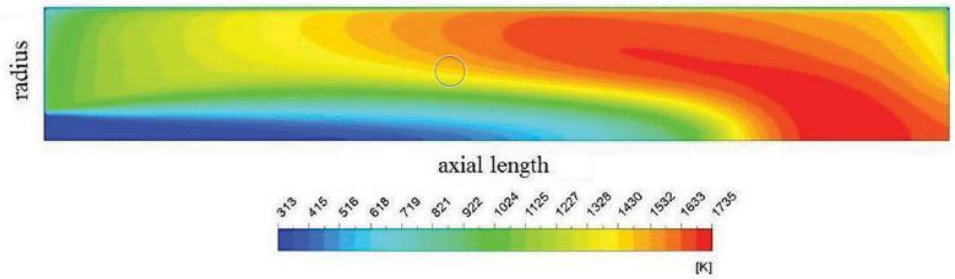

Figure 5: Temperature profile obtained by EBU/Arrhenius model.

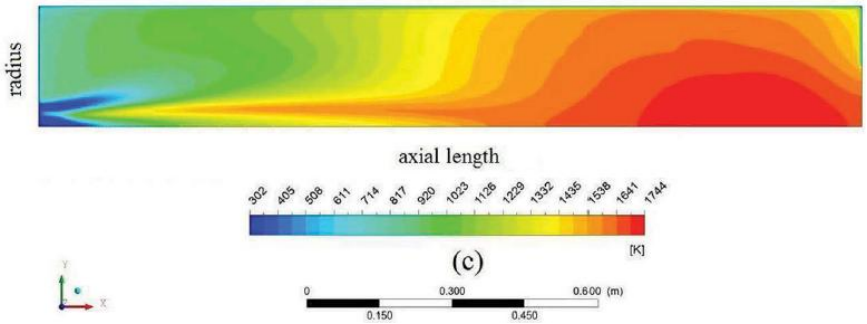

Figure 6: Temperature profile obtained by SLDF model

Figure 5 clearly shows that the best fit regarding the experimental data for the temperature was achieved with the combined EBU/Arrhenius model. This model considers simultaneously the turbulent mixing time scale (EBU) and the chemical time scale (Arrhenius) when estimating the average reaction rate. Thus, in the first half of the chamber, the jet core region presents low temperatures, resulting in a chemical limitation that delays the

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flame ignition. As temperature increases, the chemistry becomes fast and the reactions are progressively more controlled by turbulent mixing.

IV. RESULT AND DISCUSSION

1. The PDF transport model is accurate enough to predict the most important details of the flame. The simulation results and the experimental results are in good agreement with each other.
2. A non-premixed flame structure is influenced by an air micro jet. However non-premixed flame is sensitive to the fuel jet velocity rather than micro jet and co-flow jet velocities.
3. Based on the temperature profile, the air micro-jet cools down the bottom region of the flame and maintains high temperature at the upper region of the flame.

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