Low-order modeling of high-altitude relight of jet engine combustors

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Abstract

A physics-based, low-order ignition model is used to assess the ignition performance of a kerosene-fueled gas-turbine combustor under high-altitude relight conditions. The ignition model used in this study is based on the motion of virtual flame particles and their extinction according to a Karlovitz number criterion, and a stochastic procedure is used to account for the effects of spray polydispersity on the flame's extinction behavior. The effects of large droplets arising from poor fuel atomization at sub-idle conditions are then investigated in the context of the model parameters and the combustor's ignition behavior. For that, a Reynolds-averaged Navier-Stokes simulation of the cold flow in the combustor was performed and used as an input for the ignition model. Ignition was possible with a Sauter mean diameter (SMD) of 50 μm , and was enhanced by increasing the spark volume. Although doubling the spark volume at larger SMDs (75 and 100 μm) resulted in the suppression of short-mode failure events, ignition was not achieved due to a reduction of the effective flammable volume in the combustor. Overall, a lower ignition probability is obtained when using the stochastic procedure for the spray, which is to be expected due to the additional detrimental effects associated with poor spray atomisation and high polydispersity.

Keywords

ignition, spray combustion, aeroengine combustors

Introduction

Ignition is an important aspect in the operation of aviation gas turbine combustors. Ensuring safe re-ignition after a flame-out at high altitude – a so-called “high-altitude relight” – is one of the most stringent requirements in the design of combustors used in aviation propulsion systems. In aeronautical engines, the fuel is typically injected in the form of a liquid spray. Compared to gaseous flames, the presence of liquid droplets increases the complexity of the ignition process which is strongly affected by the size and location of the droplets as well as the volatility of the liquid^{1,2}, among all the other factors. The sub-atmospheric conditions associated to high-altitude relight, characterized by low pressure and low temperature, make the ignition process even more challenging. Such conditions, often associated with lower air flow velocities through the injector passages (in case airblast-type atomizers are used), have a negative effect on atomization, resulting in larger droplets and lumps of liquid that may penetrate towards the combustor liners. Large droplet sizes and low temperatures make the evaporation process very slow, limiting the availability of fuel vapor³. Therefore, much more energy is expected from the spark to ensure sufficient evaporation to have locally an ignitable fuel-air mixture, as well as to produce a flame kernel of relatively large size and increase the local temperature of the flow, leading to the kernel's successful establishment and subsequent propagation⁴. Thermal runaway is an additional peculiarity of the high-altitude ignition scenario. Immediately after the flame blow out, because of thermal inertia, the combustor's walls may still be hot. This effect can create more favorable conditions for ignition close to combustor liner, including evaporation of liquid droplets deposited on the wall. All these effects make the high-altitude conditions the most difficult scenario for ignition. As a consequence, the high-altitude ignition needs to be considered from early on in the design process of the combustor and may affect the entire operation envelope of the engine.

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Numerical simulations have become an indispensable tool to assist in the design of gas turbine combustors as they allow for an assessment and comparison of different design choices to reduce the number of expensive rig tests⁵. The forced ignition of a gas turbine combustor is an inherently transient process where evaporation, mixing as well as chemistry play a major role. Therefore, numerical methods able to accurately predict the flow, the flame transients, and mixture formation should be used. In this context the use of methods able to capture at least the large scales of turbulent motion is indispensable. Large-eddy simulation (LES) with advanced turbulent combustion modeling is, therefore, a good candidate for the prediction of ignition. The ability of combustion LES to capture the ignition process with reasonable accuracy has been demonstrated in various scientific publications^{6–8}. With the increase of computational power in recent years, high-fidelity LES has become feasible for industrial applications. Still, the ignition of turbulent flows exhibits a stochastic nature, which needs to be characterized in statistical terms⁹. Consequently, several ignition events have to be simulated to assess the ignition behavior for each ignition location and each operating condition. Despite its high computational costs, LES still allows for an evaluation of a small series of ignition events^{7,10}. Nevertheless, gas turbine designers may be interested in a large number of combustor designs in practice, as well as different operating conditions, fuels, and ignition locations. Such wide parametric studies can only be achieved using computationally inexpensive, reduced-order models which are based on the phenomena controlling the ignition transient of a flame and, at the same time, maintain key elements of stochasticity that typically characterize mixing and flame propagation. Examples of such modeling approach to gas-turbine relevant applications are the reactor based model by Sforzo and Seitzman¹¹ which evaluated the early-phase ignition of a kernel ejected from a sunken fire igniter, an approach further developed by Tang et al.¹² to include flamelet-like mapping. Alternatively, the approach proposed by Eyssartier et al.¹³ applied a series of ignition/propagation criteria to instantaneous LES flow-fields in order to assess the stochastic nature of ignition. Moreover, it is useful if such models provide designers with parameters for the evaluation of the combustion capability of the engine, such as ignition time scales and probability of ignition.

