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Large eddy simulation of a premixed flame in hot vitiated crossflow with analytically reduced chemistry

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ABSTRACT

This numerical study deals with a premixed ethylene-air jet at 300 K injected into a hot vitiated crossflow at 1500 K and atmospheric pressure. The reactive jet in crossflow (RJICF) was simulated with compressible 3-D large eddy simulations (LES) with an analytically reduced chemistry (ARC) mechanism and the dynamic thickened flame (DTF) model. ARC enables simulations of mixed combustion modes, such as autoignition and flame propagation, that are both present in this RJICF. 0-D and 1-D simulations provide a comparison with excellent agreement between ARC and detailed chemistry in terms of autoignition time and laminar flame speed. The effect of the DTF model on autoignition was investigated for varying species compositions and mesh sizes. Comparisons between LES and experiments are in good agreement for average velocity distributions and jet trajectories; LES remarkably capture experimentally observed flame dynamics. An analysis of the simulated RJICF shows that the leeward propagating flame has a stable flame root close to the jet exit. The lifted windward flame, on the contrary, is anchored in an intermittent fashion due to autoignition flame stabilization. The windward flame base convects downstream and is “brought back” by autoignition alternately. These autoignition events occur close to a thin layer that is associated with radical build-up and that stretches down to the jet exit.

Introduction

Jets in crossflow (JICF) have been studied extensively for more than 8 decades [1, 2]. They are employed, for example, in modern combustion systems for aeronautic and power applications (e.g. [3, 4]) for fuel or dilution air injection providing fast mixing between the streams. One can refer to [5] for a recent review about JICF.

In contrast, much less is known about *reactive* jets in crossflow (RJICF) [6], although early works date back to the 1970s [7, 8]. In recent studies, Wagner et al. [9–11] investigated a premixed ethylene-air jet into hot vitiated crossflow experimentally. The authors simultaneously performed hydroxide (OH) and formaldehyde (CH₂O) planar laser-induced fluorescence (PLIF) and particle image velocimetry. Building upon these experimental studies, this numerical paper aims at bringing more insight into the flame dynamics and stabilization mechanisms.

Different types of RJICF have been investigated experimentally and numerically. For experiments with an ignitable mixture in the jet (premixed), one can refer to [13, 14]. The number of experiments with pure fuel inside the jet (non-premixed) is significantly higher, for example [15–19]. Other non-premixed experimental works discuss autoignition as a flame stabilization mechanism. Sullivan et al. [20] injected different fuels in high temperature cross flows ($T_{cf} = 1775$ K). The measured

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Fig. 1. Computational mesh, boundary conditions and dimensions for the 3-D reactive jet in crossflow LES. Experimental configuration was introduced and investigated in [9–11]. Mesh overlaid with instantaneous heat release rate $\dot{q}$ contour. The total number of cells is 11 million. 3-D rendering of isosurfaces of heat release rate $\dot{q}$, hydroxide OH mass fraction and Q-criterion [12] Q visualizing vortical structures.

ignition locations were of the same order of magnitude as locations computed with 0-D reactor simulations and jet velocities. Therefore, the authors proposed autoignition as a stabilization mechanism. Experimental ignition locations of Fleck et al. [21] ($T_{cf} = 1143$ K and 1185 K), on the contrary, were one order of magnitude smaller than 0-D values. Another work [22] ($T_{cf} = 1364$ K) proposed a combination of three distinct combustion regimes for flame stabilization: upstream autoignition, premixed and non-premixed flames. These examples show that there are still open questions about the dominant flame stabilization mechanism for RJICF.

In experiments, it is often difficult or not even possible to analyze flow regions where autoignition is initialized [23]. Autoignition occurs at the most reactive mixture fraction [24], which is the mixture composition with the shortest autoignition time. Often, these mixtures are associated with very low fuel concentrations [25] that cannot be tracked. On the contrary, numerical simulations give access to such critical flow regions, provided that the dominant combustion modes are modeled correctly. For example, RJICF were simulated using large eddy simulations (LES) with one step chemistry ($T_{cf} = 1773$ K) in [26] and a hybrid Eulerian/Lagrangian approach with single step chemistry ($T_{cf} = 473$ K) in [27].

