Numerical study of the ignition behavior of a post-discharge kernel in a turbulent stratified crossflow

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Abstract

Ensuring robust ignition is critical for the operability of aeronautical gas-turbine combustors. For ignition to be successful, an important aspect is the ability of the hot gas generated by the spark discharge to initiate combustion reactions, leading to the formation of a self-sustained ignition kernel. This study focuses on this phenomena by performing simulations of kernel ignition in a crossflow configuration that was characterized experimentally. First, inert simulations are performed to identify numerical parameters correctly reproducing the kernel ejection from the ignition cavity, which is here modeled as a pulsed jet. In particular, the kernel diameter and the transit time of the kernel to the reacting mixture are matched with measurements. Considering stochastic perturbations of the ejection velocity of the ignition kernel, the variability of the kernel transit time is also reproduced by the simulations. Subsequently, simulations of a series of ignition sequences are performed with varying equivalence ratio of the fuel-air mixture in the crossflow. The numerical results are shown to reproduce the ignition failure that occurs for the leanest equivalence ratio ($\phi = 0.6$). For higher equivalence ratios, the simulations are shown to capture the sensitivity of the ignition to the equivalence ratio, and the kernel successfully transitions into a propagating flame. Significant stochastic dispersion of the ignition strength is observed, which relates to the variability of the transit time of the kernel to the reactive mixture. An analysis of the structure of the ignition kernel also highlights the transition towards a self-propagating flame for successful ignition conditions.

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1. Introduction

Driven by the need for reduced pollutant emissions, modern gas-turbine engines adopt lean combustion concepts [1]. However, using leaner...
mixtures is accompanied with the adverse effect of reduced ignition propensity [2]. This is particularly important at high altitudes, where low ambient temperature and pressure further deteriorate conditions for successful ignition, making robust relight capabilities critical for the safe operability of aviation engines. In addition, there is now strong interest in deploying alternative jet fuels, allowing for energy independence and sustainability. Their chemical properties, however, differ from conventional jet fuels, which can also have a significant impact on ignition properties and flame stabilization [3,4].

The ignition sequence in a gas turbine can be divided into several phases [5]: transition from spark and plasma phase to kernel development, followed by kernel propagation and eventually successful flame stabilization. These different processes have been studied experimentally in various configurations, such as turbulent jet flames [6], premixed swirl flames [7], and annular combustors [8,9]. However, most numerical studies of ignition have focused on kernel propagation, flame stabilization [10–12], and burner-to-burner propagation [13–15]. A main limitation of these studies is the description of the combustion initiation by kernel ignition, for which simplified models [10] based on energy and radical deposition are commonly used. A more detailed modeling of the kernel formation and initial growth is challenging as it often requires accounting for the transition from the plasma phase following the spark discharge to the fuel oxidation chemistry [16,17], involving chemical coupling processes that are not yet fully understood. Thus, these models only provide an incomplete description of ignition failures related to early kernel formation and growth. These failure scenarios can be significant in realistic gas turbines, where, for practical reasons, the ignition system is placed at the combustor wall rather than close to the fuel injection axis. In these circumstances, successful ignition strongly depends on the ability of the hot gases arising from the spark discharge to transit to a flammable region, mix with reactants and initiate the combustion, leading to a self-sustained flame.

To examine ignition mechanisms and failures at early stages of the kernel development, this study considers an experimental configuration, consisting of the ejection of a hot kernel into a stratified methane-air crossflow [18]. An important feature of this experiment is that the hot-gas kernel from the spark discharge is convected through an inert mixture prior to reaching the reactive mixture. This temporal and spatial separation of the plasma phase and subsequent combustion initiation by the ignition kernel alleviates the modeling complexity needed for the plasma phase. Similarly to realistic gas-turbine combustors, a spark ignition system is used. Although a gaseous fuel is considered, many of the key physical mechanisms of gas turbine ignition are reproduced with this configuration, such as high variability and varying local flow conditions and mixture composition.