With these ideas in mind, the low-order ignition model called SPINTHIR was developed to evaluate ignition of a full combustor¹⁴. Its development is based on experimental findings related to the advection of the kernel. Following the principles detailed in¹⁵ concerning the phases of ignition as well as experimental evidence^{16,17}, the model identifies the long-term ignition failure, where a kernel is successfully established but further flame stabilization is not possible as the kernel is advected away from the anchoring point or into regions where it is starved of fuel. The model relies on a pre-evaluated averaged cold flow field to predict ignition probabilities from a cold-start condition. For that, it tracks virtual “flame particles”, modeled so as to mimic the possible paths of a flame kernel during an ignition transient. This is based on the assumption that advection by the mean flow and turbulent transport are key drivers of this phase of the ignition process. This assumption, combined with additional rules for the production and destruction of the particles based on mixture and flame properties, replicates the motion of a flame front.

The conditions for extinction of the flame particles is central to the algorithm and key to its accuracy. The particles’ extinction criterion is based on an empirical correlation for the Karlovitz number, obtained experimentally by Abdel-Gayed and Bradley¹⁸ and implemented in the code as a critical value¹⁴. This approach has been a product of extensive validation on non-premixed flames^{14,19}, premixed flames²⁰, and more recently on kerosene spray flames²¹. Due its the main assumptions related to flame transport, it is applied with good results to spray and gaseous non-premixed conditions and high turbulence. Furthermore, the critical value for extinction was verified to be approximately 1.5 in experiments with gaseous premixed flames in isotropic turbulence¹⁸, and has been used in the code for non-premixed and spray flames^{14,19,22} and premixed flames²⁰. There is, however, little or no evidence that such value applies to spray conditions.

In fact, as a result of the contribution of droplets to stretch due to strain and curvature at the droplet-scale²³, it has been expected²⁴ and recently verified^{21,25–27} that the global Karlovitz number of spray flames at which extinction is observed differ significantly from those of premixed flames¹⁸. In recent experiments with spherically propagating flames¹, local flame extinction in polydisperse kerosene sprays was observed to be led mainly by large droplets approaching the reaction zone. It is worth noting that these experiments were carried out at flow conditions not necessarily close to those of stable spray flames commonly seen in the literature, thus exhibiting three distinct spray-flame propagation modes. Local extinction in such spray flames has been commonly attributed either to heat-sink effects occurring in the evaporative cooling of the fuel droplet, or due to the large rich region surrounding the droplet as a result of evaporation^{1,28–30}. This phenomenon was observed by de Oliveira and Mastorakos¹ mainly in the inter-droplet and gaseous-like flame propagation modes, while, in contrast, continued propagation was attributed to the presence of large droplets in the vicinity of the reaction zone in the droplet-mode propagation regime¹. As first approach to incorporate such complex combination of droplet-induced effects as fluctuations of flame speed, increased flame wrinkling at the droplet scale, and the change in the local flammability of the mixture due to the random position of the droplets in the spray, de Oliveira et al.²¹ have used a stochastic approach to evaluate the effect of local equivalence ratio fluctuations caused by the spray’s polydisperse character was evaluated. In their work, measurements of ignition probability in kerosene spray flames³¹ were used to directly evaluate the Karlovitz values at which kerosene spray flames extinguish or ignite.

The present work demonstrates the application of recent experimental findings in a canonical geometry²¹ to the practical case of an aeroengine re-igniting at high-altitude conditions. Attention is given to flow conditions where atomization of the liquid fuel within the combustor is far from normal operation conditions, that is, characterised by high Sauter mean diameter and increased polydispersity. The objectives are as follows: (i) investigate the range of Karlovitz number within the combustor for different spray conditions and, in turn, its impact on ignition probability; (ii) compare the use of the recently proposed fuel fluctuation model in SPINTHIR and assess its impact on the model's resulting ignition probability; (iii) apply the model to a real aeroengine combustor and explore the effects of spray polydispersity and spark characteristics on ignition behavior.

