Large-Eddy Simulations of Fuel Effects on Gas Turbine Lean Blow-out

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Towards the implementation of alternative jet fuels in aviation gas turbines, testing in combustor rigs and engines is required to evaluate the fuel performance on combustion stability, relight, and lean-blow out (LBO) characteristics. The objective of this work is to evaluate the effect of different fuel candidates on the operability of gas turbines by comparing a conventional petroleum-based fuel with two other alternative fuel candidates. Numerical investigations are performed to examine the performance of these fuels on the stable condition close to blow-out and LBO-behavior in a referee gas turbine combustor. Large-eddy simulations (LES) are performed at stationary conditions near LBO to examine effects of the fuel properties on evaporation, gaseous-fuel deposition, flame anchoring.

I. Introduction

Driven by the increasing concerns on air quality and the need for sustainable supplies of jet fuels, the development of alternatives to conventional petroleum-derived jet fuels is the focus of research programs in the United States\textsuperscript{1,2} and in Europe\textsuperscript{3}. Due to significant constraints associated with the aeronautical sector (extended engine life, supply infrastructures), efforts concentrate on the development of drop-in fuel, which are readily usable in the existing fleet. The certification of candidate fuels requires experimental test campaigns by engine manufacturers to evaluate their performances on three key engine operability elements: lean blow-out (LBO), cold start and altitude relight. However, the lack of predictability of the effect of the physico-chemical properties of the candidate fuels on these three processes greatly increases the cost and duration of the experimental test. The development of computational fluid dynamic (CFD) tools to better understand these fuel effects in realistic configurations is thus crucial in facilitating the certification process of alternative jet fuels.

The present study focuses on LBO, since it is of primary concern in modern lean-burn combustion chamber design. A significant body of work exists on LBO in flameholder configuration and old combustor design\textsuperscript{4,5}. Without direct knowledge of the details of the combustion process in the combustion chamber, these studies focused on deriving empirical correlations from extensive experimental test campaign. More recently, direct visualization of the flame in academic configuration experimental rigs revealed that the blow-off is closely related to the dynamics of the recirculation zone which acts as a strong stabilization mechanism.\textsuperscript{6,7} Due to the transient nature of the LBO-process, only few attempts have been made to use numerical simulations. Large Eddy Simulation (LES) was used to study LBO in a spray stabilized flame, demonstrating the ability of the simulations to capture the local flame extinction and the subsequent blow-out process.\textsuperscript{8} The same methodology was also used in order to evaluate the LBO-limit by performing multiple simulations,\textsuperscript{9} showing that LES reproduce relatively well the experimental data.

The objective of the present work is to use LES to study the LBO behavior of a realistic gas turbine combustor for different fuels and provide an understanding about the effect of the fuel physico-chemical properties on the combustion process. A conventional Jet-A fuel is first employed as a reference fuel and two alternative fuels are selected based on experimental evidence on their effect on the LBO limit. In realistic configurations, the lack of data on the spray boundary conditions gives rise to uncertainty on the CFD results.
To shed some light on the spray formation and provide guidance for the LES calculations, Volume of Fluid (VOF) simulation of the primary break-up are performed in a simplified but representative configuration.

II. Experimental Setup

The referee-rig combustor studied in this work is installed at the Air Force Research Laboratory of Dayton, and reproduces the major features of a realistic gas-turbine combustion chamber: a complex injection system composed of multiple concentric swirlers with a staged liquid injection, a multi-perforated liner and two rows of dilution jets, this is representative of Rich-burn/Quick-mix/Lean-burn (RQL) technologies. The combustor is operated in a pressurized vessel with large optical access to allow direct visualization of the reaction zone.

