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Numerical Simulation of a Turbulent Lean, Premixed Combustion with an Explicit Algebraic Stress Model

William Vicente, Martín Salinas-Vázquez, Eliseo Martínez and Alejandro Rodríguez
Instituto de Ingeniería, Universidad Nacional Autónoma de México
Ciudad Universitaria, 04510 México D.F., México

Abstract: A computational model is used in the present paper to study the influence of the turbulence modeling on the chemical species in a turbulent lean premixed flame. The simulated configuration is about a lean, premixed bluff-body-stabilized flame with a recirculation zone. To achieve the objectives, three different models were used for turbulence modeling as listed next: 1) standard k- , 2) a Reynolds Stress Turbulence Closure and 3) a state of the art Explicit Algebraic Stress Model. Comparisons with experimental data are made in terms of velocities, temperatures, as well as major and minor species. As a result, predictions show that species such as CO and OH are strongly affected by the turbulence model; whereas other species such as NO are affected slightly. On the other hand the Explicit Algebraic Stress Model offers noticeable improvements over existing models.

Key words: Turbulence, Combustion, PDF, NOx

INTRODUCTION

The join Probability Density Function (PDF) approach is an attractive tool on the numerical simulation of combustion phenomenona, i.e. flashback, stability, as well as CO and NO formation. Such combustion phenomena are governed by finite chemistry-effects and flow field interactions. To compute the PDF there are two methods: 1) supposing a determined form and then calculating the function from some of its moments and 2) calculating the function through a transport equation. Regarding the feasibility of both methods, the second approach has a better representation of the chemical reactions. However, its diffusive term –also known as term of molecular mixture- is not closed, requiring modeling procedures. Commonly, this term is modeled from the Linear Mean Square Estimation [1] or Curl model [2]. Additionally, these models postulate a proportionality between a mixture time, τ_{mix} and the turbulent parameters. In particular, the mixture time in the case of the k- model is estimated through the following relationship: $\tau_{mix} = \tilde{k} / C_D \tilde{\varepsilon}$. Moreover, this characteristic time has shown a great influence in a turbulent lean premixed flame [3]. Additionally, the precise prediction of this variable is important during the computation of the chemical species evolution.

Since the practical turbulent flow flames are abundant of anisotropies, the use of more powerful turbulent models is necessary. Fortunately, one alternative is available, the use of the Explicit Algebraic Stress Model family [4]. Consequently, this kind of models inserts anisotropic algebraic terms into traditional isotropic models like the k- standard model. In consequence, the purpose of this paper is to show the effect of this kind of model over the following parameters: 1) mixture time, 2) both velocity and temperature fields and 3) major and minor chemical species concentrations, in a turbulent lean premixed methane flame. To achieve this, the configuration studied is the methane-air, turbulent flame proposed by Nandula et al. [5]. To describe this, Nandula's flame is confined and stabilized by a cone shaped body, which acts as a bluff-body. The resulting flow-field is shown schematically in Fig. 1.

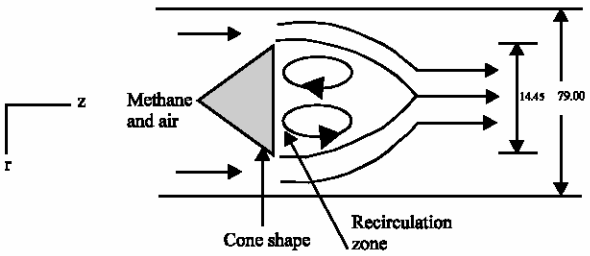

Fig.1: Experimental Configuration. r and z are Both the Radial and Axial Directions, respectively. Data are in mm

Mathematical Model: A combination of both CFD and Monte Carlo methods is used to represent the following:

* The fluid flow
* The chemical kinetics and
* Their interaction with the flow field.

For instance, a similar model to the one used here has been described in sufficient detail elsewhere [3, 6].

The chemical species evolution is simulated with the solution of a PDF equation in Favre averages [7]. In

accordance with the PDF equation, the molecular mixing term is modeled with a Linear Mean Square Estimation model [1]. On the other hand the finite chemical rates are represented by a reduced chemical system, consisting of 5 steps of reaction and 9 species [8]. Such reduced chemical system is derived from the full GRI-2.11 mechanism [9]. Also, the three routes of NOx formation are considered with the mentioned system. Finally, a look-up table method [10] is used for the chemical kinetic representation.