Methods

Low-order ignition model

The low-order ignition model SPINTHIR (“Stochastic Particle INtegrator for High-altitude Relight”), originally developed by Neophytou et al.¹⁴, predicts the ignition probability of a combustor based on the time-averaged non-reacting flow field from simulations or experiments, tracking the motion of virtual “flame particles”. The time-averaged field variables that are required as inputs to the model are the mean gas velocity $\tilde{\mathbf{u}}$, the turbulent velocity fluctuation u' , the integral length scale L_T (or equivalent, turbulent kinetic energy, defined as $k = (u_{\text{rms}}^2 + v_{\text{rms}}^2 + w_{\text{rms}}^2)$ and related to u' by $k = 3u'^2/2$, and turbulent dissipation rate, $\varepsilon = u'^3/L_T$), the mean gaseous and liquid mixture fractions, $\tilde{\xi}_g$ and $\tilde{\xi}_l$, the volumetric evaporation source term $\bar{\Gamma}_m/\bar{\rho}$ (given in s^{-1}), the arithmetic mean diameter d_{10} and the Sauter mean diameter d_{32} , all given as functions of the space variable $\mathbf{x}$.

The fluid domain is discretized by a coarse grid of cube-shaped cells of size Δx with the cell volume $V_c = \Delta x^3$. The stochastic motion of flame particles in the domain determines the state of each cell, which is defined as either hot or cold. All cells are set to the cold state at the beginning of each simulation. The growth of the flame is mimicked by the motion of the flame particles and the emission of new particles every time a flame particle enters a cell in the cold state. Once the latter occurs, the state of the cell is switched to the hot state until the end of the simulation. An ignition spark is simply modeled by switching one or more cells to the hot state, emitting one or multiple flame particles.

A flame particle is defined based on the characteristics of the two-phase flow field. The particle's motion follows a random walk given by a simplified Langevin model,

$$\Delta \mathbf{X}_p = \mathbf{U}_p \Delta t \quad (1)$$

$$\begin{aligned} \Delta \mathbf{U}_p = & - \left(\frac{1}{2} + \frac{3}{4} C_0 \right) \left(\frac{u'}{L_T} \right) (\mathbf{U}_p - \tilde{\mathbf{u}}) \Delta t \\ & + (C_0 \varepsilon \Delta t)^{1/2} \mathbf{N}_p \end{aligned} \quad (2)$$

where $\Delta \mathbf{X}_p$ and $\mathbf{U}_p$ are the displacement and velocity vectors of the particle at the time step Δt . A random fluctuation mimicking turbulent dispersion is added to the particle velocity by $\mathbf{N}_p$, a vector with uniformly distributed random direction and a length that follows the normal distribution $\mathcal{N}(0, 1)$. The evolution equation of the particle gaseous mixture fraction is

$$\begin{aligned} \Delta \xi_{p,g} = & \frac{1}{2} C_\xi \left(\frac{u'}{L_T} \right) (\xi_{p,g} - \tilde{\xi}_g) \Delta t \\ & + (1 - \xi_{p,g}) \frac{\bar{\Gamma}_m}{\bar{\rho}} \Delta t \end{aligned} \quad (3)$$

where $\bar{\rho}$ represents the non-reacting gas density. The model constants are set to $C_0 = C_\xi = 2$.

The Langevin equation describes the Lagrangian motion of fluid particles and, as such, on average, it reproduces the mean field of mixture fraction obtained by RANS. Also, the Langevin equation allows us to introduce local and instantaneous fluctuations in the temporal history of the particles, which are governed by the statistical moments of the mixture fraction, in an Eulerian sense.

Further, local flame extinction by means of turbulent strain is mimicked and introduced into the particle's behavior through an extinction criterion based on the Karlovitz number, which is defined as the ratio of chemical to Kolmogorov time scales. The Karlovitz number of a flame particle is evaluated from the empirical correlation by Abdel-Gayed and Bradley¹⁸:

$$\text{Ka}_p = 0.157 \left(\frac{u'}{S_L} \right)^2 \text{Re}_T^{-0.5}, \quad \text{Re}_T = \frac{u' L_T}{\nu}. \quad (4)$$

The turbulent velocity fluctuation is evaluated as $u' = \mathbf{U}_p - \tilde{\mathbf{u}}$, to introduce a stochastic component of turbulent strain in the extinction criterion. The condition for continued propagation of the particles is verified at each time

step as $Ka_p < Ka_{crit}$. Once Ka_p exceeds the critical value, a particle is extinguished and is no longer accounted for in the following time steps. The critical Karlovitz number Ka_{crit} was set to 0.5 in the present studies, a value that was obtained from a backwards calibration of the present model using ignition probability measurements taken in canonical experiments of spherically propagating flames in uniform droplet dispersions with aviation fuel²¹.