The test rig is pressurized at 2.07 atms and operated close to blow-out conditions at an overall equivalence ratio of $\phi = 0.096$. A 3% relative pressure drop is maintained across the injection system, corresponding to an air mass flow rate of 391.4 g/s. The inlet air temperature is 394 K while the liquid fuel temperature is 322 K. The operating conditions for the three selected fuel candidates are reported in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>Cat-A2</th>
<th>Cat-C5</th>
<th>Cat-C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalence ratio</td>
<td>0.096</td>
<td>0.096</td>
<td>0.096</td>
</tr>
<tr>
<td>Air mass flow rate [g/s]</td>
<td>391.4</td>
<td>391.4</td>
<td>391.4</td>
</tr>
<tr>
<td>Fuel mass flow rate [g/s]</td>
<td>2.563</td>
<td>2.569</td>
<td>2.51</td>
</tr>
</tbody>
</table>

Table 1. Operating air and fuel-flow rate near blow-out conditions.

The test rig is instrumented in order to measure pressure drop, wall temperature and flow split. A high speed camera is used for OH* and CH* chemiluminescence measurements up to 10 kHz. Finally, a phase-doppler particle analyzer (PDPA) is installed to investigate the spray droplet size distribution and droplets velocity.

III. Geometry and Mesh

The computational domain is shown in Fig. 1 with a cut through the combustion chamber. The four main components of the experimental configuration are included in the simulation: the large pressurized plenum, the complex injection system, the combustion chamber and the exhaust plenum. The injection system comprises two axial swirlers and a radial inner swirler. At the present low-power conditions, the fuel is fully injected through the pressure-swirl atomizer to generate a central rich zone, favorable for flame stabilization. The domain is discretized using 20 million elements with regular hexahedral elements inside the combustor and tetrahedral elements are used to represent a portion of the injector geometry. The characteristic mesh size ranges from 0.15 mm in the swirlers passages to 0.9 mm in the downstream part of the combustor.

IV. Modeling and numerics

A. Volume-of-Fluid LES solver

VOF-simulations are performed with the unstructured incompressible LES solver CLIFF developed at Cascade Technologies. Incompressible LES equations are combined with a VOF/Lagrangian Spray framework to resolved the turbulent atomization process and the subsequent droplet dispersion. Density and viscosity are assumed to be constant within each phase, and can be expressed as a function of the filtered liquid volume fraction $\tilde{\phi}$:

$$\rho = \tilde{\phi} \rho_1 + (1 - \tilde{\phi}) \rho_2,$$

$$\mu = \tilde{\phi} \mu_1 + (1 - \tilde{\phi}) \mu_2,$$

where the subscripts denote the two distinct fluid phases. The interface is simulated with a geometric unsplit VOF method that is conservative on unstructured meshes. A Piecewise-Linear Interface Calculation (PLIC) reconstruction scheme is adopted for which the surface normal $\hat{n}$ is computed from a signed distance field $G$ constructed from the VOF using a bisection/secant algorithm. The VOF representation is coupled to
the Lagrangian spray particle (LSP) method to describe the secondary breakup dynamics, which cannot be fully resolved with VOF using available computational resources. The under-resolved VOF structures represented by $n_c < 3^3$ contiguous cells are replaced by a spherical droplet of equal volume. The Lagrangian particle method is applicable to droplets with small local Weber numbers in the subsequent breakup and atomization processes. In this manner, the primary breakup and the subsequent atomization can be modeled efficiently. The Lagrangian particle motion is simulated using the Basset-Boussinesq-Oseen (BBO) equation with shear force, Basset force and added mass neglected. The further breakup of Lagrangian particles into smaller droplets is modeled by a stochastic breakup model. Note that evaporation of the Lagrangian droplets is not accounted for. The numerical method has been successfully applied to the study of a realistic jet in cross-flow injection and to the pressure-swirl atomizer used in the present combustor.

B. Multiphase reactive LES solver

Reactive simulations are performed with the low-Mach LES-solver Vida. The instantaneous Favre-averaged conservation equations for mass and momentum are solved on the LES grid with a fourth/second-order accurate spatial discretization scheme on regular/unstructured meshes, respectively. A second-order predictor-corrector scheme is used for temporal integration. Turbulent subgrid stresses are modeled with the eddy-viscosity model of WALE. Walls are considered adiabatic non-slip and the effusive cooling is modeled through a homogeneous approach in which the effusive gas-phase velocity is determined from the experimentally measured mass flow rates.

