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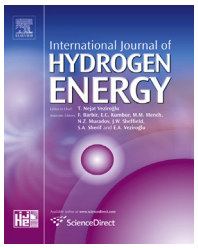

Ambient pressure effect on non-premixed turbulent combustion of CH4–H2 mixture

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ABSTRACT

The present work is devoted to the study of the effect of ambient pressure on non-premixed turbulent combustion of a mixture of 20% of hydrogen and 80% of methane. The simulations were conducted using the PDF approach and modified k-ε turbulence model. The flamelet model was used with the GRI 2.11 detailed kinetic mechanism. The flame consists of two coaxial jets of air and a jet of CH4–H2 mixture with pilot flame. After validating the model used we have varied the ambient pressure from 1 to 10 atm. We observed that the increase of ambient pressure leads to a slight increase of the flame temperature and the mass fraction of NO and a decrease in the radial and axial expansions.

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Introduction

A big part of energy conversion systems use the fossil fuels as a source. This causes emissions of pollutants such as greenhouse gases. In addition, the threat of the fuel depletion makes urgent to find solutions. To deal with this problem, renewable energies seem like an ideal solution but their adoption in the short term poses technological and financial difficulties. An intermediate solution would be the introduction of hydrogen produced from renewable energy sources such as a fuel additive to improve combustion properties of fossil fuels. Indeed, the addition of hydrogen improves the combustion properties of hydrocarbons as reported in previous studies [1–4]. Thus, it is necessary to master the various parameters of combustion of these mixtures such as the ambient pressure to achieve the improvement of combustion systems.

The choice of a numerical model to simulate turbulent diffusion flame passes through the choice of a combustion model, a turbulence model and a kinetic scheme of combustion. For the combustion model we opted for the flamelet model. This model has been widely used and its effectiveness has been demonstrated in the literature [5–7]. The turbulence model used here is the modified k-ε model with $C_{\varepsilon 1} = 1.6$. This model has been the subject of a comparative study between the RSM model and the standard k-ε model using the PDF approach, published recently by Ziani et al. [8]. The study shows that the modified k-ε model is the most accurate. Other studies confirm this result. Indeed, Frassoldati et al. [9] compared between RSM model, the standard k-ε and the modified k-ε using the EDC concept and shown that the modified k-ε turbulence model is the more accurate. Yilmaz and Onbasioglu [6] compared the LES model with the two k-ε models (standard and modified) and obtained the same

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conclusion about the accuracy of the modified k-ε turbulence model. For the combustion chemistry, the reaction mechanism GRI 2.11 is chosen. When coupled with flamelet model, this mechanism appears to be most accurate and the convergence of calculation is relatively fast [10,11]. Moreover, Ravikanti and Malalasekera [7] compared this detailed kinetic scheme with three mechanisms and reported that the GRI 2.11 gives better results especially for the prediction of NO.

Specific objectives

Brooks et al. [12] made an experimental study of the effect of ambient pressure on soot production in a turbulent diffusion flame of methane in 1998 and they published a theoretical study on the same subject in 2002. In both cases, they consider a pressure up to 3 atm. In 2005, Kobayashi et al. [13] published a study dealing with the experimental effect of pressure on the turbulent combustion velocity of the methane-air mixture in a benzene-type burner with a pressure ranging from 0.1 to 1 MPa. Conditions that approach the conditions of combustion in gas turbines. In 2007, Cohé et al. [14] made for the same type of burner a study of the effect of pressure on the structure of a premixed turbulent flame of methane enriched with hydrogen up to 20% for a pressure from 0.1 to 0.9 MPa. Griebel et al. [15] published in the same year a study on the effect of pressure on premixed turbulent combustion of methane for pressures up to 1.44 MPa with an axisymmetric burner configuration.

In the present work, the effect of pressure on turbulent diffusion flame of a mixture of 20% of hydrogen and 80% of methane is studied numerically by means of a CFD code. Our objectives are:

- the determination of the effect of pressure on the combustion temperature;
- the determination of the effect of pressure on the production of NO;
- the determination of the effect of pressure on the production of CO.

Firstly, the validation of the physical and numerical modeling (based on the modified k-ε turbulence model coupled with the flamelet model using the PDF approach) is performed by comparing the obtained results with the experimental data of Brookes and Moss [12] considering the turbulent diffusion flame of pure methane. Secondly, we simulated the combustion of a mixture of 20% of hydrogen and 80% of methane, with the same operating conditions but with new jet velocities to avoid effects of buoyancy. The ambient pressure is varied from 1 to 10 atm to study the pressure effect on this type of turbulent diffusion flame configuration.

Physical and numerical modeling

Physical modeling approaches

We have used the flamelet model for the combustion simulation. In this model the turbulent diffusion flame is considered as an ensemble of laminar flamelet. The properties of the laminar flamelet are determined by solving governing equations for a one-dimensional laminar counter flow diffusion flame. The kinetic mechanism used here is the GRI 2.11 detailed mechanism which involves 49 species in 277 reactions and includes the nitrogen chemistry. We used a probability density function to calculate the average scalar properties as follow:

$$\widetilde{\phi} = \int_0^{\infty}\int_0^{1} \phi(Z,\chi)P(Z,\chi)dZd\chi \tag{1}$$

Where ϕ is a thermochemical property (i.e. temperature, mass fraction …), $\widetilde{\phi}$ its Favre average, Z is the Mixture fraction and χ is a scalar dissipation.

Considering that the scalar dissipation and mixture fraction are statistically independent, we can write:

$$P(Z,\chi) = P(Z)P(\chi) \tag{2}$$

Where $P(Z)$ and $P(\chi)$ are respectively the Probability Density Function of the mixture fraction and the scalar dissipation.

The mean value of scalar dissipation rate is modeled by

$$\chi = C_{\chi}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{Z''^2} \tag{3}$$

where C_{χ} is a constant equal to 2.0 and $\widetilde{k}$ and $\widetilde{\varepsilon}$ are respectively the mean turbulent kinetic energy and the mean dissipation rate. The integration of the probability density function is made before the CFD calculation during the flamelet library generation. The values of this library are directly used by the CFD solver. The probability density function (PDF) gives the distribution probability of the stochastic quantities [16]. In turbulent flow, the probability density function P is a function of position in space x and time t. Then $P(u,x,t)dU$ means the probability of finding at the position x and the time t the value u in the interval $U \le u \le U + dU$. If the probability density P is known, the average value of a quantity is defined by the following formula [6,7]:

$$\overline{u} = \int_{-\infty}^{+\infty} \left(u - \overline{u}\lim_{x\to\infty}\right)^2 P(u,x,t)dU \tag{4}$$

The RANS approach (Reynolds-Averaged Navier–Stokes equations) is used in the present study. We have used the modified k-ε with $C_{\varepsilon 1} = 1.6$ for the turbulence treatment in the numerical modeling.

Computational domain and conditions

We have adopted the same geometrical configuration (Fig. 1) as the one adopted in in the experimental study of Brookes and Moss [12]. The flame consists of two axisymmetric jets of non-premixed air and fuel. The diameters of fuel and air jets are respectively $D = 4.07$ mm and d = 155 mm. The burner include annular premixed burner of 0.16 mm width.

We used the Fluent, a CFD code which uses the finite volume discritization method to perform the simulation. We considered a two dimensions axisymmetric computational domain. The Navier–Stokes equations are solved in such geometrical configuration. We used the centered scheme for the diffusion terms and first order upwind scheme for

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