In the evaluation of Ka_p , the laminar burning velocity of the spray flame, $S_L = f(\phi_p, \Omega_p, d_{32})$, is evaluated from the correlation proposed in³² based on the droplet Sauter mean diameter, d_{32} . For that, the local Sauter mean diameter of the spray $d_{32}(\mathbf{x})$ is used, and also the particle's equivalence ratio, ϕ_p , and degree of prevaporization, Ω_p ,

$$\phi_p = \phi_{p,g} + \phi_{p,l}, \quad \Omega_p = \phi_{p,g}/\phi_p \quad (5)$$

The gas-phase equivalence ratio $\phi_{p,g}$ is calculated from

$$\phi_{p,g} = \frac{\xi_{p,g}}{1 - \xi_{p,g}} \frac{1 - \xi_{st}}{\xi_{st}}, \quad (6)$$

where $\xi_{p,g}$ is obtained from Eq. 3 and ξ_{st} is the stoichiometric mixture fraction (note: $AFR_{st} = (1 - \xi_{st})/\xi_{st}$ is the stoichiometric air-fuel ratio).

The liquid-phase equivalence ratio $\phi_{p,l}$ is evaluated according to the stochastic procedure described previously²¹. Since liquid droplets are heavy compared to the gas and generally move with a velocity different from the gaseous carrier phase, the liquid equivalence ratio is not considered to be transported with the flame particles. Instead $\phi_{p,l}$ is evaluated for the cell volume at the instantaneous location of flame particle. The liquid fuel equivalence ratio in a fluid cell can be approximately computed as

$$\phi_{p,l} = \frac{\rho_l V_{l,c}}{\rho_g V_c} \frac{(1 - \xi_{st})}{\xi_{st}} \quad (7)$$

where $V_c = \Delta x^3$ is the volume of the domain cell, $V_{l,c}$ is volume of the liquid in the cell, and ρ_l and ρ_g are the densities of the liquid and the gas. Here, a dilute spray was assumed, i.e. $V_{l,c} \ll V_c$. Further assuming that the vapor fraction in the gas is small and neglecting the effect of evaporative cooling, we use constant values $\rho_g = \rho_{air} = cst$ and $\rho_l = cst$. In fact, the $V_{l,c}$ is the only variable in Eq. 7 that exhibits stochastic fluctuations, which may arise due to variations in number and size of the droplets present in the finite volume of size a cell.

In order to determine $\phi_{p,l}$, the liquid volume in a cell, $V_{l,c}$, is computed at every time step according to the following stochastic procedure. It is assumed that the droplet distribution at any location can be described using a modified Rosin-Rammler distribution that is representative of the distribution obtained after long sampling time at a location, corresponding to the time-averaged flow field. Then the accumulated liquid volume fraction is³³,

$$Q(d; \mathbf{x}) = 1 - \exp \left[- \left[\ln d / \ln X(\mathbf{x}) \right]^q \right]. \quad (8)$$

where X and q are the parameters of the distribution that are chosen independently for every point in space to best fit the local values of d_{10} and d_{32} from the time-averaged flow field. The fraction of liquid contained in droplets of size class i is $\Delta Q_i = Q(i) - Q(i-1)$, and the liquid volume fraction occupied by the corresponding droplets is $\theta_{l,i} = \theta_l \Delta Q_i$. Next we assume an arbitrary volume V_0 which contains $N_i = (\theta_{l,i} V_0) / (\pi d_i^3 / 6)$ droplets of each size class, V_0 being sufficiently large so that $N_i \gg 1$ for all size classes. Assuming that the droplets are uniformly distributed in space, the number of droplets in a sub-volume V_c (being the volume of a domain cell, Δx^3) follows a binomial distribution, which can be approximated by a Poisson distribution. Accordingly, the probability of finding exactly $N_{i,c}$ droplets in V_c can be calculated is

$$P_i(N_{i,c}) = \frac{e^{-\mu_i} \mu_i^{N_{i,c}}}{N_{i,c}!}, \quad (9)$$

where μ_i is the mean number of droplets of size i in the cell, $\mu_i = n_i V_c$, and $n_i = N_i / V_0$. Hence the number of droplets of each size class, $N_{i,c}$, in each volume cell is determined stochastically. Then the particle's liquid equivalence ratio taken equal to the liquid equivalence ratio in the volume cell is²¹,

$$\phi_{p,l} = \sum_{i=1}^{\infty} \left[\Delta Q_i \frac{N_{i,c}}{n_i} \frac{1}{V_c} \right] \phi_l \quad (10)$$

where,

$$\phi_l = \frac{\tilde{\xi}_l}{1 - \tilde{\xi}_l} \frac{1 - \xi_{st}}{\xi_{st}} \quad (11)$$

is the mean liquid equivalence ratio at the flame particles location (the liquid mixture fraction is defined as $\xi_l \equiv m_l / [m_l + m_{air}]$).

Table 1. Constant parameters used in the simulation with SPINTHIR.