Single step (and also two to four step) chemistry mechanisms are empirically reduced mechanisms [28] that are tuned to match global flame properties. For example, the scheme presented in [29] predicts the adiabatic flame temperature T_{ad} and the burning velocity s_L over a wide range of equivalence ratios; the mechanism in [30] predicts T_{ad} and autoignition delays τ_{AI} for one “design point”. For the present configuration, experimental results [9–11] indicated that both autoignition and flame propagation are likely to play a key role in the flame stabilization mechanisms. In order to model a *mix* of different combustion modes, a global mechanism is not suitable. An alternative is the tabulated flamelet approach [31] which was successfully applied to autoignition flames in combination with a stochastic fields turbulence-chemistry interaction model [32]. For more practical applications [33] however, one drawback of tabulated chemistry is the augmented complexity of the look-up table. For example, main air, cooling air and dilution air at varying inlet temperatures, and fuel injection with varying compositions/fuels can lead to four or five mixing streams. Additionally, to capture the impact of pressure [34] and strain, more dimensions need to be added to the look-up table. Hence, the computing time considerably increases [28], and simulations can become computationally unfeasible due to such high numbers of dimensions. Another alternative is an analytically reduced chemistry (ARC) mechanism (e.g. [19, 25, 35, 36]). A comparison between the tabulated chemistry approach (e.g. five transported scalars) and the ARC mechanism, used in this study [35] (18 transported species), gives an increase of computational costs for ARC by a factor of approximately 2.3. Nevertheless, ARC allows to simulate a great number of mixing streams, and accounts for pressure and strain effects on autoignition and flame propagation.

This work, for the first time, uses LES with ARC to investigate the flame dynamics and flame stabilization of a premixed ethylene-air jet in hot vitiated crossflow ($T_{cf} = 1500$ K), which was examined experimentally by Wagner et al. [9–11]. In the first section of this paper, the geometry and the boundary conditions of the investigated RJICF are presented, together with the numerical methods for the simulation: LES, ARC and the combustion model. This section also investigates the effect of the dynamic thickened flame (DTF) model on autoignition and provides a discussion on the turbulence-chemistry interaction. Second, a comparison of ARC with detailed chemistry is shown with results from 0-D reactors and 1-D flames. Then, results from LES are compared to experiments by considering jet trajectories, average velocity fields and instantaneous fields. Finally, the flame dynamics and stabilization mechanism of the RJICF are analyzed.

Fig. 2. Comparison between detailed chemistry [37] and analytically reduced chemistry (ARC_18_C2H4NARA) at 1 bar. (a) shows autoignition times τ_{AI} obtained from 0-D reactor simulations with Cantera [38]. Mixture fraction Z describes mixing between hot crossflow at 1500 K ($Z = 0$) and the cold premixed ethylene-air jet at 300 K ($Z = 1$). Two additional axis show equivalence ratio ϕ and mixing temperature. (b) shows laminar flame speeds s_L obtained from 1-D flame simulations using Cantera; fresh gas temperature at 300 K. (c) shows temperature (left) and species mass fraction (right) profiles for a 0-D reactor simulation at most reactive Z ($\phi \approx 0.55$). Symbols and lines show ARC_18_C2H4NARA and detailed chemistry.

Configuration and methodology

The RJICF configuration

Figure 1 shows an x - y cut of the computational domain with a rectangular cross-section (length 190 mm, width 76.2 mm and height 38.1 mm) for the RJICF simulations. The experiments at atmospheric pressure were conducted by Wagner et al. [9–11]. The distance between the inlet and the fuel injector is equivalent to the distance between flow straightener and fuel injection in the experiment. Besides the crossflow bulk velocity $u_{cf} = 7.6$ m/s, no information about neither the velocity profile nor turbulence intensity was given in the experimental studies. The subscript “cf” and “j” denote crossflow and jet respectively. The hot crossflow was generated in the experiments by a propane/air flame with an equivalence ratio $\phi = 0.87$. We computed a 1-D flame with Cantera [38] using detailed chemistry [37] and obtained the inlet mixture composition that is shown in Fig. 1. A crossflow temperature of 1500 K was measured along a lateral span at the jet exit location by a suction pyrometer with a thermocouple to minimize errors due to high-temperature radiation [9]; the non-uniformity was ± 15 K. The premixed ethylene-air jet with $\phi = 1.2$ at 300 K was injected through a fuel pipe with a diameter $d = 9.53$ mm. The jet bulk velocities $u_j = 9.96$ m/s and $u_j = 7.7$ m/s were computed based on the given jet-to-crossflow momentum ratios J of 8.7 and 5.2 respectively. The ratio is defined as $J = (\rho_j u_j^2) / (\rho_{cf} u_{cf}^2)$. The length of the pipe in the experiment is $\approx 33d$; particle image velocimetry measurements showed a fully developed turbulent flow profile [11].