The main objective of this study is to examine numerically the initial on-set of reactions and stochastic variability of spark kernel combustion initiation with realistic chemical kinetics, providing insight into early-stage ignition failure mechanisms that occur in partially-premixed and stratified combustion systems. The ability of the simulations to reproduce the major trends from the experimental data, such as the impact of equivalence ratio and transit time on the ignition behavior is also demonstrated. The experimental configuration under consideration is described in Section 2 and the computational setup is discussed in Section 3. Boundary conditions for the kernel ejection from the igniter cavity are discussed in Section 4. A methodology is developed to reproduce the experimentally observed ejection phenomena that is specific to this problem, by comparison between simulations and Schlieren measurements. Finally, reactive simulations are performed for various operating conditions in Section 5, comparing kernel ignition trends with experimental ignition probabilities and analyzing transition mechanisms of the kernel from a hot inert gas mixture to self-sustained propagation. The paper closes with conclusions given in Section 6.

2. Experimental configuration

The experimental configuration is detailed in [18,19]. A schematic of the facility is shown in Fig. 1. In this configuration, the stratification of the crossflow into a flammable fuel-air mixture and a non-flammable air-mixture is imposed using two streams that are separated by a splitter plate, located at a height \( h_s \) from the bottom wall, that ends 13 mm upstream of the ignition system. The spark discharge is created in a small cavity by a commercial igniter with reported energy of \( E_{\text{spark}} = 1.2 \, \text{J} \). Through thermal expansion following the discharge, the kernel transits into the crossflow. Varying \( h_s \) allows for the control of the characteristic transit time \( \tau_{\text{transit}} \), defined as the time it takes for the kernel to traverse the non-flammable air mixture and reach the flammable mixture at height.
$h_i$. Control over the flow velocity, equivalence ratio, crossflow inlet temperature and splitter plate height allows for a systematic investigation of the ignition probability over a wide range of operating conditions. Measurements of the ignition probability, Schlieren imaging and integrated OH* chemiluminescence are available. For the present study, the fuel considered is natural gas (represented by methane), and the operating point selected corresponds to a crossflow velocity $u_{in} = 20 \text{ m/s}$, crossflow temperature $T_{in} = 456 \text{ K}$, and a splitter plate height $h_i = 6.4 \text{ mm}$.

3. Computational setup

3.1. Numerical method

The simulations are performed with the finite-volume solver CharLES$^4$, solving the compressible reacting Navier–Stokes equations. For convective fluxes, a hybrid scheme is applied, consisting of a fourth-order central scheme and a second-order essentially non-oscillatory scheme [20] which minimizes the numerical dissipation [21]. Chemical source terms are evaluated using finite-rate kinetics with a semi-implicit Rosenbrock–Krylov scheme [22,23].

3.2. Computational domain and boundary conditions

The numerical domain is 73 mm long, with a rectangular cross section of 30 mm width and 50 mm height, compared to $54 \times 86 \text{ mm}$ in the experimental setup. It was verified that the reduced cross section considered in the simulation does not induce any significant confinement effects. Lateral and bottom walls are modeled with adiabatic no-slip boundary conditions, and a constant pressure ($P = 1 \text{ bar}$) is imposed at the outlet. The domain inlet corresponds to the location where the splitter plate ends. To reproduce the inflow condition, a constant axial velocity of $u_{in} = 20 \text{ m/s}$ is applied. Turbulent velocity fluctuations are superimposed with intensity of $u' = 2 \text{ m/s}$ based on experimental root-mean-square (rms) velocity levels [19] with an integral length of $h_i/2 = 3.2 \text{ mm}$, leading to a turbulent Reynolds number ranging from $Re_t = 100 – 380$ for conditions evaluated with respect to kernel temperature and crossflow air temperature.

A pure air stream is imposed below the splitter plate height ($z < h_i$) and a premixed methane-air mixture at an inlet temperature $T_{in}$ is prescribed above. The kernel ejection is modeled by a temporally varying boundary condition embedded at the bottom wall, which is further detailed in Section 4.

The domain is discretized with a uniform grid size of $\Delta = 0.25 \text{ mm}$ in the three spatial directions, resulting in a total of 7 millions hexahedral elements. The subgrid stress contribution is neglected.