ξ_{st}	0.0657	-
ν	$2.075 \cdot 10^{-5}$	m^2/s
Δx	3	mm
Δt	0.5	ms

Figure 1. Fuel distribution in a sector of a developmental rich-quench-lean combustor. Flammable regions are depicted in green.

In order to monitor individual ignition attempts, it is convenient to define an ignition progress factor, Π , as the number of burned cells divided by the number of cells in the combustor. Since hot cells cannot switch back to the cold state, Π increases monotonically. An ignition event is considered to be successful if the ignition progress factor passes a critical threshold, i.e. the model's criterion for ignition success is $\Pi > \Pi_{crit}$. The threshold, Π_{crit} , is case dependent and needs to be chosen accordingly. The probability of ignition, P_{ign} , is evaluated by performing a large number of simulations for the same condition.

Simulation set-up

Constant parameters used in SPINTHIR in the present work are summarized in Table 1. The stoichiometric mixture fraction ξ_{st} corresponds to a kerosene-air mixture. The gas density ρ_g and the viscosity ν correspond to pure air at the operating conditions, neglecting the effect of fuel vapor in the mixture. The cell size Δx and the time step Δt were set according to the guidelines presented in Ref. ¹⁴. The flame speed, $S_L(\phi_p, \Omega_p, d_{32})$, used in the extinction criterion (Eq. 4), was evaluated using the correlation developed by Neophytou et al. ¹⁴ (Eqs. 7-9 in Ref. ¹⁴) from 1-D freely propagating laminar flames, adjusted for the gaseous laminar burning velocity of kerosene ³⁴. A comparison between the measurements and the values obtained from the correlation is given in ²¹.

In the ignition simulation performed with SPINTHIR the spark location placed at the top of the combustor near the injector location (shown in Fig. 2d). The effect of the spark size on ignition capability of the combustor was investigated by performing calculations with spark diameters of $d_{spark} = 10, 16$, and 20 mm. A total of 500 ignition attempts were carried out. The code is conveniently designed so it is computationally inexpensive, allowing for parametric studies to be easily carried out. For example, each case comprising of all ignition attempts requires around 10 CPU hours (Intel Core i7, 2.4 GHz).

Two different versions of the ignition model are tested. In the first version, which corresponds to the model originally published by Neophytou et al. ¹⁴ (referred to in this paper as *original* SPINTHIR model), the liquid equivalence ratio is evaluated without considering stochastic fluctuations; hence $\phi_{p,l} = \phi_l(\mathbf{x})$, computed according to Eq. 11. In the second version of the model (referred to as *modified* SPINTHIR model), $\phi_{p,l}$ is computed from Eq. 10 considering the stochastic effect of a polydisperse spray. All other features of the model are kept the same in both versions. The criterion for ignition success used the ignition progress factor Π . The critical ignition progress factor was $\Pi_{crit} = 0.15$ for the original SPINTHIR model (where $\phi_{p,l} = \phi_l(\mathbf{x})$), and $\Pi_{crit} = 0.05$ for the *modified* model, considering the fuel fluctuation model due to the spray (Eq. 10). This threshold is geometry specific, as indicated in a previous work ¹⁴, and can be verified in the future through experimental and high-fidelity reacting simulation data.

Non-reacting flow field

SPINTHIR was tested by simulating the ignition at conditions resembling those of high-altitude relight of a realistic Rolls-Royce rich-quench-lean (RQL) combustor. The time-averaged cold flow field, necessary as input for

Figure 2. Combustor cross-section gas velocity fields used in SPINTHIR, obtained by interpolating the RANS solution data to a regular grid, shown at the cross-section $y = 0$.

SPINTHIR computations, was obtained from a computational fluid dynamics (CFD) simulation using the Rolls-Royce proprietary finite volume code PRECISE-UNS, described by Anand et al.³⁵. The geometry and the numerical mesh of the combustor consist of a single sector with diffuser and annuli regions included. In the simulation, an Eulerian-Lagrangian approach was employed, which combines an Eulerian description of the gas-phase with a Lagrangian simulation of the fuel droplet motion. The Reynolds-averaged Navier-Stokes (RANS) framework with $k-\epsilon$ turbulence model³⁶ was used for the gaseous flow. Typical RANS equations for cold flow were solved, together with a scalar equation representing the mixture fraction of fuel released by droplet evaporation. The Lagrangian tracking of fuel droplets (dispersed liquid phase) was performed using material-point approximation, two-way coupled with the gaseous phase. The modeling of the dispersed liquid phase included the standard sphere drag correlation³⁷, stochastic dispersion, and the Abramzon-Sirignano evaporation model³⁸. Further details on the Eulerian-Lagrangian approach implemented in PRECISE-UNS, numerics and solution strategy can be found in Ref.³⁵ and references therein.

