Statistical Analysis of Pulsating Methane Flames issued into Hot Co-flow by LES with FGM

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Abstract
This work presents a statistical analysis of an auto-igniting impulsively started jet flame issuing into hot and vitiated co-flowing oxidizer. This analysis uses data from a high-fidelity Large-Eddy Simulation with multidimensional detailed tabulated chemistry. The results are first validated against the (statistically) steady jet experiment from the German Aerospace Center, then the computed ignition delay times and spots are cross-checked with the same experiment, but now for a transient injection. A good agreement is achieved between the LES and the experiments, convincing to go further with the statistical analysis. For the statistics, the probability density functions and conditional means of temperature and important species-concentrations are evaluated during the pulses. Initial observations yield that the ignition-related species HO_2 and CH_2O show different properties than the flame related species OH. The probability of finding a high concentration of the ignition-related species increases until the flame becomes stabilized then decreases afterward. It is observed that these high species-concentrations first appear in the most-reactive mixture fraction before the ignition, later are visible towards the stoichiometry. After the flame stabilizes, mostly low-concentrations of these species are found in the fuel-rich zones.

Introduction
Direct injection and ignition play a significant role in many combustion systems including Diesel and gasoline engines. The ongoing chemistry in these systems is governed by ignition and mixing dynamics. Even small perturbations of temperature, pressure, turbulence intensity, gas composition and scalar dissipation rate influence ignition, hence the combustion [1]. This leads that the ignition dynamics determine the efficiency and the safety of the combustor. A detailed overview of studies on AI is given in the review paper by Mastorakos [1].
The studies showed that the self-driven ignition, or auto-ignition (AI), takes place in the form of local ignition kernels emerging at the most-reactive mixture fraction, away from stoichiometry, at low scalar dissipation rates (SDR) [2]. This work combines the high-fidelity flow fields that are obtained from high-resolution Large-Eddy Simulation (LES) with advanced tabulated chemistry approach Flamelet Generated Manifolds (FGM) [3], which enables an accurate description of the AI in a transient jet flame.

In the present work, the experiment from DLR (German Aerospace Center) [4-5] is reproduced. The objectives are; i. to validate the models by comparing the LES data against the experimental ones for (statistically) steady jet, and by cross-checking the predicted and measured ignition delay and flame stabilization times for transient jet; ii. to present a time-history of a transient flame's statistical behavior during an injection-cycle.

Modeling

For the combustion model, eight auto-igniting unsteady one-dimensional counter-flow flames (flamelets) are precomputed with the GRI-3.0 mechanism [6] using FlameMaster by Pitsch [7]. Flamelet simulations consider methane on the fuel side and hot and vitiated hydrogen/air mixture on the oxidizer side and vary the Scalar Dissipation Rates (SDR) in a range from 0.1 to 1000 1/s. These selected SDRs are chosen such that the S-curve is correctly described. The Lewis number is assumed to be unity. The ignition history is used to fill the manifold's composition and progress spaces controlled by the mixture fraction Z and the progress variable $Y_p = Y_{CO2}+Y_{CO}+Y_{HO2}$, and the third dimension includes the local effect of SDR on AI.

The pressure dependency is considered in the manifold by analytical functions [8], where the fit parameters of these functions are first pre-computed from the reference and perturbed flamelet simulations, then are re-computed in the LES simulations to adjust temperature, gas constant, heat conductivity and reaction source terms. In the perturbed flamelet simulation, the oxidizer and the fuel inlet temperatures are increased by 500 K and 100 K, respectively.

The manifold is accessed in the subsequent LES calculations by the transported mixture fraction, progress variable, total energy, and the computed SDR. The sub-grid fluctuations of Favre-filtered mixture fraction are considered via the top-hat filtered density function (FDF) method [9]. The flame is thickened to the order of the LES grid size by the artificial thickened flame (ATF) method [10].

Setup

In the experiment by Papageorge et al. [4-5], a high-velocity fuel (U_f = 177 m/s) emanates into a laminar co-flowing oxidizer of hot exhaust products of a lean hydrogen/air mixture (U_{co} = 4 m/s) at atmospheric pressure. The injector nozzle has a 1.5 mm diameter, leading to a jet-Reynolds number of 16,000 and a local-Mach number of 0.65. Further information is given in Table 1.

Table 1. Boundary conditions for the fuel and the oxidizer.

Fuel		Oxidizer				
Z_{st}	T_f [K]	T_o [K]	X_{N2}	X_{O2}	X_{H2O}	X_{OH}
0.034	290	1495	0.719	0.102	0.178	0.001

Experimentalists [4-5] measured the mixture fraction and temperature fields for 300 injections-cycles using high-speed Rayleigh scattering. They determined the AI delay times and ignition kernels for each realizations.

