Application of a PDF Method to Transient Reactive Jets

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1 Introduction

In this work a stand alone Probability Density Function (PDF) method is used to study ignition of premixed hydrogen/air mixture by hot turbulent jets. The case under consideration is a statistically transient premixed reactive turbulent jet. In this case, chemical reactions occur at small scales which are not resolved either in a large-eddy simulation (LES) or a Reynolds-averaged Navier-Stokes (RANS) method and must be modeled. PDF methods, however, achieve closure at the level of one-point, one-time joint PDFs and have been used extensively to simulate combustion and reactive flows [1]. Convection and reactions are treated without the need for modeling [2, 3]. Yet, the equation for the joint PDF contains unclosed terms such as the effects of pressure gradients and the mixing process of molecular diffusion which need to be modeled [2].

The applications of ignition initiation by hot turbulent jets are found in explosion protection, nuclear safety, pulse detonation engines, supersonic combustors etc. [4, 5]. The motivation of the current work is explosion protection [6]. Due to internal explosion in an electrical equipment, hot exhaust gas may issue into the combustible environment from the enclosure through inevitable gaps which may lead to accidental explosion. An experimental and numerical study of an ignition process was conducted by Sadanandan [6], where a jet of hot exhaust gas impinges through a narrow nozzle into a quiescent hydrogen/air mixture by initiating an explosion in another chamber. It was shown that the ignition first appears at the jet tip. The aim of the current study is to investigate qualitatively the conditions and processes that lead to ignition. The results of these first investigations will be used as a basis for quantitative simulations of ignition processes in our following work in order to understand and prevent accidental explosions.

The impact of turbulence and mixing in autoignition of non-premixed fuel, released from a nozzle into a turbulent hot co–flow of air in a pipe was investigated experimentally by Markides and Mastorakos [7]. It was shown that decrease in turbulence intensity and increase in turbulence lengthscale intend to reduce the autoignition length.

The simulations performed include stationary variable-density inert jets, transient variable-density inert jets and transient reactive cases. We have performed calculations for stationary non-reactive variable density jets using PDF methods for various range of density ratios in [8]. In the current paper, we present

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simulations of transient variable-density jets. We found good agreement of jet penetration distance after injection with findings of experimental analysis [9]. Finally, the numerical results concerning transient ignition of a premixed hydrogen/air mixture, which is initiated by a hot jet, are presented. The results show, at the beginning where the turbulent mixing is at its high, the hot jets cools down and reaction rate cannot compensate the heat dissipation due to turbulent mixing. Therefore, ignition is suppressed. Further downstream, as turbulence frequency is decreased re-ignition takes place. These observations are in accordance with the experimental findings in [5, 10] and the explanation of turbulence effects on ignition length in [7].

2 PDF Approach

In order to model turbulent flow, we used a PDF method which has been developed for the joint velocity-turbulence frequency-composition PDF model [2, 3]. The modeled PDF equation is solved by using a Monte Carlo particle-cell technique. In this method, the flow is modeled by an ensemble of notional particles. The evolution of notional particles is governed by a set of stochastic differential equations.

We use the simplified Langevin model (SLM) [2] for the velocity evolution. Here we use same model equations and constants as explained in [3], with the exception of the model constant $C_{\omega 1}$. Different values for the turbulence model parameter $C_{\omega 1}$, which controls the spreading rate of the jet, have been reported in the literature [11]. Using a value of 0.70 as in [11], sufficient agreement with experimental results for the steady state condition has been achieved [8]. For the transient cases the same model constant is used. Molecular mixing is modeled by the interaction by exchange with the mean (IEM) model [12]. In the IEM model C_ϕ is a model constant which controls the molecular mixing rate. Increasing the value of C_ϕ increases micro-mixing rate. For the calculations performed the values of 2, 3 and 4 is used for C_ϕ for different cases. We adopted a projection method [**?**] to obtain the mean pressure gradient. To reduce the number of dependent variables in the simulation, a reduced description of the thermochemical state is applied. We use the REDIM method for this purpose [13]. For the reactive case in the current work it is sufficient to describe the state with a one-dimensional manifold and we use a manifold which is equivalent to a one dimensional premixed hydrogen/air flamelet. The manifold is parametrized with the specific mole number of H_2O, ϕ_{H_2O} which is defined as w_{H_2O}/M_{H_2O}, where M_{H_2O} is the molar mass and w_{H_2O} is the mass fraction of H_2O. Thus, ϕ_{H_2O} and enthalpy are the only additional variables that has to be solved in the reactive simulations.