Combustion is modeled with the flamelet/progress-variable (FPV) approach in which the thermo-chemical properties are parameterized as a function of filtered mixture fraction $\tilde{Z}$, filtered reaction progress variable $\tilde{C}$ and mixture fraction variance $\tilde{Z}''^2 = \tilde{Q} - \tilde{Z}^2$:

$$\frac{\partial \tilde{p} \tilde{Z}}{\partial t} + \frac{\partial \tilde{p} \tilde{u}_j \tilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \tilde{p} \tilde{D} + \frac{\mu_t}{S_{Cl}} \right) \frac{\partial \tilde{Z}}{\partial x_j} \right] + \tilde{S}_z$$

$$\frac{\partial \tilde{p} \tilde{Q}}{\partial t} + \frac{\partial \tilde{p} \tilde{u}_j \tilde{Q}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \tilde{p} \tilde{D} + \frac{\mu_t}{S_{Cl}} \right) \frac{\partial \tilde{Q}}{\partial x_j} \right] - \left[ 2 \rho D \frac{\partial \tilde{Z}}{\partial x_j} \frac{\partial \tilde{Z}}{\partial x_j} + 2 \rho D \frac{\partial \tilde{Z}''}{\partial x_j} \frac{\partial \tilde{Z}''}{\partial x_j} \right] + \tilde{S}_Q$$

$$\frac{\partial \tilde{p} \tilde{C}}{\partial t} + \frac{\partial \tilde{p} \tilde{u}_j \tilde{C}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \tilde{p} \tilde{D} + \frac{\mu_t}{S_{Cl}} \right) \frac{\partial \tilde{C}}{\partial x_j} \right] + \tilde{\omega}_c$$

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*http://www.cascadetechnologies.com/pdf/VIDA.pdf*
where \( \overline{\rho} \) and \( \overline{\mathbf{u}} \) are the filtered density and velocity component, respectively. \( \overline{D} \) is the scalars diffusivity, \( \mu_t \) is the subgrid scale viscosity and \( Sc_t \) is the turbulent Schmidt number kept equal to 0.9. The last term of the right hand side of Eqs. [3] and [4] is the source term due to evaporation, while the last term in Eq. [5] is the reaction progress variable source term.

The progress variable is defined as \( C = Y_{CO_2} + Y_{CO} + Y_{H_2O} + Y_{H_2} \). The flame structure is obtained from the solution of steady laminar non-premixed flamelet equations, which are solved along the entire S-shaped curve. Cooling effects of the liquid phase on the flame is considered by computing an effective gaseous fuel temperature \( T_{fuel,g} = T_{fuel,l} - \Delta h_v(T_{evap})/c_p,l(T_{evap}) \), where \( \Delta h_v \) is the latent heat of evaporation and \( c_p,l \) is the specific heat capacity of the liquid.

The spray is modeled using a Lagrangian approach where the droplet motion is described by the Basset-Boussinesq-Oseen (BBO) equation and the evaporation rate is based on equilibrium calculations of isolated droplets. Secondary droplet break-up of Lagrangian particles into smaller drops was found to be important since the low injection velocity and the high flow velocity issued by the swirler result in a large droplet Weber number (ranging between 2 and 20). Secondary breakup is modeled by a stochastic approach where the radius of the droplets is assumed to be a time-dependent stochastic variable with a given initial-size distribution. The critical Weber number is set to a numerical value of 6 based on experimental observations. The spray boundary conditions consist of a ring of 0.9 mm radius located 0.1 mm from the atomizer nozzle. A Rosin-Rammler distribution is used with a Sauter Mean Diameter (SMD) prescribed by the empirical correlation:

\[
SMD = 2.25 \sigma^{0.25} \mu_L^{0.25} \dot{m}_L^{0.25} P_L^{-0.5} \rho_a^{-0.25}
\]

where \( \sigma, \mu_L, \dot{m}_L \) are the fuel-dependent liquid surface tension, viscosity and mass flow rate, respectively, \( P_L \) is the pressure drop across the nozzle, and \( \rho_a \) is the air density.