Analytically reduced chemistry (ARC)

The LES was performed with an ARC mechanism that was recently derived by Felden et al. [35] from the detailed scheme of Narayanaswamy et al. [37] (164 transported species) tailored for ethylene-air combustion. The ARC mechanism (18 transported species) is referred to as ARC_18_C2H4NARA below. A two-step reduction procedure was carried out utilizing the reduction tool YARC [39, 40]. First, species and reactions reduction lead to a skeletal mechanism with 29 species. Second, to further reduce the skeletal mechanism, a quasi-steady-state approximation was applied to 11 species, resulting into ARC_18_C2H4NARA that comprises these 18 transported species: N_2 , H , H_2 , O , OH , O_2 , H_2O_2 , H_2O , HO_2 , CO , CH_3 , CH_2O , CO_2 , CH_4 , C_2H_2 , C_2H_4 , C_2H_6 and CH_2CO .

Figure 2a compares autoignition times for two chemical mechanisms: the detailed mechanism [37] and the ARC mechanism used in this study. The autoignition time τ_{AI} is shown in logarithmic scale over mixture fraction Z . τ_{AI} was obtained from 0-D reactor simulations using Cantera and it is defined at the highest temperature gradient. Z describes the mixing between the hot crossflow at 1500 K ($Z = 0$) and the cold premixed ethylene-air jet at 300 K ($Z = 1$), without chemical reactions between fuel and oxidizer. Each Z value corresponds to one species composition or equivalence ratio ϕ , and mixing temperature, both shown with two additional axes. ARC_18_C2H4NARA and the detailed mechanism are in very good agreement. Both predict the most reactive mixture fraction Z_{mr} , which is the Z with the shortest autoignition time, at ≈ 0.11 .

Figure 2b compares laminar flame speeds s_L over equivalence ratio ϕ for the same two chemical mechanisms presented in (a). These results were obtained from 1-D freely-propagating flame simulations using Cantera. The fresh gas temperature was set to 300 K for all ϕ . Results for ARC_18_C2H4NARA and the detailed scheme are in excellent agreement. Figure 2c

Fig. 3. The effect of the dynamic thickened flame (DTF) model on the onset of autoignition. Top: autoignition time τ_{AI} normalized by autoignition time obtained on a flame-resolved grid (right vertical dashed line) $\tau_{AI, resolved}$ for three mixture fractions Z . Bottom: thickening factors F applied by the DTF model. Results obtained by 0-D reactor simulations (symbols) with AVBP. The left vertical dashed line shows grid resolution on the windward side of the RJICF.

shows temperature and species mass fraction profiles obtained with Cantera 0-D reactor simulations using the two schemes. The mechanisms are in excellent agreement; both predict a thin region of formaldehyde CH_2O and hydroperoxyl HO_2 just before the temperature increases suddenly.

Large eddy simulations (LES)

Compressible reactive LES were performed using the explicit cell-vertex code AVBP [41] with the step Taylor-Galerkin scheme TTGC [42] giving third-order accuracy in space and time. The classical Smagorinsky approach was used to model the Reynolds sub-grid scale stress tensor. The time step of 5×10^{-8} s is based on the acoustic CFL condition. At the inlets and the outlet, we used Navier-Stokes characteristic boundary conditions (NSCBC). We imposed a flat velocity profile without turbulence at the crossflow inlet and simulated the entire distance of 110 mm between flow straightener and jet. The crossflow temperature was set to 1500 K.