3 Results and Discussions

Simulation results of transient non-reactive variable density case will be considered first. Calculations are performed for an axisymmetric inert jet of helium/air mixture to quiescent air at ambient temperature. The density ratio of the jet to the ambient gas is 0.26. The inlet condition corresponds to top hat flow having the exit velocity of $300\,\mathrm{m/s}$. The nozzle diameter is 1 mm. The jet tip position Z_t at time t is proportional to the square root of the time after injection of the jet and is given by the following relation [9]

$$Z_t = \Gamma \left(\frac{\dot{M}}{\rho} \right)^{\frac{1}{4}} t^{\frac{1}{2}}, \tag{1}$$

where $\dot{M}$ is the nozzle exit momentum flow rate, ρ is density and t is time. In this equation Γ is a constant. Analysis of experimental data has shown that this constant has a value of 3 ± 0.1 [9]. Fig. **??** shows the normalized jet tip position of the simulation results against the squared root of the time

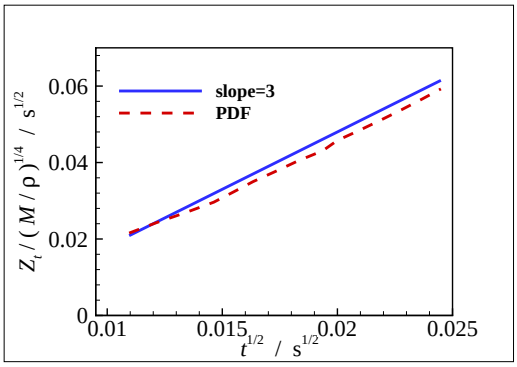

Figure 1: Normalized penetration distance after injection of variable-density inert jet.

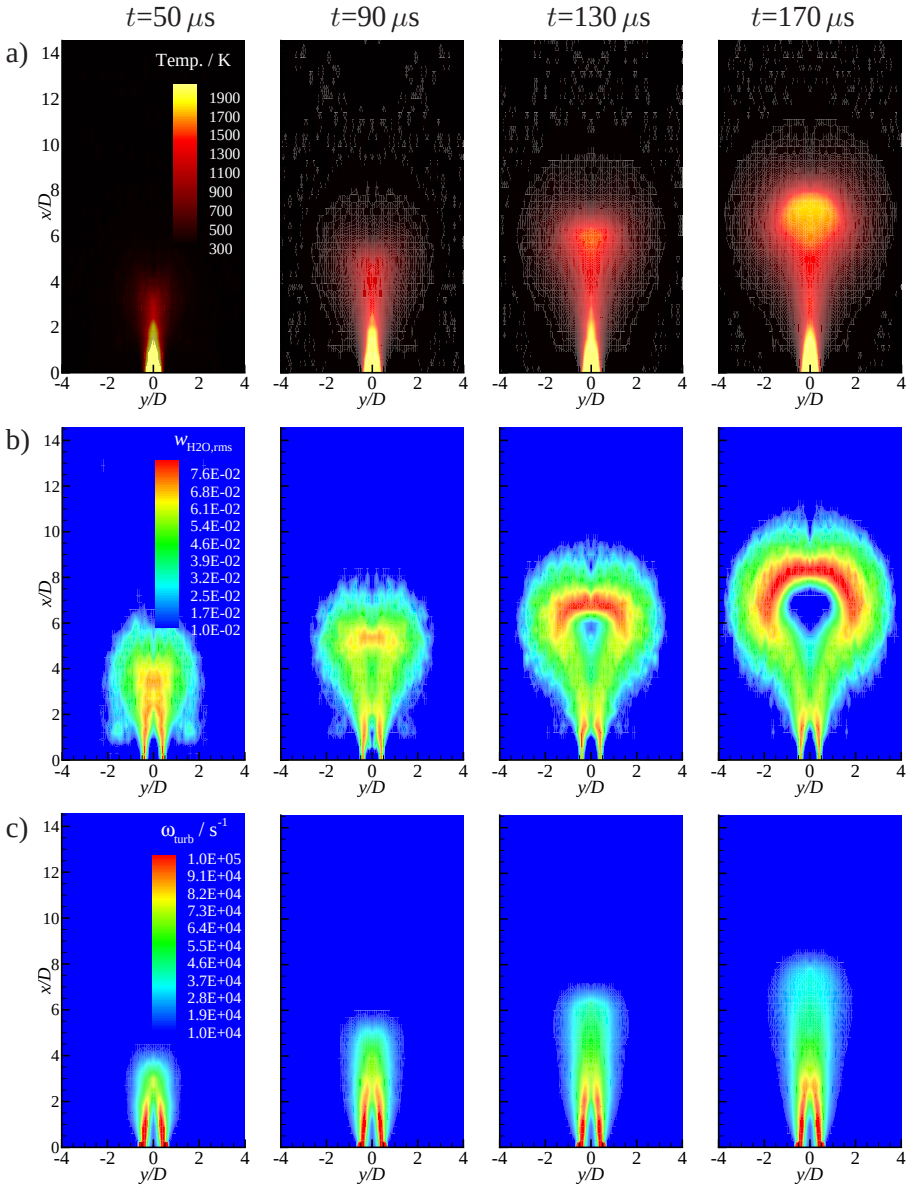

Figure 2: Imaging of ignition event. a) Mean temperature. b) RMS of mass fraction fluctuation of H_2O, $w_{H_2O,rms}$. c) Turbulence frequency.