The liner cooling system was included in the simulations by using both direct modeling (e.g. slot cooling for the tiles) and distributed source/sink terms at the corresponding walls (liners with film cooling). The flow split between the cooling streams were provided by Rolls-Royce and computed with low-order network tools.

The CFD simulation was carried out by imposing periodic conditions on the lateral boundaries of the combustor's sector. Velocity profiles obtained from simulations of the compressor were imposed at the inlet, whereas an outlet condition was used at the combustor's exit. The operating condition was representative of sub-idle operation of the engine, corresponding to a static pressure $p = 38400$ Pa and a temperature $T = 263$ K. The fuel spray at the injector was assumed to follow a Rosin-Rammler distribution with distribution parameters X and q of $100\mu\text{m}$ and 6, respectively, resulting in a d_{32} of $50\mu\text{m}$. The droplet temperature at the injection location was assumed to be equal to 400 K. The higher value compared to the gas-phase temperature is justified by the thermal inertia of the combustor walls that contribute to keep the liquid temperature at injection above the ambient temperature.

The discretization schemes were of second order in space for all flow variables but the turbulence model variables, for which an upwind scheme was employed. A hexa-dominant unstructured mesh of approximately 20M cells was used. The computational mesh, provided by the Combustion Aerothermal Methods group at Rolls-Royce plc., was built according to best-practices developed by the company over more than ten years of experience in simulations of aero-engine combustors. Best practices are the results of extensive studies on configurations similar to the one investigated in this work to ensure mesh independence and accurate representation of the flow through the injector, including swirl and spray opening angle, and in the diffuser area as well as mixing in the region downstream of the dilution holes. Accuracy in the simulation of the flow field and mixing was achieved through refinements in the injector and in high shear regions.

Results and discussion

First, the Reynolds-averaged, non-reacting flow field is discussed. Figure 1 shows the fuel distribution in the combustor at the condition studied (with injected SMD equals $50\mu\text{m}$), with green isocontours representing an overall mixture within the gaseous flammability limits ($0.5 < \phi < 3.6$, see Ref.³⁹) and blue and red isocontours representing regions below the lean limit and above the rich flammability limit, respectively. The evaporation of kerosene fuel at the present sub-atmospheric conditions is very slow, so that the fuel is almost entirely present

Figure 3. Combustor cross-section fields used in SPINTHIR obtained by interpolating the RANS solution data to a regular grid: (a) equivalence ratio, (b) Sauter mean diameter, and (c) turbulent kinetic energy. Numbers 1 and 2, indicated in (a) refer to the center of the combustor and the spark location, respectively.

in the liquid form. Consequently, the equivalence ratio field directly indicates the presence of droplets. Near the injector and within the spray cone the overall mixture is very rich. Due to the annular periodicity of the combustor, the spray cones of the adjacent injectors also intersect with this sector, giving rise to the pattern of high equivalence ratio best seen in Fig. 1b. Figure 2 shows the Reynolds-averaged velocity field, normalized by the maximum absolute velocity found in the combustor. The injection regions and dilution jets characterized by a high velocity magnitude can be clearly seen in Fig. 2c.

In the next step, ignition simulations with SPINTHIR are explored. Figure 3 shows flow variables relevant to the ignition model in the combustor middle plane: the fields of (a) the (total) equivalence ratio, (b) Sauter mean diameter (SMD), and (c) turbulent kinetic energy. A high concentration of fuel can be seen in (a) in the vicinity of point 1, which is caused by the merging of the two adjacent injection cones in the annular combustor with the injection cone of the current sector. This region is also characterized by high turbulent kinetic energy levels, which is mainly induced by the high velocity of the dilution jets (c). Overall, the SMD remained very uniform within the combustor (b), except in the region closest to the injector and at points downstream of it, where some slight segregation of the droplets based on their momentum may also occur due to the flow. One should note that, as the images depict an axial cut of the combustor, the full spray cone might not be fully represented. In terms of SMD, for example, regions of very small fuel volume fraction as those occurring inside the cone, will be characterised by low SMD values.

As a step towards understanding the non-linear effect of atomization on the combustor's ignition performance, a parametric study considering three distinct Sauter mean diameters was carried out. For this investigation the *modified* model with stochastic spray modeling was used. Further, the cold flow field obtained from RANS was used, as shown previously in Figs. 1–3, while the d_{32} field was scaled by 50% and 100%, that is, representing an injected SMD of 75 and 100 μm , respectively. The representative Rosin-Rammler volume fraction curves are illustrated in Fig. 4 for reference, with their resulting effect on the cell's PDF of $\phi_{c,1}$ shown in (b). A characteristic effect of increasing the spray SMD on the variance of equivalence ratio (Fig. 4b) is a shift of the distribution towards lean conditions, and the appearance of a longer tail at richer conditions than the mean. The latter effect represents events in which very large, but scarce droplets of diameter around 400–600 μm are accounted for in the cell. It should be noted that a better prediction of the spray cone and the recirculating flow can be obtained by using Large Eddy Simulations.