V. Fuel description

The present study considers three fuels, namely a conventional petroleum-derived Jet-A fuel (Designation: Cat-A2, POSF 10325) and two test fuels: a fuel with a very narrow boiling characteristic (Cat-C5, POSF 12345) and a fuel with low cetane number (Cat-C1, POSF 11498). Key properties and compositions of the three fuels are given in Table 2. Compared to Cat-A2, Cat-C5 and Cat-C1 have a similar and higher H/C ratio. All three fuels differ in term of molecular weight where Cat-C5 is low than the conventional fuel while Cat-C1 is significantly higher.

Chemically, Cat-C5 has a significantly higher content of branched hydrocarbons and aromatics than Cat-A2, but has almost no cycloparaffins. Cat-C1 is composed only of iso-Paraffins with about 16% of highly branched-chain hydrocarbon (iso-cetane). The physicochemical properties and combustion chemistry models for all fuels are obtained from studies conducted within the context of the National Jet Fuel Combustion Program (NJFCP) and implemented in the LES solver.

<table>
<thead>
<tr>
<th>Composition (mass fraction [%])</th>
<th>Aromatics</th>
<th>iso-Paraffins</th>
<th>n-Paraffins</th>
<th>Cycloparaffins</th>
<th>Alkenes</th>
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<tr>
<td>Cat-A2</td>
<td>18.66</td>
<td>29.45</td>
<td>20.03</td>
<td>31.86</td>
<td>&lt;0.001</td>
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<tr>
<td>Cat-C5</td>
<td>30.68</td>
<td>51.58</td>
<td>17.66</td>
<td>0.08</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>Cat-C1</td>
<td>&lt;0.01</td>
<td>99.63</td>
<td>&lt;0.001</td>
<td>0.05</td>
<td>0.32</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>H/C</th>
<th>Mol. Weight</th>
<th>( T_{90} - T_{10} )</th>
<th>( \mu_l(322 \text{ K}) )</th>
<th>( \sigma(322 \text{ K}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cat-A2</td>
<td>1.90</td>
<td>159</td>
<td>67.8</td>
<td>1.17</td>
</tr>
<tr>
<td>Cat-C5</td>
<td>1.93</td>
<td>135</td>
<td>2.9</td>
<td>0.56</td>
</tr>
<tr>
<td>Cat-C1</td>
<td>2.16</td>
<td>178</td>
<td>45.5</td>
<td>0.98</td>
</tr>
</tbody>
</table>

Table 2. Properties of fuels studied.
VI. High-fidelity primary break-up simulations

The simulation is conducted for the Cat-A2 fuel in the operating conditions described in Section II. To reduce the computational cost, for the breakup simulation a reduced domain comprising the primary zone of the referee rig combustor and the swirl chamber of the pressure swirl atomizer (Fig. 2) is used. The mesh resolution is reduced to 25 µm within and at the vicinity of the atomizer nozzle in order to capture the development of the liquid sheet. Boundary conditions are extracted from time-averaged data on the full combustor non-reacting simulations. The velocity field on the reduced domain is shown to reproduce the main flow structure of the full domain simulations: a strong inner recirculation zone (IRZ) induced by the rotational motion of the flow and a high shear region close to the injector nozzle.

![Computational domain used for the VOF simulation along with details on the refined region around the atomizer nozzle.](image)

An instantaneous view of the spray is shown in Fig. 3 using an iso-surface of VOF = 0.5. Due to the interactions with the surrounding turbulent flow, the continuous liquid sheet is shown to rapidly breakup into long ligaments and large droplets. The subsequent conversion of the VOF into Lagrangian droplets as well as the secondary break-up are not represented. Although the nominal pressure swirl atomizer has a 90 degree angle, the interaction of the liquid sheet with the IRZ induces a larger angle, and particles are rapidly convected toward the shear layer between the IRZ and the flow issued from the radial inner swirler. In the shear layer, droplets are subjected to a large acceleration resulting in secondary break-up.