(dashed line) and a plot of Eq. (1) (solid line). It can be seen that there is very good agreement between simulation results and Eq. (1).

The second test case is transient ignition of hydrogen/air mixture by a hot jet. In the current study, the hot jet is exhaust gas of hydrogen/air near equilibrium and the corresponding exit temperature is about $2000\,\mathrm{K}$. The flow at nozzle exit is assumed to be a fully developed turbulent pipe flow having streamwise velocity of $300\,\mathrm{m/s}$ at the jet centre. The ambient is quiescent cold ($300\,\mathrm{K}$) stoichiometric mixture of hydrogen/air. As it is mentioned before, the specific mole number of $\mathrm{H_2O}$ is chosen as reaction progress variable.

In the experimental measurements a strong cooling down of exhaust gas due to the nozzle walls is observed. For a quantitative comparison of experimental data and results from a simulation, it is essential to account for this effect. However as a first stage we intended to study the behaviour of our applied models, before regarding this complicated case from the experiments and we assumed a configuration of an ignition case that can be described with a one-dimensional manifold, as explained above. The heat loss at the nozzle can be accounted for with a two-dimensional manifold, which will be identified and applied in our following work for the quantitative simulations.

Fig. 2a) shows the temperature evolution at different time instants after the hot jet injection. It is observed that after injection of hot gas, near the nozzle exit there is first a cooling down due to turbulent mixing as it was shown also in [5]. Although turbulent mixing also provides combustible material to the hot jet, heat dissipation due to the mixing cannot be compensated by reaction rate. Further downstream when the mixing rate decreases re-ignition occurs at the jet tip as it is reported in [5]. RMS of mass fraction fluctuation of $\mathrm{H_2O}$, $w_{\mathrm{H_2O,rms}}$ is shown in Fig. 2b). Two regions with higher values of $w_{\mathrm{H_2O,rms}}$ are observed. In the region close to the nozzle at the shear layer a high value of $w_{\mathrm{H_2O,rms}}$ corresponds to the turbulent mixing of the jet. Further downstream at the jet tip a secondary emergence of higher value for $w_{\mathrm{H_2O,rms}}$ mostly corresponds to the reaction and approximates the location of the flame front. From the temperature field (Fig. 2a)) and $w_{\mathrm{H_2O,rms}}$ (Fig. 2b)) it can be seen that the ignition length from the nozzle (where temperature rises due to reaction and then is sustained) is about $5D$. Fig. 2c) shows the turbulence frequency field. In the location where ignition occurs, it can be seen that turbulence frequency is much reduced compared to the high values close to the inlet, hence, the reaction rate compensates the heat dissipation due to turbulent mixing and leads to a self-sustaining flame propagation.

Furthermore, we have studied the effect of mixing model constant C_ϕ which controls micro-mixing rate. The typical value of this constant is 2. Yet, in premixed combustion a wide range of values for C_ϕ (1-12) has been reported [11, 14]. Rowinski and Pope [11] investigated sensitivity of this parameter for the range of 2 to 4 in the IEM model. In the current study we used the same values to investigate the sensitivities of the results to this parameter. Mean temperature evolution for different values of C_ϕ (2, 3 and 4) is shown in Fig. 3. In all cases ignition length is about $5D$ which means ignition length is not much sensitive to this parameter for the range of C_ϕ studied in this work. However, it can be seen that for lower values of C_ϕ (i.e. lower rate of micro-mixing) initial cooling down of temperature is more pronounced. Same behaviour was also reported in [11].

To further investigate the impact of micro-mixing and turbulent mixing on reaction the scatter plot of temperature against $w_{\mathrm{H_2O,rms}}$ is illustrated in Fig. 4 for simulations with different values of C_ϕ. The plot is color-coded by turbulence frequency. For each case of C_ϕ the simulation results are shown for the time when after re-ignition temperature rises again to a specific value, here $2000\,\mathrm{K}$. It can be seen that for the case with the value of C_ϕ=2 the points with higher turbulence frequency (red points) is concentrated in the region on the map where having temperature in the range of $1000\,\mathrm{K} - 1600\,\mathrm{K}$. While for C_ϕ=4 the points with higher turbulence frequency (red points) is scattered up to $1900\,\mathrm{K}$. The observation of higher turbulence frequency in the region with high temperature indicates that higher