A mean profile of a fully developed turbulent pipe flow with isotropic turbulence (intensity $u'/u_j = 0.1$) was imposed at the jet inlet. A priori simulations with and without fuel pipe showed a non-negligible change in jet trajectories. Simulations were performed for different lengths of the jet pipe. No change in jet trajectory was observed for pipe lengths of $2d$ and $4d$, and therefore, the simulated pipe length is $2d$.

No information about wall boundary conditions, such as wall temperature was available from the experiments. In the LES, heat loss $\dot{q} = (T_{\text{wall}} - T_{\infty})/R_w$ was imposed at the domain walls, with reference temperature $T_{\infty} = 300\text{ K}$ and thermal resistance $R_w = 0.02\text{ K/W}$. This led to wall temperatures T_{wall} of approximately 700 K.

The unstructured computational grid, which has a total number of 11 million tetrahedral cells, is presented in Fig. 1. A first estimation of the required mesh resolution was done based on the LES filter size Δ . Pope [43] showed that at least 80% of the turbulent kinetic energy should be resolved; a ratio between filter width and integral length scale (Δ/L_t) of approximately 0.083 would resolve 80% of the turbulent kinetic energy [43]. L_t is of the order of the largest eddies in the domain and was estimated as 4.8 mm, which is half the diameter of the fuel injector pipe. Using Pope's criterion, a filter width of $\Delta \approx 0.4\text{ mm}$ was computed. This is just a first estimation and the choice of integral length scale might appear to be somewhat arbitrary. Therefore, we performed LES on four different meshes with characteristic cells sizes of 0.2 mm, 0.3 mm, 0.5 mm and 1 mm. For all four meshes, we observed grid independence with regard to average jet trajectories. However, for average velocity magnitudes along the trajectories, grid independence was reached only for $\Delta x = 0.2\text{ mm}$ and 0.3 mm. Hence, we used a grid size of $\Delta x = 0.3\text{ mm}$ in the leeward side of the jet. Moreover, we deployed a coupled velocity/temperature wall-model that is based on the Van Driest formulation [44] and the extension of Schmitt et al. [45], which is suitable for non-isothermal configurations.

The flame thickness for a 1-D propagating flame at $\phi = 1.2$ and a fresh gas temperature of 300 K is approximately 0.25 mm. A cell size of $\approx 0.06\text{ mm}$ would discretize the flame front with 4-5 cells. This, however, would increase the cell count

Fig. 4. Heat release rate $\dot{q}$ contour overlaid with isoline at thickening factor $F = 3$ (yellow). This highlights regions where the DTF model applies flame thickening.

Fig. 5. (a) contour of total kinetic energy that is composed of the resolved part of the turbulent kinetic energy k_{re} and the modeled sub-grid energy k_{sgs} . (b) the ratio between k_{re} and total kinetic energy.

by a factor of approximately 37. Moreover, the LES time step would decrease, both leading to a significant increase of computational costs. Therefore, the turbulence/ flame interaction was modeled with the dynamic thickened flame (DTF) model which has been proven to perform well in endless studies, e.g. [19, 25, 28, 29, 35, 46]. The model thickens the flame front to a minimum of 4.5 cells while maintaining the correct laminar flame speed of 0.73 m/s. The sub-grid scale flame wrinkling was modeled with the efficiency function of Colin et al. [46]. The effect of the DTF on autoignition is an open question at the moment; in [25] it was shown that flame thickening can delay the onset of autoignition. Therefore, Fig. 3 investigates the influence of the DTF model on autoignition times τ_{AI} for varying grid size Δx at three mixture fractions Z . τ_{AI} is normalized by the autoignition time that was obtained on a flame-resolved grid $\tau_{AI, resolved}$ $\Delta x = 0.05$ mm. The bottom plot shows the corresponding thickening factors F applied by the DTF model. The DTF parameters for the 0-D reactor simulations were the same as in the actual RJCF simulation. For a grid size of 1 mm and $Z = 0.15$, thickening factors of 21 are applied and τ_{AI} is delayed up to a factor of 6. It is also shown that the DTF model does not delay the onset of autoignition for the characteristic mesh size of the windward flame ($\Delta x = 0.2$ mm), which is highlighted with the left vertical dashed line. Indeed, as shown in an instantaneous snapshot of heat release rate $\dot{q}$ contour in Fig. 4, flame thickening (yellow isoline) is only applied in the high heat release rate region of the propagating upper windward flame and the leeward flame, but not in the lower windward reaction zone that is associated with autoignition chemistry. In this zone, the flame-turbulence interaction is not modeled by the DTF model. Therefore, a posteriori, we computed the ratio between the resolved scales and the total fluctuating energy. Figure 5a shows the total kinetic energy that is composed of a resolved part k_{re} and the non-resolved sub-grid energy k_{sgs} , which was computed using $1/(C_V \Delta)^2 v_t^2$ [47] with constant $C_V = 0.17$ and eddy viscosity v_t . (b) shows the ratio between k_{re} and total kinetic energy. In the region of interest, the modeled scales contribute less than 2% to the total kinetic energy and therefore, the sub-grid turbulence-chemistry interaction in the autoignition driven reaction zone is neglected for this study.