In-house LES and DNS solver PsiPhi [11,12] has been used for the LES in this work. Favre-filtered governing equations are solved with a low-storage explicit Runge-Kutta scheme. Convective fluxes of momentum are treated with a central differencing scheme blending over into a TVD scheme (MUSCL [13]) for Mach numbers greater than 0.2, and the rest with total variation diminishing (TVD) scheme.

The computations use an 80x45x45 mm^3 domain, which consists 48 Million equidistant cells with 0.15 mm spacing. The simulation requires 0.2 million compute hours per pulse cycle using 1296 cores in parallel through MPI.

The unresolved fluxes in momentum and scalars are estimated from eddy-viscosity and eddy-diffusivity approaches at a Turbulent Schmidt number of 0.7, respectively. Turbulent viscosity is determined by Nicoud's σ-model [14], and the Lewis number is assumed to be unity.

Results

The simulated (statistically) steady jet flame with the experimental line-plots have been initially compared. Then, the transient jet flame has been validated by comparing the ignition delay and flame stabilization times of simulations over 20 pulse-cycles to the experiments. In both cases, a good agreement between the predictions and the experiments has been observed, providing evidence that this model is suitable for this study.

For the statistical analysis, the second injection cycle is selected for post-processing. The hydroperoxyl HO_2 and formaldehyde CH_2O are chosen to study the ignition since they indicate the start and the progress of the AI. The time-history of the joint-Probability Density Function (JPDF) of the simulated normalized Y^*_{CH2O} over the mixture fraction is shown in Fig. 1. The Y^*_{CH2O} peaks in the stoichiometric mixture fraction, however, the probability of this species is highest in the lean-mixture, which coincides with the most-reactive mixture fraction, which has a value of 0.021. After the AI at 2.3 ms, the probability of this species increases towards the stoichiometry. It is also observed that the Y^*_{CH2O} shows an increase in its probability on the rich-zones just after the flame stabilizes at 4 ms.

The flame front can be identified by the mass fraction of hydroxyl OH. In the LES, the flame and ignition show quite distinctive statistical behavior. This can be seen in Fig. 1 from the time-history of the JPDF for the computed normalized Y^*_{OH} and the mixture fraction. Contrary to the Y^*_{CH2O}, the probability of high OH concentrations is observed on much leaner-mixture than the most-reactive one. This probability increases until the flame stabilized, then remains constant, however, on a wider mixture fraction spectrum.