This was validated by performing simulations with the Vreman eddy-viscosity model [24], showing marginal impact of subgrid stress modeling on the flow and kernel properties at this level of grid resolution. The subgrid contribution of turbulence chemistry interaction is also neglected and the transport of scalars with chemical source terms is directly resolved on the grid. It was verified on laminar flame computations that the grid resolution is adequate to capture the chemical scales of the reaction zones and to recover the flame structure.

3.3. Chemical kinetics

The methane-air oxidation and NOx chemistry are described by a reduced mechanism consisting of 22 transported species and 21 species in quasi-steady state approximation [25], based on the GRI 3.0 mechanism [26], which was validated for non-premixed, premixed and auto-igniting flames [25,27].

4. Kernel ejection model

The kernel formation process comprises an energy deposition phase with plasma formation in the igniter cavity followed by a rapid expansion into the main stream. Correctly describing this process requires the accurate modeling of the plasma physics [17] which is beyond the scope of this work. However, in order to capture the key physical processes that are relevant for ignition, only the post-expansion behavior of the kernel is considered in this study, by formulating a numerical methodology based on the zero-dimensional model from Sforzo et al. [18]. The methodology is developed and calibrated specifically for this problem using the available experimental data, but it can be also applicable to other ignition problems provided that sufficient data about the kernel formation is available either from experiments or high-fidelity spark discharge simulations [17].

4.1. Zero-dimensional thermodynamic model

The model describes the kernel formation by idealized transformations, which are schematically illustrated in Fig. 2. In a first step, the air inside the igniter cavity ($V_0 = 0.2 \text{ cm}^3$) receives an energy deposition, $E_{spark} = 1.2 \text{ J}$, from the spark discharge.
Assuming an isochoric heat addition, the intermediate equilibrium state of the kernel is computed using the air plasma mechanism from Schulz et al. [28], leading to a post-discharge temperature \( T_1 = 5300 \text{ K} \) and pressure \( P_1 = 1 \text{ bar} \). The second step considers an isentropic expansion of the ionized mixture to the main flow pressure \( (P_2 = 1 \text{ bar}) \) leading, under the assumption of chemical equilibrium, to a final temperature of \( T_2 = 3300 \text{ K} \). This equilibrium hypothesis appears to be reasonable when comparing the typical life-time of plasma atomic species \((O(10 \mu s))\) to the transit time of the kernel to the flammable region \((\tau_{\text{transit}} = O(100 \mu s))\) [29]. The resulting composition, given in Table 1, shows good agreement between equilibrium obtained with the reduced mechanism and the air-plasma mechanism. It was found that all mole fractions of the ionized species and electrons are below \( 10^{-7} \). Thus, the reduced mechanism equilibrium composition and temperature without considering plasma ionized species are used as boundary condition for the kernel in the simulations. From mass and total enthalpy conservation, the final volume \((V_2 = 1.5 \text{ cm}^3)\) and velocity of the kernel \((U_2 = 3350 \text{ m/s})\) are also deduced. However, it was experimentally reported [18] that only a fraction of the total kernel volume may actually enter into the main chamber and other non-idealities such as shock waves and wall losses can reduce the initial kernel velocity. Therefore, these two values are later adjusted (Section 4.4) by matching estimations of kernel volume and trajectory obtained from high-speed Schlieren measurements.

### 4.3. Kernel inlet forcing

In the experiments, a significant variability of the transit time is observed, which may be attributed to the stochastic variability for one spark discharge to another. For the conditions considered here \((h_t = 6.4 \text{ mm})\), the mean transit time to the splitter plate height is \( \tau_{\text{transit}} = 40 \mu \text{s} \) [19], and a dispersion of \( \pm 10 \mu \text{s} \) was reported in the measurements, which corresponds to a typical deviation of 25%. To mimic this dispersion numerically, a random forcing with 20% turbulent intensity is imposed on the kernel boundary condition, with a length scale matching the kernel diameter.