Fig. 6. Experimental [11] (a) and LES (b) contours of velocity magnitude $|u| = \sqrt{u_x^2 + u_y^2}$ in the central plane for non-reactive (left) and reactive (right) jets in crossflow. Solid lines show streamlines originating at the windward jet edge, the jet center, and the leeward jet edge. (c) shows velocity magnitude $|u_y|$ along normalized y-coordinate of jet-center trajectory. Jet-to-crossflow momentum ratio $J = 8.7$.

Comparison to experiments

Figure 6a and b show the average velocity magnitude $|u| = \sqrt{u_x^2 + u_y^2}$ contours obtained from experiments [11] and LES, respectively ($J = 8.7$). Experimental and LES jet equivalence ratios are both $\phi = 1.2$. Non-reactive and reactive results are presented in the left and the right part of the figure, respectively. In each of the four fields, the isolines show streamlines originating at the windward jet edge (left isolines), the center of the jet, and the leeward jet edge (right isolines). Results from experiment and LES are in good agreement. Both show a low-velocity region just upstream of the windward streamline for the non-reacting and reacting case. The low flow velocity region in the wake of the jet increases for the reactive case for experiment and LES. Figure 6c shows the velocity magnitude $|u_y|$ along the y-coordinate of the jet-center trajectory, which is highlighted by an arrow in (a). For the non-reactive case, $|u_y|$ is slightly under-predicted close to jet exit and over-predicted for $(y/d)|_{\text{trajec}} > 1$. For the reactive case, the velocity is slightly under-predicted by LES between $1.5 \leq (y/d)|_{\text{trajec}} \leq 2.5$. However, the correct divergence of streamlines in the reacting flow due to gas expansion in the combustion products was correctly reproduced.

Figure 7 compares instantaneous snapshots from experiments (left) and LES (right) showing a zoom of the windward side of the jet. The LES snapshot was arbitrarily chosen from the simulated sequence and resemble the experimental data presented in [10]. Contours of velocity magnitude $|u|$, vorticity ω_z , formaldehyde CH_2O , hydroxide OH and the product of the two $\text{OH} \times \text{CH}_2\text{O}$ are presented from top to bottom. Species distributions from experiments were obtained from planar laser-induced fluorescence (PLIF); one can refer to [9–11] for a detailed description of PLIF measurements and PLIF image post-processing. Species from LES are given in mass fraction. For $J = 5.2$, experimental fields were only available for $\phi = 1.0$ and LES were only performed at $\phi = 1.2$. However, typical flame dynamics were reported independent of ϕ [11]. Therefore, the difference is acceptable for the purpose of comparing dynamics. For all others figures, experimental and numerical ϕ are identical though. Wagner et al. [9–11] defined three distinct flame regions: (i) a preheat zone, (ii) a reaction zone and (iii) a post-flame zone. Zone (i) is located close to the cold premixed jet and only CH_2O is present. In (ii), CH_2O and OH overlap; this zone is tracked by $\text{OH} \times \text{CH}_2\text{O}$. Zone (iii) is located close to the hot crossflow and only OH is present. In Fig. 7, the flame front (ii) is highlighted with black isolines at $\text{OH} \times \text{CH}_2\text{O} = 3 \times 10^{-8}$. This instant shows a characteristic interaction of the flame with a coherent structure of the flow (highlighted with boxes): the preheat zone (i) is thickened by a vortical structure that is visible in both ω_z contours, and the flame front is rolled up by this vortex.

