Improvement of Calculations for Turbulent Premixed Flame Characteristics Determination using PDF Monte Carlo Simulation

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Abstract
This study aims at simulating turbulent premixed flame in a constant-pressure vessel (P = 1 atm) where the turbulence is supposed to be homogeneous and isotropic. The mixture of gas is composed by iso-octane-air. The realized CFD were based on Lagrange approach in Monte Carlo simulations. We focused on calculations of; flame radii $R_F$, the flame propagation velocity $St$, flame-brush thickness $\delta_t$ and flammability limit. During the study, influencing crucial parameters such as, the equivalence ratio $\phi$ and the turbulence intensity $u'$ were considered. Results show that the equivalence ratio enhances the flame propagation when passing from lean to stoichiometric flames. Also, the turbulence intensity yields a notable growth for the flame characteristics mentioned above. Moreover, we noticed that the flammability limit is strongly depending of the turbulence intensity and the equivalence ratio. More precisely, we remarked that the minimum ignition energy (MIE) was situated quite smaller than the stoichiometric condition. But, it increased with the turbulence intensity.

Keywords: Monte Carlo Simulation; Premixed Flame; Turbulent

Introduction
Although the trend nowadays is towards more and more renewable energy such as; solar energy (thermal and/or photovoltaic), wind energy, geothermal energy and especially biomass [1-4], the fossil energies used in combustion in various installations still retain their importance [5-8]. However, although turbulent premixed flames were well studied [9-11], and for more than 50 years ago, we think that many aspects of the problem remain misunderstood. Indeed, significant practical problems still remain not resolved in spark-ignition engines, explosions and stationary power gas turbine. In this context many works in literature are dealing with spherical expanding laminar/turbulent flames. Shu, et al. [12] developed an experimental study of laminar ammonia-methane-air premixed flames based on expanding spherical flames in a constant pressure chamber. They focused on the laminar flame speed, the Markstein lengths and the flammability limits. They found that the laminar flame speed correlated with the methane volume fraction. Also, when increasing methane content in the fuel mixture, upper and lower flammability equivalence ratio limits were boarded. Moreover, Bradley, et al. [13] focused on extending the measurements of turbulent burning velocity over a wide range of fuels and pressures using schlieren high speed photography to define the rate of burning and the smoothed area of the flame front. They obtained correlations of turbulent burning velocity normalised by the effective rms $\mu'$, for a certain range of Karlovitz stretch factor $K$ and different negative strain rate Markstein numbers. They concluded that $\mu'$ increased when $K$ decreased. In addition, authors identified different burning regimes from mixed
turbulence/laminar instability at low K values to that corresponding to high K values for which $\mu'$ is reduced due to localised flame extinctions. Nie, et al. [14] studied the flame height and the flame brush thickness of lean turbulent premixed Bunsen methane/air and propane/air flames. They observed that under fuel-lean conditions the Bunsen flame height and the centreline flame brush thickness decrease when increasing the equivalence ratio. However, the turbulence intensity plays a marginal role on these two parameters. Many other results reported in literature showed that the flame propagation velocity $S_t$ is always increased by the root mean square (r.m.s.) $u'$ [15-17]. Indeed, the pioneers Damköhler [18] and Shchelkin [19] in this domain attributed the $S_t$ increase, under $u'$ effect, to the local flame surface area growth due to small-scale eddies. Also, in a previous paper, it was found that the flame burning velocity ratio $S_d/S_L$ followed a linear tendency according to the Damköhler model with $n = 1$ [20]. Concerning the flame-brush thickness $\delta$, it is well known that this characteristic is quite affected by the equivalence ratio, but, more seriously by the turbulence intensity $[9,11,21]$. It is well known that the flame front propagation is governed by the success of the flame kernel initiation. The latter flame stage is seriously affected by flammability limits. Indeed, physical phenomena such as the flame stretch and the preferential diffusion controlled by turbulence, which influence seriously the flame burning velocity, are fundamental for understanding the flame extinction $[22]$. Hence, regarding what was reported in literature, the main object consists at knowing the behaviour of the flame, its propagation, the flame laminar speed, the flame burning velocity and the so-called flame-brush thickness constitute crucial data for more apprehending this type of combustion $[23-25]$.