### 4.4. Cold flow kernel ejection: parameters calibration

The aim of the calibration is to find suitable values for the remaining controlling parameters of the kernel boundary conditions \((U_{\text{ker}}\) and \(\tau_{\text{pulse}}\)), through comparisons against experimental results. To this end, non-reactive simulations are performed. It was verified that the feedback from chemical reactions (typically through heat release) is not strong enough to influence the kernel kinematics at early stages \((t = 0 - 500 \mu \text{s})\), therefore the calibration is expected to remain valid for reactive conditions. The boundary conditions are selected by matching kernel volume and kernel trajectory with experimental estimations obtained by edge tracking the Schlieren images. A similar methodology is used in the simulations, where the kernel boundary is determined by thresholding line-of-sight (LOS) results of numerical Schlieren data \((\nabla p/p)\). The kernel volume \(V_{\text{ker}}\) issuing from the boundary condition scales as \(V_{\text{ker}} \propto U_{\text{ker}} \Delta t\), whereas the kernel transit time scales with the injected momentum \(J \propto U_{\text{ker}}^2 \Delta t\). Based on this scaling, the two parameters are adjusted to match these criteria. Final values of \(U_{\text{ker}} = 2000 \text{ m/s}\) and \(\tau_{\text{pulse}} = 3 \mu \text{s}\) are obtained and used for all following calculations. The comparison of one experimental kernel ejection and an unforced numerical sequence (without superimposing any kernel velocity fluctuations) is shown in Fig. 3. Note that the bright emission obscures the experimental Schlieren results at early

### Table 1

Post expansion \((T_2 = 3300 \text{ K, } P_2 = 1 \text{ bar})\) equilibrium kernel composition in mole fractions. Comparison between a) air plasma mechanism [28] and b) reduced methane-air mechanism [25].

<table>
<thead>
<tr>
<th></th>
<th>(X_{N_2})</th>
<th>(X_{O_2})</th>
<th>(X_{NO})</th>
<th>(X_N)</th>
<th>(X_O)</th>
<th>(X_{NO_2})</th>
<th>(X_{N_2O})</th>
</tr>
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<tbody>
<tr>
<td>(a)</td>
<td>0.72</td>
<td>0.12</td>
<td>0.049</td>
<td>(8 \times 10^{-5})</td>
<td>0.11</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>(b)</td>
<td>0.74</td>
<td>0.14</td>
<td>0.054</td>
<td>–</td>
<td>0.062</td>
<td>(3 \times 10^{-5})</td>
<td>(4 \times 10^{-6})</td>
</tr>
</tbody>
</table>
Fig. 3. Time sequence of kernel trajectory. Comparison between (a) experimental Schlieren images with edge tracking lines (green line) and centroid (red point) and (b) LOS integration of numerical Schlieren for an unforced kernel ejection with threshold line used to define kernel boundaries. The horizontal white line indicates the height of the splitter plate. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. Temporal evolution of (a) kernel diameter and (b) height of the kernel centroid. Comparison between fits from experiments (○), unforced case (●) and five forced cases (⋯).

instant \( t < 40 \mu s \). This comparison shows that a good qualitative agreement is obtained in terms of kernel size, shape and temporal evolution, resulting in a comparable transit time with measurements. A quantitative comparison of kernel diameter is performed by comparing Schlieren results and LOS integration for the unforced kernel ejection, and five forced cases (20\% kernel random velocity fluctuations). The resulting kernel diameter, shown in Fig. 4, is close to the experimental range, and the forcing has a marginal impact on the resulting kernel diameter. Similarly, the trajectory of the kernel centroid of Fig. 4 shows good agreement between simulations and measurements for the unforced case. For the five forced cases, the forcing leads to a dispersion of the trajectories. The dispersion level can be quantified by evaluating the transit time of the leading edge and centroid of the kernel to the height of the splitter plate. Over the ensemble of cases considered in this study, the kernel transit time is \( t_{\text{le}} = 51 \pm 11 \mu s \) for the leading edge and \( t_{\text{cent}} = 137 \pm 25 \mu s \) for the centroid compared to \( 40 \pm 10 \mu s \) and \( 120 \pm 15 \mu s \), reported for the experiments.

5. Reactive cases

Four operating conditions are chosen to investigate different ignition behaviors. These conditions are: \( \phi = 0.6 \), corresponding to zero ignition probability in the experiments; \( \phi = 1.2 \), for which the probability of ignition reaches a maximum \( P_{\text{ign}} = 80\% \) and \( \phi = 0.8 \) and \( \phi = 1.0 \) having intermediate behaviors. For each equivalence ratio, five kernel ejection realizations are simulated, compared to typically \( O(100) \) kernel events to construct converged probabilities in the experiments. Note that a different initial crossflow field is randomly selected to start each simulation, to capture the potential ignition variability due to mixing layer fluctuations. The number of realizations is limited by the CPU cost for one simulation, which is about 40,000 CPU hours on the NASA HPCC Pleiades cluster (Ivy Bridge architecture), leading to a total cost for all calculations of 800,000 CPU hours.