The reactive flow aerodynamics is simulated via Favre-averaged continuity and momentum equations. On the other hand the turbulent convective term ($\tau_{ij} = u_i'' u_j''$), resulting from the average of the convective terms, is represented by mathematical models. Finally, the turbulence models used in this study were the following: 1) k- standard, 2) a Reynolds Stress Transport Model [11] and 3) EASM [4]. As mentioned earlier, the EASM model introduces anysotropic algebraic terms to typical isotropic models. For example, if the k- model is used, the Reynolds stresses are represented by:

$$\tau_{ij} = \frac{2}{3}\tilde{k}\delta_{ij} - \alpha_1^*\left(\frac{\tilde{k}^2}{\tilde{\varepsilon}}\right)\tilde{S}_{ij} - \alpha_2^*\left(\frac{\tilde{k}^3}{\tilde{\varepsilon}^2}\right)(\tilde{S}_{ik}\tilde{w}_{kj} + \tilde{S}_{jk}\tilde{w}_{ki}) + \alpha_3^*\left(\frac{\tilde{k}^3}{\tilde{\varepsilon}^2}\right)\left(\tilde{S}_{ik}\tilde{S}_{kj} - 1/3\tilde{S}_{kl}\tilde{S}_{kl}\delta_{ij}\right) \quad (1)$$

where:

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) \quad \tilde{w}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i}\right) \quad (2)$$

are the mean rate of strain and mean vorticity tensors respectively. On the other hand the α_i^* coefficients (for i = 1, 2, 3) are obtained from S_{ij}, w_{ij}, k, and some flow parameters. Certainly, these parameters may be expressed as follows: 1) constant values: simple EASM model or 2) variables in function of space and time: dynamic approach EASM model [4].

Numerical Method: The simulation is a two-dimensional domain on the bluff body. Simplifying the problem, just a half of the total diameter of the bluff body is considered in the radial direction and the axial direction extends to 4.6 diameters. In particular, a 40x45 (radial x axial) mesh is used. Additionally, grid resolution studies were made to guarantee a better numerical accuracy. Finally, flame aerodynamics equations are solved through a finite volume method, using a SIMPLE-type algorithm [12] on the solution of the pressure-velocity coupling.

The PDF is simulated in every computational cell with 100 particles (group of vectors). For simplicity, the steady state consideration is assumed on the estimations of the mean values, to avoid stochastic fluctuations. Finally, auxiliary tests were performed to show that the mean values were independent of the number of particles per cell.

RESULTS

It is shown that the characteristic mixture time has an important effect on the evolution of both chemical species and temperature [3]. Therefore, the local mixture time or mixture frequency, ($\omega_{mix} = 1/\tau_{mix}$), induces the approaching of the scalar probability toward its mean values with a smaller or bigger rate. As a consequence, the chemical rates of production/destruction of the species may become fast enough to relax the concentrations into equilibrium, as they have a competition for mixing between themselves. In consequence, the precedent process produces a narrower reaction zone as ω_{mix} is increased.

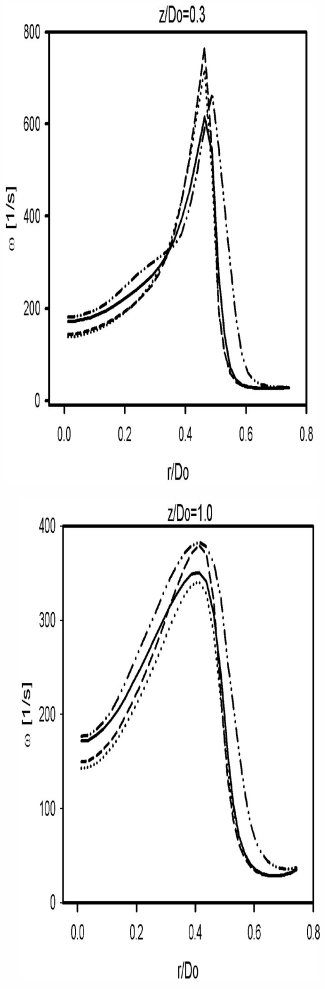

Fig. 2: The Radial Evolution of Mixture Frequency at Axial Station z/Do=0.3 and 1.0, where Do is the Cone Diameter. ——— Standard k- , Simple EASM, ····· Dynamical Approach EASM – – – – and —·· — RSTM

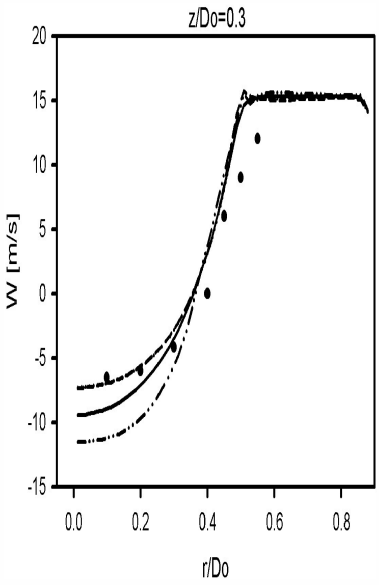

Fig. 3: The Radial Evolution of the Axial Velocity at Axial Station z/Do=0.3 and 1.0. ——— Standard k- , ····· Simple EASM, – – – – Dynamical Approach EASM, — · · — RSTM and • Experiment