The investigated simulation in this paper is based on Monte Carlo method. This method is powerful when simulating the transport equations of joint probability density functions (pdf’s) in turbulent reactive. The whole space is the product of phases and thermochemical variables $[26,27]$. Indeed, it was proven that the fluid particle, the probabilistic particle and the stochastic particle present almost the same trajectories in real, conditional and stochastic spaces respectively $[28]$. Hence, the principal objective in this work was to simulate turbulent premixed flame of iso-octane/air using Monte Carlo method in a lagrangian approach. For this purpose we tried to extend the simulation time as long as possible. As it is explained below this method requires multi-level modelling; on the correlated velocity field, on the turbulent diffusion and on the chemical kinetics of reaction and reaction rate. The parameters affecting the flame development are the equivalence ratio and the turbulence intensity (rms). Appropriate treatments of the temperature field inside the combustion chamber permit the access to determine the up-mentioned flame characteristics.

### Formulation and Operating Conditions

The governing equations for this problem are; the mass conservation equation written in spherical coordinates (Equation 1) (because of the spherical symmetry problem), the joint PDF transport equation (Equation 2) and the perfect gas equation (Equation 3).

$$\frac{\partial \bar{p}}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho \bar{u}_r \right) = 0 \quad (1)$$

$$\frac{\partial}{\partial t} \left[ \rho \bar{v} \right] + \frac{\partial}{\partial r} \left[ \bar{u}_r \rho \bar{v} \right] = - \frac{\partial}{\partial r} \left[ \left( A \bar{v} \right) f_{\bar{v}} \left( \bar{v}, \bar{v} \right) \right]$$

$$- \frac{\partial}{\partial \phi} \left[ \left( \bar{\theta}_\phi \right) f_{\bar{\theta}} \left( \bar{v}, \bar{v} \right) \right] \quad (2)$$

with respectively:

$$A_i = \frac{1}{\rho} \left( \frac{\partial \bar{T}_{ij}}{\partial x_j} + \rho \bar{F}_i \right) \quad (3)$$

$$\bar{\theta}_u = \frac{1}{\rho} \left( \frac{\partial \bar{J}^u_k}{\partial x_k} + \rho \bar{\omega}_u + \bar{S}_u \right)$$

$$P = \rho \frac{r T}{M} \quad (3)$$

$\rho$ is the density, $u_r$ is the radial velocity vector. In equation (4) $\bar{O}$ is the sample space variable corresponding to $O$ and $\bar{V}$ is the sample space vector corresponding to $V$. $f_{\bar{O}}$ is the joint PDF of velocities and scalars. The terms $A_i$ and $\bar{\theta}_u$, which are characterized by stochastic processes, contain respectively the following physical terms: $\bar{\theta}_k$ is the viscous stress tensor, $\bar{F}_i$ is the external force per volume unity, $P$ is the pressure, $\bar{J}^u_k$ is the diffusive fluxes, $\bar{u}_k$ is the reaction rate and finally $S_u$ is the source term which provokes ignition. In equation (3), $T$ is the temperature and $M$ is the mean molecular weight of mixture.

The turbulence is supposed homogeneous and isotropic described by $K$-$\varepsilon$ frozen model $[29,30]$. However, we don’t take into account the interaction between flame and walls, and for overcoming this we suppose that the vessel is big enough and the kernel flame is ignited in the middle so that it can be developed far from the side walls. Chemistry
is simplified to a one stage global reaction and the reaction rate is calculated using Westbrook and Dryer formula [31]. Also, radiative transfers are not considered. Ignition energy comparable to that given by a spark in real case is deposited in a reduced zone characterized by a certain radius \( R_{ign} \) and during a certain time \( \Delta t_{ign} \). The spark ignition is selected to decrease linearly versus the time according to experimental observations and to decrease as a parabolic function like the variation of the loss of heat between the electrodes. Then, the whole energy produced by ignition is obtained by making the sum of the variations of enthalpy on all the elementary shells located inside the ignition radius. Before each run, we have fixed the kinetic energy of turbulence \( K \), the dissipation rate of turbulence \( \varepsilon \), the equivalence ratio \( \Phi \), the grid size \( dr \), the time increment \( dt \), the ignition radius \( R_{ign} \), the ignition time \( \Delta t_{ign} \), a constant characterizing the mixing frequency and the energy activation \( E_a \). The turbulence intensity \( u' \), the turbulent scale length \( L_t \) and the turbulent time scale \( \tau_t \) are calculated in function of \( K \) and \( \varepsilon \) according to the \( K-\varepsilon \) frozen model:

\[
L_t = 0.16 \frac{k^{3/2}}{\varepsilon} \quad (4)
\]

\[
\dot{\varepsilon} = 0.3 \frac{k}{\alpha} \quad (5)
\]

0.16 and 0.3 are two constants chosen on experimental considerations.

