STUDY OF METHANE PROPAGATING FLAME CHARACTERISTICS USING PDF-MONTE CARLO MODEL AND REDUCED CHEMICAL KINETIC SCHEME

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ABSTRACT
The main purpose of this work is to simulate turbulent premixed and stabilized flame in an adiabatic combustion chamber. The turbulence is supposed to be isotropic and homogeneous and the chemistry is represented by a four-step scheme of methane combustion.
The simulation, based on Monte Carlo scalar P.D.F transport method, was used to study the spherical flame propagation characteristics under different equivalence ratio and turbulence intensity. So we have investigated the flame mean radius, the turbulent flame radius, the flame propagation velocity and the flame brush thickness and our results were compared to different experiments done in a nearly spherical vessel. Good agreements were obtained.
Keywords: premixed turbulent combustion, methane, flame velocity, flame radius, flame thickness.

1. INTRODUCTION
Due to their fundamental importance for premixed combustion theory, turbulent flame characteristics were a subject of a large number of investigations for many decades.[1]
The main purpose of this work is to simulate a premixed turbulent flame in a constant volume vessel. The adopted conditions are similar to those realised in many experiments. The Monte Carlo scalar PDF transport method that is the basis of our numerical simulation has been used for few decades by many authors [2], [3], [4], [5] to simulate ignition delay and the flame growth in turbulent combustion case. Nowadays, this method continues to be efficient for calculating flame characteristics taking into account turbulence and chemistry interaction using reduced chemical kinetic mechanisms [6], [7]. For our case, turbulence is supposed to be homogeneous and isotropic with turbulence time scale of the order of 10^{-3} s and the chemistry is described by the four-step chemical kinetic mechanism of Jones & Lindstedt [8].The mixture is composed of methane as fuel and air as oxidizer.
The calculation domain is divided into a given number of cells. Initially, each one contains Ni particles. These particles move in the domain thanks to the following velocities:

- Gas expansion velocity due to temperature gradient between burned gases (hot products) and 'fresh gases'.
- Turbulent diffusion where a correlation velocity deduced from turbulence spectrum is respected.

An electric spark ignites the flame in a chosen region (e.g., the middle) of the vessel. During this period energy excess will be deposed, making temperature grow highly in this region, [4]. Flame front position is determined when finding a 'pitchfork' of temperature in the vicinity of 600 K, which corresponds to silicon oil vaporisation temperature in the experimental case. A fractal treatment method, [9], [10], allows us to calculate the flame mean radius, the flame turbulent radius, the flame-brush thickness and the flame propagation velocity.

2. FORMULATION
The equations that determine our problem are respectively:

- the mass conservation equation written in spherical coordinates, whose solution gives us the expansion velocities due to temperature gradient between hot products and fresh gas:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{1}{r^2}\frac{\partial (r^2 \overline{\rho}\widetilde{u}_r)}{\partial r} = 0 \qquad (1)$$

- the Lagrangian joint PDF transport equation:

$$\frac{\partial}{\partial t}(\rho(\underline{\psi})\, f_{\underline{u},\underline{\Phi}}(\underline{v},\underline{\psi})) + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[\rho(\underline{\psi}) V_i\, f_{\underline{u},\underline{\Phi}}(\underline{v},\underline{\psi})\right] =$$
$$-\sum_{i=1}^{3}\frac{\partial}{\partial v_i}\left[\rho(\underline{\psi})\left\langle A_i \middle| \underline{V},\underline{\psi}\right\rangle f_{\underline{u},\underline{\Phi}}(\underline{v},\underline{\psi})\right]$$
$$-\sum_{\alpha=1}^{N}\frac{\partial}{\partial \psi_\alpha}\left[\rho(\underline{\psi})\left\langle \theta_\alpha \middle| \underline{V},\underline{\psi}\right\rangle f_{\underline{u},\underline{\Phi}}(\underline{v},\underline{\psi})\right] \qquad (2)$$

where $A_i = \frac{1}{\rho}\left(\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_j} + \rho F_i\right)$ $i,j = 1,3$ and $\theta_\alpha = \frac{1}{\rho}\left(\frac{\partial J_k^\alpha}{\partial x_k} + \rho \dot{\omega}_\alpha + S_\alpha\right)$ $\alpha = 1,N$