Fig. 7. Comparison between experiments (left) and LES (right). Instantaneous contours of velocity magnitude $|u| = \sqrt{u_x^2 + u_y^2}$, vorticity ω_z , CH_2O , OH , and the product of the two $\text{OH} \times \text{CH}_2\text{O}$, used as a flame front marker in the experiments [9–11]. OH , CH_2O and $\text{OH} \times \text{CH}_2\text{O}$ from experiments obtained with PLIF; species from LES in mass fraction. Isolines at $\text{OH} \times \text{CH}_2\text{O} = 3 \times 10^{-8}$ show flame front. Jet-to-crossflow momentum ratio $J = 5.2$.

Flame dynamics

Figure 8 shows seven instantaneous snapshots of a continuous sequence in a 2-D x - y -cut through the jet centerline with $\Delta t = 0.3$ ms. Hydroxyl (OH) mass fraction, temperature T and velocity magnitude $|u|$ are presented from top to bottom. The flame is visualized by a heat release rate $\dot{q}$ isoline at $1.6 \times 10^9 \text{ W/m}^3$. On the leeward side, the flame is attached more robustly compared to the windward side. The flame root is located near the shear layer very close to the fuel exit. It propagates into the bulk flow of the jet further downstream. This is in very good agreement with experimental results that showed a leeward flame stabilized by flame propagation [9–11]. In contrast, the lifted windward flame exhibits a significantly more complex behavior. OH contours on the windward side show a very thin concentration spanning from the jet exit to the flame tip (see t_0); this was observed for all snapshots of the entire simulation. OH is an important species in autoignition layers prior to flame stabilization [48]. This thin OH layer can be associated with radical build-up prior to autoignition. Indeed, the temperature increases upstream of the flame front close to this thin reaction zone, as shown in the zoom of the T contour at $t_0 + \Delta t$. The velocity magnitude snapshots show that this autoignition layer is located close to the shear layer between jet and crossflow. This is in agreement with results from Wagner et al. [9], proposing flame stabilization due to autoignition in the shear layer of the windward jet. The most upstream point of the windward flame base is referred to as “autoignition flame base”, marked with circles at $t_0 + \Delta t$ and $t_0 + 2\Delta t$ in the $|u|$ contour. As highlighted from $t_0 + 3\Delta t$ to $t_0 + 5\Delta t$, the upstream part of the windward flame propagates into the bulk jet, which was also reported in the experiment, as shown in the top left part of Fig. 7. Finally, the two flame fronts merge at $t_0 + 6\Delta t$, creating an isolated propagating flame front.

Figure 9 shows the time evolution of the windward and leeward flame base heights. The dashed lines highlight the time-averaged flame positions for the leeward ($y_{\text{flame}}/d \approx 0.3$) and windward side ($y_{\text{flame}}/d \approx 1.1$). The positions are in good agreement with experiments [11] that showed leeward and windward flame heights of approximately 0.21 and 0.98. The

Fig. 8. An instantaneous sequence in a 2-D x - y -cut trough jet centerline, visualizing from top to bottom: OH mass fraction, temperature T and velocity magnitude $|u| = \sqrt{u_x^2 + u_y^2}$. Flame visualized by heat release rate $\dot{q}$ isoline at $1.6 \times 10^9 \text{ W/m}^3$. The time between snapshots is $\Delta t = 0.3 \text{ ms}$. Jet-to-crossflow momentum ratio $J = 8.7$.