The flame propagation velocity is calculated by differentiating the flame radius as function of the time:

\[
S_f = \frac{dR_c}{dt} \quad (6)
\]

The flame-brush thickness is evaluated using the following expression:

\[
\delta_f = \frac{1}{\max(dC/dx)} \quad (7)
\]

In the last expression \( C \) is the progress variable, which is equal to zero in the fresh gas and, it is equal to 1.0 in the burned gas.

**Mote Carlo Method**

Because of the spherical symmetry of the problem, we carried out the numerical simulation in 1-D spherical case (a long an axis \([0, R]\)). This domain should be divided into \( N \) cells. Initially, each cell should contain \( N_i \) particles. The pressure, supposed constant, is equal to \( 10^5 \) Pa. The micro-scale mixing imbedded in \( \delta_t \) (in the second right hand side of (Equation 2)) occurs in a closed form and has to be modelled. The modified Curl micro-scale model was chosen based on coalescence–dispersion of particles [32]. Coalescence –dispersion models are also known as particle-interaction model in which mixing takes place by pairs: two particles \( P_i \) and \( P_j \) selected randomly from the ensemble of \( N \) particles in a given cell, mix with a certain probability \( P_{m} \) during a time step \( \Delta t \). After mixing, the particles will have new scalar values, equal to the mean of their values before the mixing stage. Moreover, Monte Carlo particles are able to roam the domain randomly thanks to the expansion velocity and to the turbulent diffusion. The type of PDF that we use in this work, is the evolution PDF (transported PDF), called Pope’s method [28,33,34]. This method uses Monte Carlo particles solver, and the form of the PDF may freely evolve. Contrary to presumed PDFs, there is no preset shape in our case. The Monte Carlo method represents the PDF with an ensemble of “stochastic elements” distributed throughout the flow field, from which the moments of interest may be calculated. Particularly, in Lagrange approach, the elements (particles) are free to roam the physical domain as dictated by a stochastic hydrodynamic field. Moreover, the composition of elements changes only due to mixing and reaction. The particles enclosed in every cell are moved according to the local time step determined by the minimum of the flow time scale and the mixing time scale. In this context, Raman, et al. [35] performed some numerical tests to determine the optimal global time step, the optimal space step, and to estimate the increase in computation load with the number of particles per cell and, consequently the number of particles in the whole domain. They concluded that the tracking time scales linearly with particles, size grid and global time step. It was for Raman, et al. [35] that for the propane-air a time step of \( 2.10^{-4} \) s yields consistent results for both reacting and non-reacting cases. Concerning statistical error, it can be noticed that it evolves like \( N^{-1/2} \), according to the central limit theorem. So, for a large number of particles, the error tends to zero, but the computational load increases hyper linearly. This result was also mentioned by Pope [28]. It is to be highlighted that the stochastic particles move in the calculation domain thanks to types of speeds:

- Gas expansion mean velocity due to temperature gradient between burned gas and fresh gas.
- Turbulent diffusion correlated velocities, based on Box and Müller transformation [36].

**Results and Discussions**

**Mesh Effect**

First of all, we tested the grid mesh size effect on the flame formation and propagation. For this, we varied the grid size \( dr \) at the vicinity of the optimal value stated by Raman, et al. [35], whereas, all the other simulation parameters were constant. Figure 1 shows that the grid size has a quiet little
effect on the flame kernel formation. Furthermore, for these values the flame kernel was born and propagated without any difficulty.