Figure 4 compares the spray characteristics of the VOF simulation 5 mm downstream of the injection system with the one obtained in the full geometry LES simulation with the injection methodology described in Section II, and PDPA measurements. The predicted droplet position is in good agreement for the two simulations and the experiments. Both axial and radial droplet velocities components are well predicted in the two simulations. Simulations indicate that droplets are close to equilibrium at this location, especially for the full reactive LES, which predicts smaller droplet diameter. The SMD is found to be slightly under-predicted in the VOF simulation whereas the offset is larger for the full reactive LES. In the latter, the injection droplet size distribution is obtained from an empirical correlation whose applicability to a wide range of injector design and operating conditions is subjected to uncertainty.

VII. Results and Discussions

A. Spray data validation

The comparison between simulation and experiments presented in Section VI focused on a position close to the injection system, where the effect of the burnt gas recirculation on the spray is expected to be small. In order to validate the reactive LES and evaluate the fuel effects on the spray characteristics, radial profiles of droplet axial and radial velocities as well as SMD are plotted in Fig. 5 at three axial positions downstream of the injector for all three candidate fuels. LES is shown to correctly reproduce the spray angle as well as the magnitude of the velocity components. However, in accordance with the results presented in Section VI, the
SMD is under-predicted. Note that the radial profiles of SMD exhibit a bi-modal shape close to the injection system, which is not predicted by the LES. Further experimental analysis indicates that droplets are hitting the inner walls of the injection system and could lead to the formation of a liquid film, eventually atomizing at the lip between the inner passage and the first axial swirler. This atomization process is not included in the present LES where droplet/wall interactions are modeled with droplets reflection. Comparison of the

Figure 3. Side (left) and front (right) view of the developing liquid sheet represented by an iso-surface of VoF = 0.5.

Figure 4. Comparison between VOF, LES and experiments for radial profiles of droplets count, SMD, axial velocity and radial velocity in a plane 5mm downstream of the injection system for Cat-A2 fuel.
three different fuels reveals very little fuel effect close to the injection system, while further downstream, SMD values for Cat-C5 are found to be higher and its sample number is lower. This suggests that small droplets are evaporating faster for Cat-C5.

B. Fuel effect on flame position

The flow field in the referee combustor rig is representative of modern combustor designs where the strong swirl induced by the injection system generates a large IRZ, which extends upstream within the injection system and interacts downstream with the first row of the dilution holes. The IRZ advects hot gases toward the injection nozzle acting as a flame stabilization mechanism, however the lack of pre-vaporized fuel and the high velocity within the injection system results in a lifted flame as shown in Fig. 6. For Cat-A2 and Cat-C5 fuel, the flame mostly lies in the downstream part of the primary zone while for Cat-C1 the flame sits in the shear layer between the hot recirculating gases of the IRZ and the incoming fresh gases. The flame is sustained by clusters of droplets evaporating and generating locally stoichiometric mixture. The
temperature of the IRZ is much lower than the flame temperature due to the lean equivalence ratio of the primary zone ($\phi_{\text{prim}} \simeq 0.16$) and the intermittent emission of fresh gases from the dilution holes. Because of the very low liquid mass flow rate near the LBO limit, the droplet injection velocity is low and droplets are rapidly entrained by the swirling air. The spray then interacts with the PVC forming clusters of droplets, which lead to a periodic variation of the evaporation rate. The PVC frequency, $f_{\text{PVC}} = 520 \text{ Hz}$, is evaluated using a probe (see cross in Fig. 1) and this frequency is insensitive to the fuel or operating conditions.

Figure 6. Instantaneous field of temperature and mixture fraction in the combustor central cut plane for Cat-A2 (top), Cat-C5 (middle) and Cat-C1 (bottom) at $\phi = 0.096$ along with the droplets within a 1mm slab.