- the perfect gas equation:

$$\overline{P} = \overline{\rho}\,\frac{R\,\widetilde{T}}{M} \qquad (3)$$

ρ is the density, $\widetilde{u}_r$ is the Favre averaged radial velocity corresponding to the expansion velocity due to the temperature gradient between hot products and fresh gas. In equation (2), $\underline{\Phi}$ and $\underline{u}$ are respectively a scalar vector and a velocity vector in the physical space and to which correspond respectively the vectors of random values, $\underline{\Psi}$ and $\underline{V}$ in the conditional space. $F_{\underline{u},\underline{\Phi}}$ is the PDF of velocities and scalars. The change terms that characterized the stochastic process A_i and θ_α present the following terms: τ_{ij} that is the strain tensor, F_i is the stirred force per volume unity, P is the pressure, J_k^α represents the diffusive fluxes, $\dot{\omega}_\alpha$ is the reaction rate and finally S_α is source term. In equation (3), $\widetilde{T}$ is Favre averaged temperature and M is the molar mass of the mixture.

3. PDF-MONTE CARLO METHOD

The use of probability density functions (PDF) constitutes a potential solution to describe the evolution of turbulent reactive flows in which fluctuation terms need statistical treatment. The type of PDF that we use in this work is the evolution PDF (transported PDF) called Pope's method [2]. This method uses a Monte Carlo particle solver and the form of the PDF may freely evolve.
It can be highlighted that the high dimensionality of underlying PDF scalar transport equation requires Monte Carlo stochastic solution methods. Monte Carlo method evokes the representation of the PDF with a whole of elements distributed throughout the flow field, and from which the moments of interest may be calculated. In Lagrangian case, the elements (particles) are free to roam the physical domain as dictated by the hydrodynamic field, and the composition of the elements changes only due to mixing and reaction.[11]

4. CHEMICAL KINETICS

Detailed chemical kinetic descriptions of hydrocarbon combustion may require the tracking of hundreds of chemical species and thousands of reaction steps. For the foreseeable future, CPU time and computer memory limitations will prohibit implementation of fully detailed descriptions of

combustion chemistry into CFD simulations of combustion hardware. As a result, it is important to minimize this number while retaining essential features of the detailed chemistry.
Reduced chemical kinetic mechanisms, that can represent important aspects of the behaviour of these detailed mechanisms using few enough scalars that they can be implemented into CFD simulations, offer large potential improvement in the modelling of practical combustion devices [12]. The feasibility of these mechanisms in the simulation of internal combustion engines (ICE) was demonstrated in a previous study.[13]
In the present study, the four-step reaction mechanism of Jones & Lindstedt [8] was chosen thanks to its good results in ICE simulations [13]:

$$CH4 + 1/2\ O2 \rightarrow CO + 2\ H2$$
$$CH4 + H2O \rightarrow CO + 3\ H2$$
$$H2 + 1/2\ O2 \leftrightarrow H2O$$
$$CO + H2O \leftrightarrow CO2 + H2$$

5. RESULTS AND DISCUSSION

In this section we try to study more precisely the turbulent flame front characteristics as: the flame mean radius, the flame turbulent velocity and the flame-brush thickness which are very important for the turbulent combustion. The predicted values are compared to the experimental results realised by many authors. The geometry studied was a parallelepiped vessel with a constant volume. Ignition occurs in the middle of the domain then a flame kernel grows spherically.
To detect more precisely the flame front evolution, we have chosen a cell size (Δr = 0.25 mm) and a calculation time step (Δt = 0.1 ms) which remain constant along the time and overall the domain. Turbulent time scale and turbulent length scale values are equal to those used in experimental cases.

5.1. Flame propagation velocity

The flame propagation velocity is defined as the differential of the flame mean radius vs. time. In Figure 1 are compared the flame propagation velocities found by our simulation and experimental results presented by Kobayashi et al. [17] and Aldredge et al.[18]. There is a very good agreement between experimental and simulation results.
Concerning equivalence ratio effect on flame propagation velocity, it has been known for many decades in laminar combustion regimes, that the flame burning velocity is maximal when the equivalence ratio is around stoichiometry value [19] and [20]. Besides in recent work Bradley [16] affirmed that for turbulent case the flame propagation velocity, which strongly depends on burning velocity, increases with ER. These declarations are justified in Figure 1(a). We can remark that in the case of lean flames (ER = 0.9), the flame propagation velocity increases slowly.
In the case of turbulence intensity effect, it's obviously clear that the flame propagation velocity increases with turbulence intensity. These results are confirmed by theory. In fact, a high level of turbulence intensity makes micro-scale mixing more efficient and turbulence diffusivity stronger, so the flame will be much faster.
In order to discover the effect of the turbulence-chemistry interaction on turbulent premixed flame characteristics, we have represented the flame velocity ratio St/SL versus u'/SL (see Figure 1(b)). In comparison with the experimental results of Kobayashi et al.[17], we can affirm that the flame-burning velocity ratio varies function of the dimensionless turbulence intensity, responding to Damköhlers' model in the case of n = 1. Thus, the expression takes the following form:

$$S_t / S_L = 1 + C_1\, u' / S_L \qquad (4)$$

This formula is similar to that given by Gülder [10] for a fixed Damköhler number. This finding is in agreement too with Zimont-Lipatnikov's model.[21]

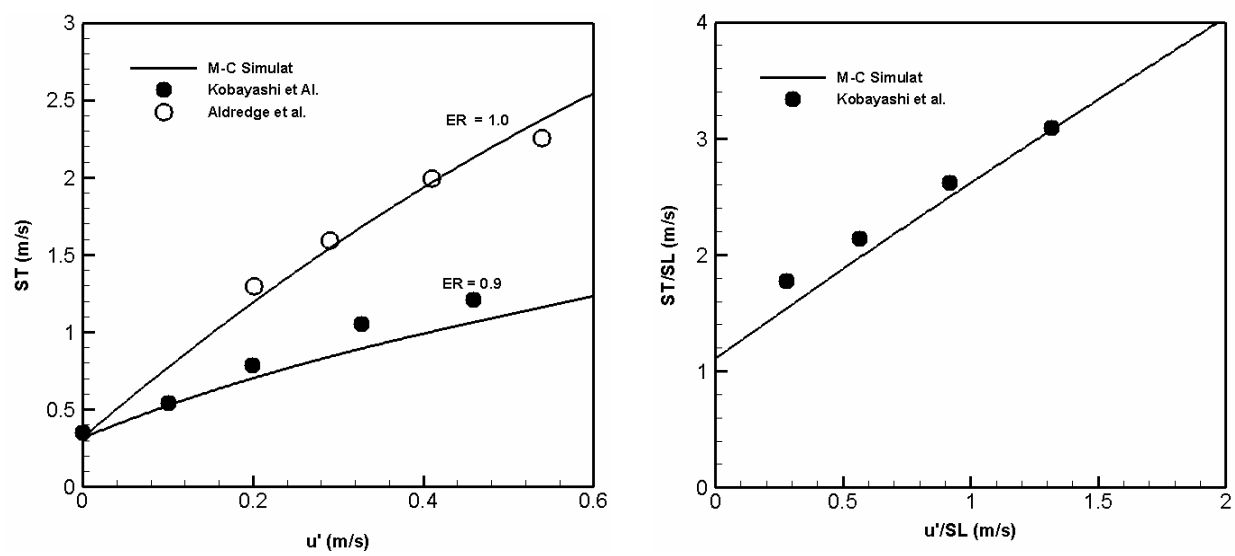

Figure 1. Turbulent flame propagation velocity.

5.2. Flame mean radius

The flame mean radius (R_f) is defined by Lecordier [9], as the radius of a circle that contains the same surface of burned gas (S_b).

$$R_f = \sqrt{\frac{1}{\pi} \times S_b} \tag{5}$$

Figure 2 shows the flame mean radius evolution function of time for different turbulence intensities and different equivalence ratios. First of all we see clearly that the predicted values found by our simulation are in good agreements compared to the experimental ones.

In order to study the equivalence ratio ER effect on flame mean radius, one maintains the turbulence intensity u' constant and varies the equivalence ratio. The effect of this last parameter on flame mean radius is shown in Figure 2. It is worth noting that for lean flames the flame mean radius is fairly linear. However, when ER enhances (around stoichiometry) the flame burning velocity and the flame mean radius increase. These results are in perfect agreement with those announced by Hainsworth [15] and Bradley [16].