inset of Fig. 9 shows an instantaneous snapshot of OH (gray contour), flame front (blue isoline at $\dot{q} = 1.6 \times 10^9 \text{ W/m}^3$), windward flame base (green dot) and leeward flame base (red dot). The flame base height y_{flame} is defined as the flame front at minimum y . The leeward flame base varies only slightly around its mean height. The windward flame, on the contrary, shows a strong intermittent behavior: the flame height slowly increases, followed by an abrupt shift of the flame base to lower y_{flame} . These sudden shifts are due to autoignition events. The windward flame front is constantly convected downstream and is intermittently “brought back” by autoignition, which governs flame stabilization on the windward side. A similar behavior was observed in [49] for a lifted methane flame in hot vitiated coflow. The authors reported “sudden jumps” in flame lift-off height associated with autoignition of mixtures located upstream of the “old” flame position. The solid blue line corresponds to the autoignition length $l_{\text{AI,mr}}$ computed with the shortest autoignition time $\tau_{\text{AI,mr}}$ and the bulk jet velocity u_j . This length is one order of magnitude smaller than the time-averaged flame base height (green dashed line). This difference can be explained as follows. First, heat is released at the most reactive mixture fraction Z_{mr} , which is located on the oxidizer side ($Z = 0.1$, see Fig. 2a). This results in low heat release that can be observed close to the jet exit (see Fig. 4) and that matches with the $l_{\text{AI,mr}}$. Of course, such small heat release rates are difficult or even not possible to detect in the experiment, but in LES. It is expected that the heat released at Z_{mr} rises the temperature of neighboring richer mixtures which become the most reactive ones and eventually auto-ignite. Once higher Z start to auto-ignite and significant heat is released, the flame becomes “visible” and appears lifted on the windward side. The detailed underlying mechanism will be investigated in future work.

Conclusion and outlook

This numerical paper analyzes an RJCF with a premixed ethylene-air jet at $\phi = 1.2$ and $T = 300 \text{ K}$ injected into a hot vitiated crossflow at 1500 K . The RJCF was recently investigated experimentally by Wagner et al. [9–11] proposing autoignition and flame propagating as dominant flame stabilization mechanisms. The present study is a follow up of this

Fig. 9. Time evolution of windward and leeward flame heights y_{flame} . Dashed lines show average y_{flame} . The inset shows an instantaneous snapshot of OH contour, the flame front highlighted by isolines, and the two flame bases. The blue line shows autoignition length computed with $\tau_{\text{AI,mr}}$ at Z_{mr} and the jet bulk velocity. $J = 8.7$.

experimental work and aims at bringing more insight into the flame dynamics and the complex stabilization mechanism by the use of 3-D LES in combination with ARC and the DTF model.

First, 0-D and 1-D Cantera simulations compare two chemical mechanisms for ethylene-air combustion: (i) a detailed mechanism and (ii) the ARC mechanism used in this study. ARC is in excellent agreement with detailed chemistry and captures the non-trivial autoignition chemistry associated with radical build-up prior to ignition. Moreover, the effect of the DTF model on autoignition is investigated for varying grid sizes Δx and mixture compositions. The model has no impact on autoignition times for the characteristic Δx used in this study. However, the model can significantly delay autoignition for bigger Δx . Second, results from LES are compared to experiments. 2-D time-averaged velocity fields and jet trajectories are in very good agreement for non-reactive and reactive simulations. Moreover, LES successfully reproduce characteristic flame-vortex interactions.

Finally, a dynamic flame analysis is presented. It shows a leeward flame that is anchored stably in the shear layer close to the jet exit. Further downstream, the flame transverses the shear layer and propagates into the bulk jet containing a flammable mixture. The windward flame, in contrast, shows a much stronger dynamic behavior. The lifted flame base is shifted downstream and is “brought back” by autoignition intermittently. These autoignition events occur close to a thin layer of OH radicals that spans over the entire windward side down to the jet exit for all instants of time. Further downstream, the windward flame can also propagate into the bulk jet leading to flame fronts merging with the leeward flame inside the jet. The understanding of flame dynamics and flame stabilization can be particularly important for practical applications, such as combustion systems in stationary gas turbines. In such systems, the dynamic flame behavior has a strong influence on the thermoacoustic stability [50, 51]. Recently, it was shown that temperature fluctuations of the crossflow can lead to very strong spatial fluctuations of the heat release rate zone due to a modulation of the autoignition time of the mixtures. The resulting heat release rate fluctuations depend on the mean crossflow temperature, as shown in [33]. These results were obtained in conditions similar to the present one. Therefore, future work could address the effect of upstream temperature fluctuations on these particular RJICF flame dynamics.

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