A comparison between the three investigated cases (SMDs of 50, 75, and 100 μm) is shown in Fig. 5 in terms of S_L and Ka computed from the Reynolds-averaged, mean flow variables. In this approach, S_L and Ka shown are the values used by the original SPINTHIR model. Moreover, Fig. 5 visualizes that the region of high S_L and low Ka shrinks as the SMD of injected droplets increases. This shows how poorer atomization, as caused by lower liquid fuel temperatures at sub-atmospheric operating conditions, will have a strongly detrimental effect on the ignitability of the combustor. Nevertheless, in the *modified* model, $\phi_{p,1}$ (the quantities required for the evaluation of S_L and Ka) are evaluated stochastically; hence, ignition of the regions of high mean Ka , shown in black, is still possible.

Note that the flame particles' gaseous mixture fraction, ξ_p , exhibits stochastic fluctuations, which deviate from the mean mixture fraction $\tilde{\xi}$. The governing Lagrangian equation (Eq. 3), on average, reproduce the Eulerian mean mixture fraction field obtained by RANS. The Lagrangian formulation thus allows us to introduce local and

Figure 4. (a) Rosin-Rammler volume fraction distributions and (c) typical resulting PDFs of liquid equivalence ratio for the particles considering the model in Eq. 10 and three conditions corresponding to injected SMDs of 50, 75, and 100 μm .

instantaneous fluctuations in the temporal history of the particles, which are locally equivalent to the statistical moments of the mixture fraction. In addition to these gas-phase fluctuations, liquid-phase fluctuations modeled with the present stochastic approach due to the spray will also add to the fluctuations of the particles' mixture fraction. In the present case, the fluctuations of the gaseous mixture fraction are small compared to the variance that arises due to the spray.

Figure 6 shows the probability density functions of equivalence ratio, flame speed, and Karlovitz number stochastically computed in SPINTHIR considering the fuel fluctuation model and the velocity fluctuations seen by the flame particles. Point data is given for two locations within the combustor: at the (a) combustor center and at the (b) spark location (points 1 and 2 in Fig. 3a). The PDF at the spark location is relevant for the initial survival and subsequent growth of the kernel, whereas the PDF in the center region of the combustor eventually determines if a substantial fraction of the combustor volume can be reached by the flame, i.e. if the critical value of Π attained to achieve successful ignition. It can be seen that the effect of increasing the injected SMD is more detrimental at the combustor center location (Fig. 6a); a higher reduction in probability of values $Ka < Ka_{\text{crit}}$ is observed in this case due to the higher average equivalence ratio. An initial test was performed to compare the performance of the modified SPINTHIR with its original version. The ignition events are monitored using the ignition progress factor Π . Figure 9 shows Π in terms of the time after the spark for a test with the (a) original and the (b) modified model (with the fuel fluctuation). For the condition studied ($d_{\text{spark}}=10$ mm, $\text{SMD}=50$ μm), most of the ignition attempts in both cases (a,b) resulted in quenching of the flame particles soon after the “spark” was initiated, that is, within the first few time steps of the simulation. Failure to ignite the combustor in (a) was also observed in cases where a large burned region took place ($\Pi = 0.1$, approximately), although this type of failure was less frequent than the rapid quenching of the spark region. Ignition events were in turn characterized by an initial slow propagation of the flame particles, followed by their rapid growth in number. As shown in Fig. 7, the flame particles representing the kernel generated by the spark (i) were captured by the recirculation zone of the burner downstream of the fuel injection, igniting that region (iii), and only then spreading throughout the combustor (iv-vi). In contrast, in a typical ignition failure event (Fig. 8), the flame particles propagated towards the recirculation zone (ii-iii) but fully extinguished without ever igniting it (iv) – alternatively, the particles simply advected downstream the combustor. It should be noted, when interpreting the present results, that the underlying Reynolds-averaged flow field remains constant throughout the simulation of an ignition event, in line with the present low-order approach. The reader is cautioned to the limitations of the model when interpreting its results, as no feedback between the flame particles and the flow field is accounted for. One should note that additional factors impacting the ignition probability results are related to the model's lack of capability to capture, for instance, a sequence of interconnected ignition, extinction, and re-ignition events, where hot walls and products may remain in the combustion chamber affecting the subsequent ignition attempt.