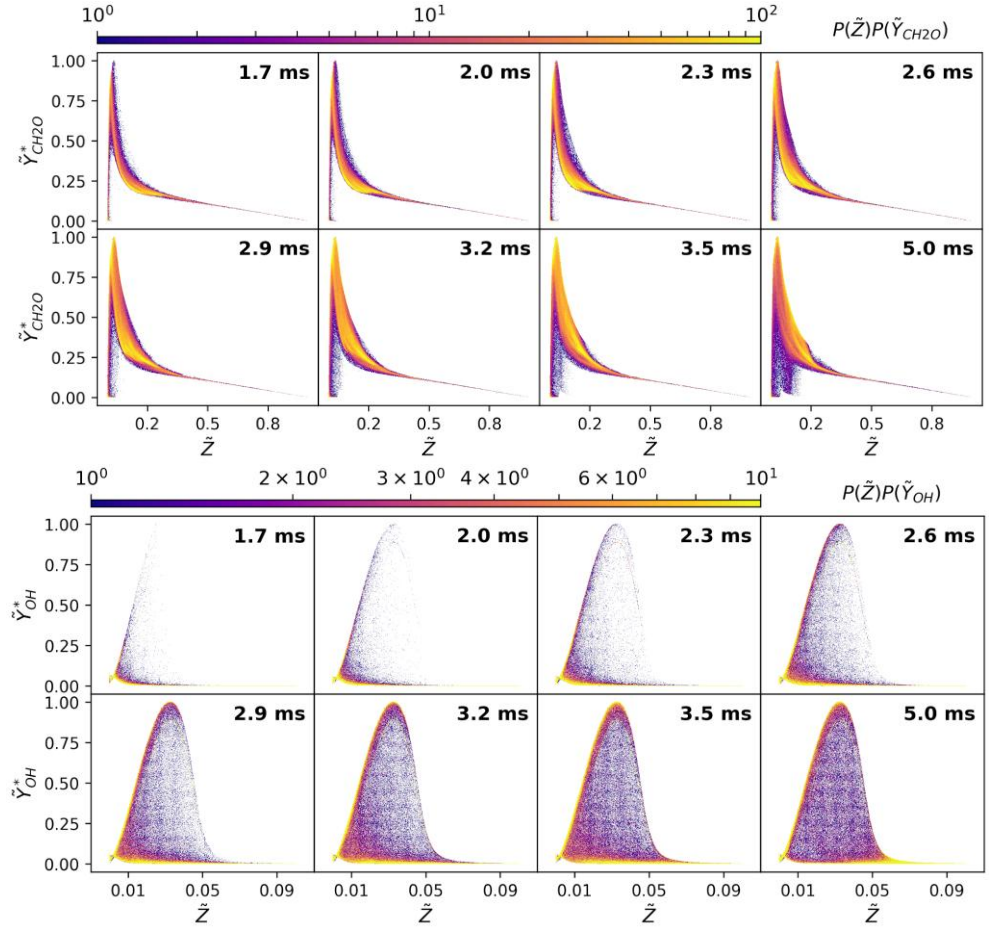
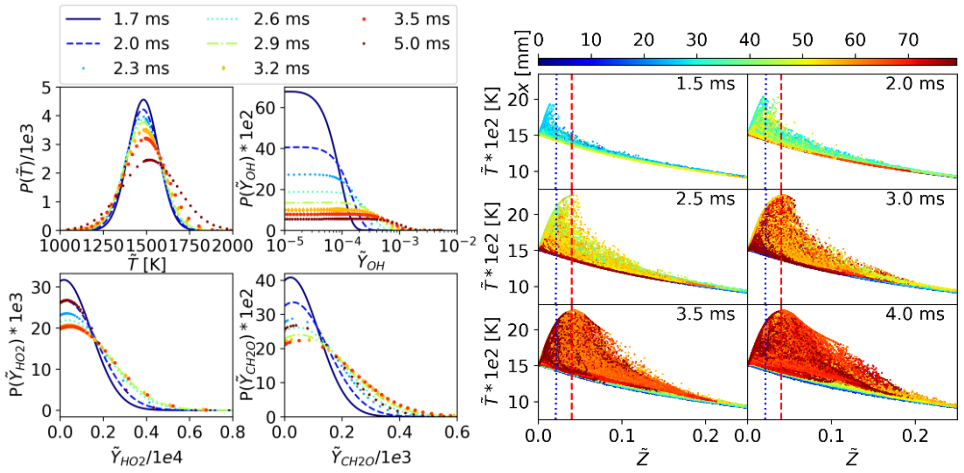


Figure 1. The time-history of normalized Y^*_{CH2O} (top) and Y^*_{OH} (bottom) over the mixture fraction colored by their JPDF.

The time-history of the PDFs of the predicted temperature, ignition related species Y_{HO2} and Y_{CH2O} and flame related species Y_{OH} are given in Fig. 2a. The highest temperature probability decreases until the AI, meanwhile, the distribution of the probability becomes wider over time. At the same time, similarly, the probability of higher Y_{OH} increases and is available on wider mixture fraction spectrum. On the other hand, the probability of finding high concentrations of ignition related species HO_2 and CH_2O increases until the flame stabilizes then decreases afterward.

It should be noted that the ignition-related species form even after the AI since the freshly injected gas must also ignite. However, the quantity of the ignition spots that form during the steady injection is fewer than the spots that form during the transient injection, which is due to the vortex pinch-off. Hence, the ignition-related species-concentrations could not maintain their high-values at later times.

Figure 2b shows the scatter plots of the temperature over the mixture fraction at several times of a pulse, colored by the distance from nozzle-exit. It can be seen that a temperature increase is visible even before the AI, however, this increase is not enough to trigger AI. Before the AI, the high-temperature values emerge on the most-reactive mixture fraction at an axial distance of x=30 mm. During the ignition, the AI kernel expands from this mixture to the richer zones. After a stable flame is established, the clustered high temperatures move to further downstream positions of x>60 mm.



(a) (b)

Figure 2. The time-evolutions of PDFs of the temperature and relevant species (a), and of the temperature over the mixture fraction, colored by the distance from the nozzle-exit (b) during an injection. Dotted and dashed lines denote most-reactive and stoichiometric mixture, respectively

Conclusions

A good agreement was obtained between the LES and the experiments of the (statistically) steady and pulsed auto-igniting jet flames. The tested combustion model performed reasonably well, imposing low computational costs. The estimated AI delay times and ignition kernels were in a good agreement with the experiments, which normally require more costly combustion models.

Statistics showed that the ignition-related species HO_2 and CH_2O started forming at lean-zones, then formed at the richer-zones after the flame became stabilized. These species also form in a much larger quantity at the initial injection phase than the steady injection phase.

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