**Figure 1:** Effect of the grid size on the flame growth.

### Minimum Ignition Energy (MIE)

To test the influence of the ignition energy \( I_{en} \) on the flame we carried out different runs with different ignition energies. Figure 2 illustrates that \( I_{en} \) plays an important role either on the flame kernel birth or on the flame propagation. Indeed, on one hand, more \( I_{en} \) is bigger more the flame kernel is early formed. On the other hand, it can be noted that high the ignition energy is, high the acceleration of the flame propagation is. This result can be attributed to the increase of temperature (reaching 2800 K) in the ignition zone of \( R_{ign} \) radius. However, in order to more apprehend the problem of ignition fail (flammability limit) it is capital to optimise the minimum ignition energy (MIE) provided by the spark during the ignition step [22]. Obviously this phenomenon is not suggested in SI engine, although it is well recommended in order to bring down the number of accidents in mines and in industry. However, the ignition success/fail is not depended only on MIE. Indeed, the MIE may correlate with the equivalence ratio and also with the turbulence intensity. Figure 3 shows the variation of MIE with the equivalence ratio \( \Phi \). This curve is similar to what was published in literature by Lewis and von Elbe [37]. MIE minimal founded in our case iso-octane/air flame is 0.4 mJ for \( \Phi = 0.95 \) and rms \( u' = 0.2 \) m/s. The value founded by Lewis and von Elbe for \( \text{CH}_4/\text{air} \) laminar flame was 0.3 mJ for \( \Phi = 0.9 \). The little difference can be attributed to the weak turbulence in our case. In the same context, Figure 4 shows the variation of MIE versus the equivalence ratio for different turbulence intensities \( u' \). It can be noted that when increasing \( u' \) MIE increases, but the equivalence ratio corresponding to MIE is always at the vicinity of 0.9-0.95. This shows that the turbulence plays a negative role on the flame kernel formation, and in many case the flame can't resist to the wrinkling and stretching effects caused by turbulence, and leading to flame extinction [38, 39].
Figure 5: Evolution of the temperature as function of elapsed time for different radii from the ignition zone.

Figure 6 shows the variation of the flame radius versus elapsed time, for different equivalence ratios and for a given turbulence intensity. One observed that lean flames exhibited quite linear radius. However, when we go near the stoichiometric flames, radius becomes more and more parabolic. Hence, the flame is accelerated when reaching stoichiometric condition.

Figure 7 shows the turbulence intensity effect on the flame radius evolution for a given equivalence ratio. One noticed that radii become more parabolic when increasing the turbulence intensity $u'$. This result could be attributed by a turbulent diffusion more efficient when the turbulence is more intense. Indeed, the micro-scale mixing becomes more efficient. Figure 8 illustrated a good agreement between our results and those obtained experimentally by Groff in similar conditions [40].

Flame Propagation Velocity

Figure 9 shows the influence of the equivalence ratio on the flame propagation speed $S_t$. Lean flames ($\Phi = 0.7$ and $\Phi = 0.8$) this figure exhibit almost constant speed. However, when increase the equivalence ratio, the flame propagation velocity increases and tends to an asymptotic value in the case of a moderate turbulence ($u' = 1.2$ m/s). In Figure 10 the effect of the turbulence intensity is tested for a given equivalence ratio. Even in the case of lean flame the increase of the flame propagation speed is notable. Furthermore, the growth of speed can reach un-controlled level with intense turbulence (no asymptotic tendency in this case). In Figure 11 we carried out comparisons with results found by Lipatnikov and Chomiak [41], and Bradley, et al. [42].
of iso-octane-air mixture is equal to 358 K. The pressure is equal to $10^5$ Pa. The equivalence ratio is equal to 0.8 and the turbulence intensity value is $u' = 2.36 \text{ m.s}^{-1}$. We observe that the curve obtained by Monte Carlo simulation is in a satisfactory agreement with both F.S.C. model [41] and experimental [42]. However, the agreement is better with Bradley, et al. [42] when the flame radius is ranging between 15 and 30 mm.

In Figure 13 are plotted the dimensionless flame brush thickness as function of the dimensionless time for different equivalence ratio and for a fixed turbulence intensity $u'$. As it is shown $\delta_t/L_t$ increases rapidly at the beginning and tends to an asymptotic value. Also, one noticed that this limit value increases when the equivalence ratio decreases in perfect predictions with the combustion regimes diagram. In addition, it is to be highlighted that this phenomenon appears only when the flame becomes developed enough ($t/\tau_t > 2.0$).

Conclusion

We carry out numerical simulation of premixed turbulent spherical flame using Monte Carlo method in lagrangian approach. Results show that for optimal space step of $2 \times 10^{-4}$ m and optimal time step of $10^{-4}$s the calculation load is acceptable. Moreover, we remark that the MIE is situated closed the stoichiometric condition ($\Phi \approx 0.95$). The premixed flame characteristics such as, flame radius, flame propagation speed and flame brush thickness are strongly influenced by the turbulence intensity, but less by the equivalence ratio. The flame propagation speed is almost constant for lean flames but increases to an asymptotic value. But, in case of high intensity of turbulence the growth becomes uncontrollable. The same bending effect seen for the flame propagation speed is also observed with the flame brush thickness.

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