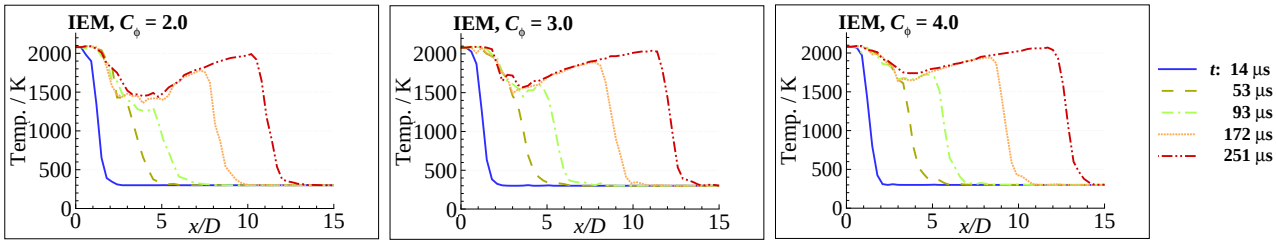

Figure 3: Mean temperature along the centreline at different times for simulations with various C_ϕ.

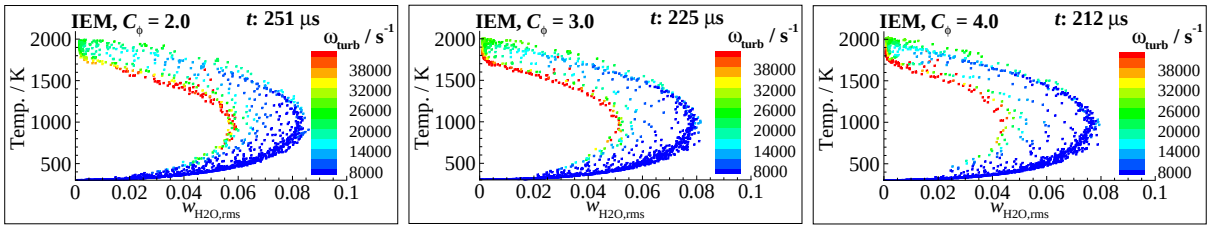

Figure 4: Scatter plot of temperature against RMS mass fraction fluctuation of H_2O for simulations with various C_ϕ. The plot is color-coded by turbulence frequency $\omega_{\mathrm{turb}}/\mathrm{s}^{-1}$.

micro-mixing (using higher values of C_ϕ) leads to higher reaction rate, consequently, heat release due to reaction dominates the heat dissipation caused by turbulence.

4 Conclusion

Here we reported an application of a stand alone Probability Density Function (PDF) method to study ignition of premixed hydrogen/air mixtures by hot turbulent jets. The results show the influence of turbulence on mixing and ignition processes. The simulations performed include hot turbulent jets with various conditions at inlet boundary. Here due to limited space only one example is presented. In the current study, the hot jet is exhaust gas of hydrogen/air near equilibrium and the corresponding exit temperature is about $2000\,\mathrm{K}$. The heat loss at the nozzle is not accounted for. The flow at the nozzle exit is assumed to be a fully developed turbulent pipe flow having streamwise velocity of $300\,\mathrm{m/s}$ at the jet centre. The ambient is quiescent cold ($300\,\mathrm{K}$) stoichiometric mixture of hydrogen/air. The results show at the beginning where the turbulent mixing is at its high the hot jet cools down and reaction rate cannot compensate the heat dissipation due to turbulent mixing, therefore, ignition is suppressed. Further downstream, as turbulence frequency is decreased re-ignition takes place. These observations are in accordance with the experimental findings in [5, 10] and investigation of turbulence effect on the ignition length by Markides and Mastorakos [7]. Although the results were not presented explicitly, the influence of jet velocity was also investigated in the current studies. The investigation has shown that the ignition length increases by increasing nozzle exit velocity, not only due to a higher transport. Also the higher jet velocity leads to increased turbulent mixing which suppresses the ignition and, therefore, additionally increases the ignition length. This is in accordance with the other results presented in this paper. However, a detailed analysis of the dependence of the ignition length on parameters like stoichiometry or temperature of the jet was not performed in this study.

Future work should address further the impact of inlet condition (turbulence, velocity profile, inlet geometry, temperature, etc.) on ignition delay time. An extension to two-dimensional manifolds would also allow to account for heat losses at the nozzle, which will be part of future work for a better description of the experimental configuration [5]. Using conditions that are close to experiments will allow more quantitative investigations of the turbulent ignition process. This information may provide

more insight about the mechanisms behind ignition processes initiated by hot jets in order to prevent accidental explosions which is the main motive of the ongoing research.

Acknowledgements

This work was supported in part by Underwriter Laboratories Inc. Northbrook, Illinois and in part by the Deutsche Forschungsgemeinschaft within the Research Group FOR 1447.

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