To obtain a better understanding about the combustion regime and the interactions with the spray, the conditional integrated progress variable source term $\langle \int_{V} \dot{\omega}_{c} | Z \rangle$ and the conditional integrated evaporation source term $\langle \int_{V} \dot{S}_{z} | \tilde{C} \rangle$ are plotted in Fig. 7. Most of the evaporation is found to occur on the fresh gas side (low values of $\tilde{C}$) for all three fuels, but a higher portion of it occurs in the burnt gases for Cat-C1. This highlights the fact that the Cat-C1 flame is located closer to the injection system and more droplets penetrate the flame front. The conditional integrated progress variable source term indicates that because of the very lean operating conditions, most of the reaction occurs below the stoichiometric mixture fraction ($Z_{st} \simeq 0.063$ for all fuels). However, the distribution is shifted towards higher mixture fraction for Cat-C1, consistently with the flamelet tables.

Time-averaged statistics are collected over two flow-through times in the primary zone and Fig. 8 shows the mean temperature (top) and progress variable source term (bottom) for all three fuels. Velocity streamlines are superimposed on the temperature field to highlight the recirculation zones while iso-contours of the evaporation source term of mixture fraction are added on the $\dot{\omega}_{C}$ field. The flow pattern is very similar for all fuels, but the temperature in the recirculation zones are different. Specifically, temperatures in both inner and outer recirculation zones are higher for Cat-C1 with a larger progress-variable source region in the shear layer between the IRZ and the incoming fresh gas compared to Cat-A2. Note that because of the very lean
equivalence ratio, the time-averaged temperature of the IRZ is far below the stoichiometric temperature. The equilibrium temperature obtained from the equivalence ratio of the primary zone ($\phi_{PZ} = 0.16$) is of $\simeq 960$ K for Cat-A2 and Cat-C5 and $\simeq 975$ K for Cat-C1. Most of the evaporation is found to occur upstream of the mean reaction zone for all candidate fuels.

![Figure 7. Integrated progress variable source term (left) and evaporation rate (right) conditioned on $\tilde{Z}$ and $\tilde{C}$ respectively.](image)

![Figure 8. Time-averaged field of temperature and mixture fraction in the combustor central cut plane for Cat-A2 (up), Cat-C5 (middle) and Cat-C1 (down) at $\phi = 0.096$.](image)
The differences in flame stabilization can be related to the ignition behavior of the coupled liquid/gas system. A 0D pseudo-batch reactor is used to evaluate the effect of the initial droplet size and initial gas temperature on the ignition delay of the system. This reactor solves the coupled liquid/gas equations. The results indicate that the Cat-C1 candidate fuel is the fastest igniting spray mixture. Amongst the three candidate fuels, Cat-C1 is the only one exhibiting a negative temperature coefficient (NTC) behavior. In sprays, the evaporation process induces a reduction in the gas temperature that results in a rapid increase in the ignition delay for Cat-A2 and Cat-C5, but not for Cat-C1 which eventually ignites faster.

VIII. Summary

The effect of fuel at conditions near lean blow-out is studied by comparing the flame obtained with two candidate fuels with a conventional Jet-A fuel in a realistic configuration using Large Eddy Simulations. To obtain a better understanding about the spray injection characteristics, a VOF simulation of the primary break-up is performed with the Jet-A fuel which shows the strong interaction between the thin liquid sheet and the recirculation generated by the swirled injection system. The methodology employed in the LES is found to relatively well reproduce the feature of the VOF and compare well with experimental data downstream. Reactive simulations are performed with three candidate fuels at condition near to blow-off. Comparison of spray data against PDPA measurement are in good agreement. LES results indicate that the flame is weakly stabilized in the primary zone of the combustion chamber with pockets of evaporating droplets allowing intermittent diffusion flame structure. Due to the very low-equivalence ratio, the mean temperature of the primary zone is low inducing long droplets evaporation time. The temperature is found to be significantly higher for Cat-C1 fuel with a flame stabilized closer to the injection system allowing for more burnt gas recirculation. This change in flame position results of the faster ignition delay time of Cat-C1 at low temperature.

Ongoing work focus is on performing transient simulations to analyze the fuel effect on the blow-out process and evaluate the capability of LES to reproduce the trends obtained experimentally.

Acknowledgments

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References