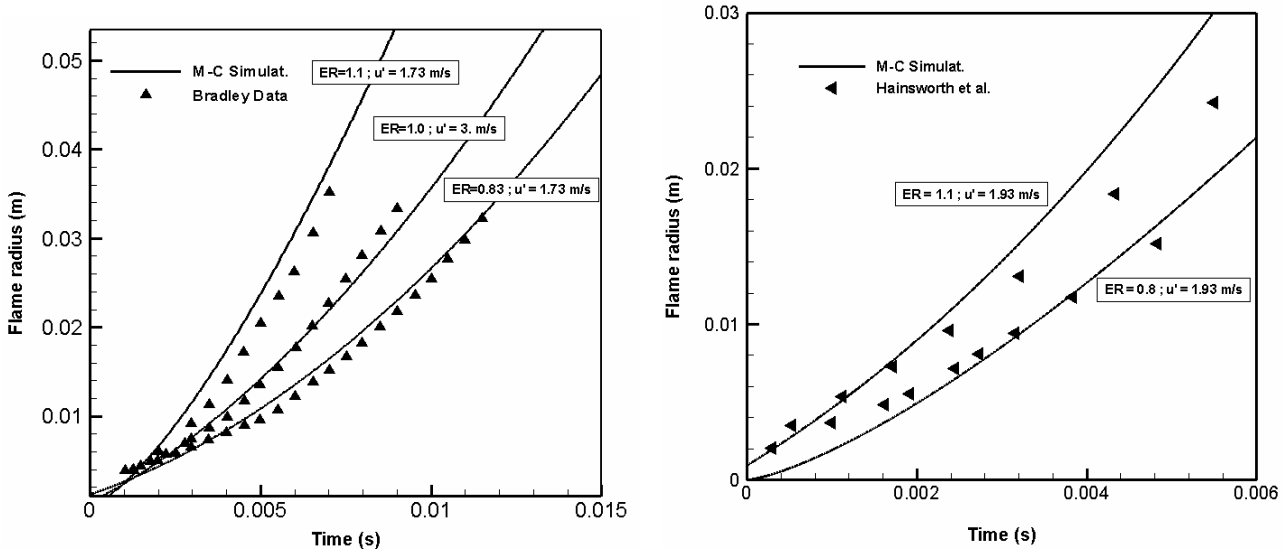

Figure 2. Flame mean radius evolution vs. time.

5.3. Flame brush thickness

Figure 3 shows the flame-brush thickness (δ_t) evolution vs. time. The agreement between simulation and experimental results is satisfactory. The asymptotic tendency of δ_t, affirmed by Galzin [3] and Liptanikov & Chomiak [1], is observed in our simulation. The increase of δ_t is mainly controlled by the turbulent diffusion law, whereas flame propagation reduces δ_t and it can reach approximately constant values after the development phase. However, this constancy of δ_t can be caused by other effects (e.g. turbulence decay or wall influence) rather than by reaching the regime of turbulent flame propagation characterized by a fully-developed δ_t.

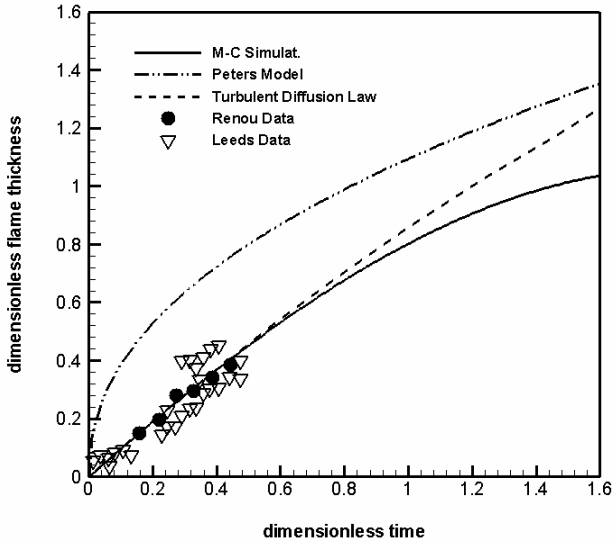

Figure 3. Flame brush thickness evolution vs. time.

6. CONCLUSION

Turbulent premixed combustion was numerically simulated in an adiabatic constant volume vessel. Simulation was based on the PDF-Monte Carlo method. Turbulence was supposed to be homogenous and isotropic. The chemistry was described by a four-step reaction mechanism of methane combustion. Confrontation with many experimental results gave satisfactory agreements, especially on mean flame radii, turbulent propagation velocity and flame-brush thickness.

Finally, it will be very interesting, in a next work, to study the propagation flame characteristics by more considering turbulence-chemistry interactions. Also, it would be useful to take into account more detailed chemistry allowing us to evaluate pollutant emissions.

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