5.1. Ignition behavior

As a first metric to assess the kernel transition to a propagating flame, we examine the temporal evolution of the total heat release rate in the domain, normalized with the overall maximum value observed at \( t = 2 \) ms. Figure 5 shows the comparison for the different operating conditions. For all cases, a steep increase is observed at early instants \( t < 0.15 \) ms, corresponding to the kernel transit phase from the bottom wall to the mixing layer. During this phase, the dilution by inert air from the crossflow leads to exothermic recombination of radicals that are initially present in the kernel. A second phase is observed for \( t \geq 0.1 - 0.5 \) ms. During this time interval, the kernel travels through a fuel-air mixture, and thus starts entraining reactive mixture in hot regions of the kernel. This is illustrated in Fig. 6, showing mid-plane temperature fields at different time instances. Around \( t = 0.5 \) ms, the temperature fields of Fig. 6 show that the kernel is fully engulfed into the premixed mixture but has not grown significantly yet. Some ignition events
occur, as shown by the heat release isocontours in Fig. 6. They preferentially occur in the downstream (right part) of the kernel. This region of the kernel is not directly exposed to the incoming crossflow. It results in lower strain rates and entrainment, that are more favorable to non premixed-ignition [30]. From these local ignition events, full kernel ignition may eventually start, which translates into a rapid increase in the heat release rate for $\phi = 1.0$ and 1.2 after 0.5 ms (Fig. 5), and significant spatial growth of the hot kernel region and reacting zone (Fig. 6) for $t > 0.5$ ms, indicating successful ignition events for these operating conditions. Conversely, for $\phi = 0.6$, a plateau in the heat release is observed, the hot region shrinks under the effect of mixing with the surrounding cold environment, without any onset of a strongly reacting front that is characteristic of a self-propagating kernel.

To compare the ignition propensity, a qualitative metric for successful ignition characterization is defined. Experimentally, the ignition success criterion is based on a visual inspection of the OH* chemiluminescence signal for $t > 2$ ms. Since these measurements are only qualitative, a direct comparison with simulations of this particular metric is difficult. Instead, this work defines an Ignition Propensity (IP) as a qualitative measure by evaluating the normalized total heat release rate at $t = 2$ ms. Figure 7 shows the direct correlation between these two metrics for the ensemble of cases considered. These results indicate that the chemical impact of varying the equivalence ratio is adequately captured in the simulations. However, we note that certain kernel ignition failures are not captured in the simulations, and could be attributed to an overestimation of the actual kernel temperature or the underestimation of the turbulent mixing rate.

5.2. Detailed analysis of ignition sequence

A detailed analysis of the ignition sequence is performed for two ignition realizations at $\phi = 0.6$ and $\phi = 1.0$, previously shown in Fig. 6. Based on a fuel stream tracer $\xi_f$, which is equal to 1 at the fuel inlet, the mixture fraction is evaluated as $Z = Y_{CH_4}^{\phi} \xi_f$, where $Y_{CH_4}^{\phi}$ is the fuel mass fraction at the fuel-air crossflow inlet. Another tracer from the kernel could also be used to fully describe the mixing in this three-stream problem. However, this was found not to be necessary for the analysis of the ignition process. Mean temperature and integrated heat release rate are extracted in the kernel region from solutions at different times ($t = (0.5, 1, 1.5, 2)$ ms) and conditioned on $Z$. The evolution of the conditional mean temperature and integrated heat release rate is shown in Fig. 8, along with probability density functions (PDF) for mixture fraction. The temperature levels are significantly lower than the initial kernel temperature, because of the dilution by cold air from the crossflow. For the lean case (Fig. 8a), at $t = 0.5$ ms the temperature is initially high at low mixture fraction, and decreases quasi-linearly with mixture fraction, showing the mixing by entrainment of fresh reagents into the ignition kernel.