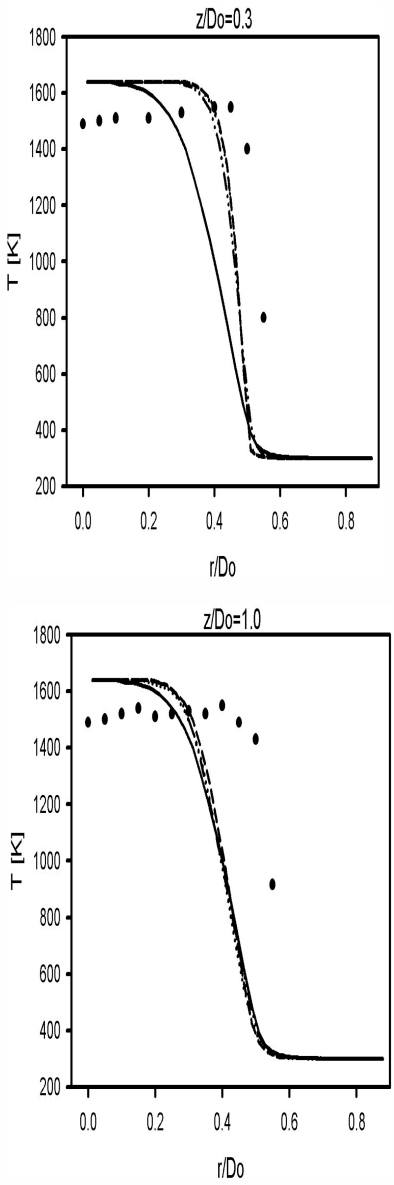

Fig. 4: Radial Evolution of Temperature at Axial Station z/Do=0.3 and 1.0.——— Standard k- , ····· Simple EASM, – – – Dynamical Approach EASM, — · · — RSTM and • Experiment

For instance, Fig. 2 illustrates the radial evolution of the mixture frequency at the axial station z/Do=0.3 and 1.0. Additionally, the k- model predicts the lowest values for the frequency of mixture in the shear layer, creating a wider reaction zone. Also, at the axial station z/Do=1.0, ω_{mix} values for all models are similar. Finally, values of ω_{mix} are related to the turbulent model behavior, according to its definition. On Figure 3, the velocity fields are presented at two different axial stations. Herein, differences are found, most of them are at the recirculation zone (r/Do<0.3), where the EASM results approach the closest to the experimental ones.

Figure 4, shows the temperature profiles at the two coincident axial stations. In this case, discrepancies between the k- model and the other three models are remarkable. For example, differences are greater that 100% at the shear layer zone. Similarly, the over predictions of temperature at the recirculation zone, are in al cases because we did not consider the radiation heat losses related to the process.

The accuracy of the concentrations estimation of the minor species like CO, OH and NO, as well as main species like CH4, is improved as observed in the temperature profiles, (Fig. 5). Additionally, their corresponding profiles approach closer to the

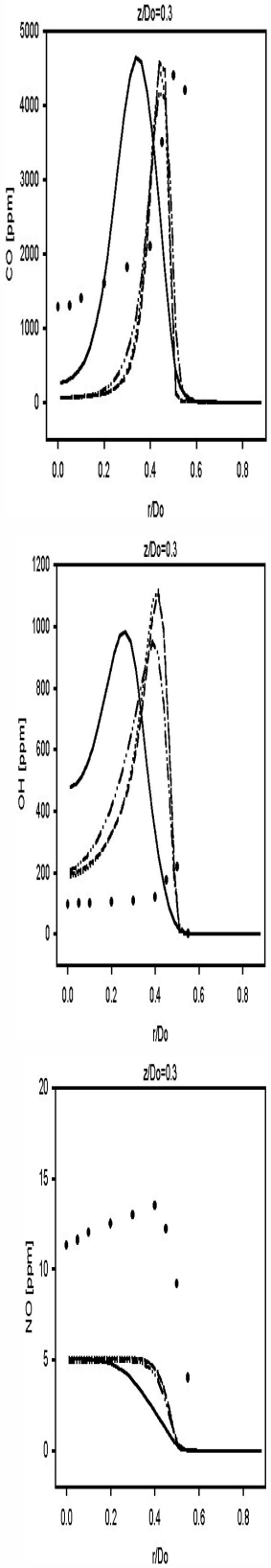

Fig. 5: The Radial Evolution of CO, OH and NO at Axial Station z/Do=0.3.——— Standard k- , ····· Simple EASM, – – – Dynamical Approach EASM, — · · — RSTM and • Experiment

experimental ones at the shear layer. Therefore, the improved representation of the combustion reached here is directly related to the turbulent models performance.

All minor species are affected by the turbulence models. However, the NO concentration at the recirculation zone has a uniform concentration value, which is not affected by the turbulence model. To explain this, the NO-related reactions work too slowly to relax the NO concentration into the equilibrium, whereas mixing works faster.

CONCLUSION

The study of a lean premixed methane flame, computed with different kind of turbulence models is performed in this paper. Such turbulence models supply the characteristic mixture time required to compute the probability density function junction.

The performed simulations show the influence of the turbulence model, mainly, in the shear layer, where reactions take place. Minor species like CO and OH are more affected by the turbulence models than the NO; this is because the chemical rates for the NO-related reactions work too slowly to relax the NO concentration into the equilibrium, whereas mixing works faster.

EASM models are a good alternative in the simulation of turbulent reacting flows. Furthermore, the EASM models have an additional advantage -over models of second order closures- consisting of reduced computational requirements.

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