For non-premixed flames, the ignition is expected to preferentially occur around the most reactive mixture fraction [30], which is located at very lean conditions for methane at atmospheric pressure [27,31]. In the present case, the reactivity is further enhanced at very lean conditions by the high temperature. Based on 0D autoignition computations, the most reactive mixture fraction is $Z_{nr} \approx 0.004$, assuming a temperature of 2100 K for the kernel after dilution at $Z = 0$. Consistently with this picture, the initial peak in the conditionally integrated heat release rate occurs at very lean
conditions, around $Z = 0.008$, as shown in Fig. 8a. At subsequent instants, because of further fuel-air mixture entrainment, the mixture fraction distribution shifts towards richer mixtures, as shown by the mixture fraction PDF in Fig. 8a. Accordingly, the conditionally integrated heat release rate shifts towards richer regions, but the total integrated heat release plateaus. As a result, the temperature remains close to the mixing levels, without significant increase in the reaction region, indicating a failed transition to a sustained flame propagation.

For the stoichiometric case, a similar behavior is observed for the mean temperature and integrated heat release rate (Fig. 8b) for the first instant ($t = 0.5$ ms). However in this case, the integrated heat release rate dramatically increases and a continuous transition towards higher mixture fraction conditions occurs. This propagation in mixture fraction space strongly resembles the scenario that is observed for counterflow non-premixed flames [32], thus indicating a non-premixed ignition mode.

At $t = 2$ ms, the heat release rate peaks near the mixture fraction of the fuel stream, indicating that the kernel transitions to a premixed burning mode at the crossflow fuel-air stream equivalence ratio. This is supported by the mean temperature evolution (Fig. 8b), evolving from mixing levels at $t = 0.5$ ms to reach levels close to the stoichiometric adiabatic flame temperature at $t = 2$ ms.

![Fig. 8. Mixture fraction PDF (top), conditional mean temperature (middle), and integrated heat release rate (bottom) conditioned on mixture fraction at four different instants ($t = [0.5, 1, 1.5, 2]$ ms) for (a) lean condition and (b) stoichiometric condition. The vertical line indicates the mixture fraction of the crossflow fuel-air stream.](image)

5.3. Impact of the kernel transit time

The previous analysis highlights the significant reduction of temperature levels by air entrainment in the kernel. The amount of air entrainment is related to the residence time of the kernel in the lower crossflow stream, which is controlled by the kernel transit time. In turn, it impacts the global reactivity of the kernel, as evidenced from the negative correlation obtained between IP and $\tau_{transit}$ for the ensemble of cases (Fig. 9). This suggests that the kernel transit time is one of the key parameters in the variability of the ignition behavior.

6. Conclusions

In this work, computations of multiple realizations of kernel ejection into a stratified crossflow are performed to examine effects of flow composition and stochastic variability of the ignition kernel. Kernel ejection conditions are identified based on a zero-dimensional thermodynamic model. To account for non-idealities of the plasma igniter, a calibration step is included with experimental results for non-reacting conditions. Several kernel ejection realizations are simulated at four different operating conditions by varying the crossflow equivalence ratio. The strong dependency of the ignition behavior to the crossflow equivalence ratio is well reproduced numerically, capturing systematic ignition failures for the leanest conditions.

The detailed analysis of the kernel structure shows that the kernel ignition is typical of a non-premixed forced ignition process [30]. Ignition is initially triggered at lean conditions for all cases, where the mixture reactivity is the highest under the combined effect of high auto-ignition propensity of methane-air mixture at very lean conditions and high temperature. Depending on the conditions, reacting regions may propagate towards richer mixtures close to the overall equivalence ratio of the premixed fuel-air stream, eventually leading to a sustained premixed propagation mode.

Significant variability is also observed between realizations. It is strongly related to the kernel transit time in the crossflow, which controls the kernel dilution by cold air and in turn its reactivity. A good
correlation is obtained between experimental ignition probability and numerical ignition intensity. However, no ignition failure is observed in simulations for $\phi \geq 0.8$, which requires further investigations, by analyzing the sensitivity of the ignition onset to kernel temperature, turbulent mixing and kernel dilution.

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