The original and the modified SPINTHIR models are further compared in terms of the predicted ignition probability (Fig. 9) for the case of injected SMD of 50 μm . While the original model predicted a P_{ign} of 18% (a), with the modified model (b) a significantly lower probability of approximately 4% was obtained, which seems in agreement with practical experience with this type of combustor at the given operating conditions. In addition, a high fluctuation of the particle's equivalence ratio (attributed to the presence of large droplets at the tail of the Rosin-Rammler distribution as shown in Fig. 4) led to an effectively smaller flammable region in the combustor. In other words, for an injected SMD of 75 and 100 μm , a reduction of the local equivalence ratio at the cell tends to shift towards lower values, as shown in the PDF of Fig. 4c. This overall reduction of flammability explains the lower values of Π for ignition cases obtained in (b) in relation to (a).

Figure 5. Combustor cross-section fields of flame speed and Karlovitz number calculated from mean flow variables, ignoring the variance of the liquid equivalence ratio. Both fields are given for injector SMDs of (a) 50 μm , (b) 75 μm , and (c) 100 μm .

Figure 6. Probability density functions of equivalence ratio, flame speed, and Karlovitz number for injection SMDs of 50, 75, and 100 μm at two distinct locations: (a) combustor center, (b) spark location (Points 1 and 2, Fig. 3).

Figure 7. Example of an ignition sequence in SPINTHIR, with yellow and red particles representing the burning and extinguished virtual flame particles in the domain, respectively – $d_{32}=50\text{ }\mu\text{m}$, $d_{\text{spark}}=10\text{ mm}$. Time instants from (i) to (vi) correspond to 1, 10, 20, 30, 40, and 50 ms.

Figure 8. Example of a failed ignition sequence in SPINTHIR – $d_{32}=50\text{ }\mu\text{m}$, $d_{\text{spark}}=10\text{ mm}$. Time instants from (i) to (iv) correspond to 1, 2.5, 4, 5.5 ms.

Finally, the overall ignition behavior of the engine is given in Fig. 9 for various conditions with different spark diameters and injected SMDs, while using only the modified version of SPINTHIR. Additionally, the probability

Figure 9. Ignition progress factor in terms of time after the spark for the (a) original and (b) modified SPINTHIR model – $d_{32}=50\text{ }\mu\text{m}$, $d_{\text{spark}}=10\text{ mm}$.

of initiating a flame in the combustor, denoted as P_{flame} , that is, achieving a small flame with $\Pi > 0.01$, as well as the resulting ignition probability, P_{ign} , are given in Fig. 11a-b, respectively, calculated based on the results of Fig. 10. For the lowest SMD case (SMD= $50\mu\text{m}$), increasing the spark diameter guaranteed a higher ignition probability (Fig. 9b) by increasing the likelihood of more flame particles initiated at the spark surviving local quenching and continuing to propagate. This effect is seen in Fig. 9 for the three SMD cases. However, increasing the spark diameter was not enough to guarantee ignition (as measured by P_{ign}) in cases with coarser sprays. In those cases, although increasing d_{spark} led to higher P_{flame} for SMD of 75 and $100\mu\text{m}$ (Fig. 11a), the presence of large droplets suppressed further propagation of the flame particles beyond $\Pi = 0.05$, as seen in Fig. 10 middle and right columns. This occurred due to extremely low values of S_L caused by the large droplets. Nevertheless, there is evidence that ignition might occur even in conditions of extremely high SMDs. The fact that the model was not able to capture ignition events at such conditions suggests that additional models must be taken into account in conditions with extremely poor atomization. In order to do so, one may be able to couple consecutive ignition attempts, for example, to account for vapor fuel build-up within the combustor chamber, which is believed to occur in real applications and could have a significant impact on the model.

Conclusion

The effect of the spray polydisperse character was investigated in the context of the low-order ignition model SPINTHIR applied to a sector of a Rolls-Royce developmental RQL gas-turbine combustor at relight conditions. RANS simulations of the combustor at non-reacting conditions were carried out, and the data was used as an input for the ignition model SPINTHIR to predict the combustor's ignition behavior. In order to achieve low computational cost, the Reynolds-averaged flow field is constant – this is a key assumption of the present modelling approach.

To incorporate droplet-induced effects on flame extinction in SPINTHIR, which is achieved through the Karlovitz number-based extinction criterion, an additional model was used to evaluate the spray polydispersity taking an stochastic approach, where the local equivalence ratio at each of the model's cells is evaluated based on the cold-flow spray characteristics. To illustrate the difference between the *original* and the newly proposed *modified* SPINTHIR models, probability density functions (PDF) of equivalence ratio, flame speed, and Karlovitz number were evaluated at the spark location and at the center of the combustor. Overall, using a stochastic formulation, the presence of large droplets manifests in the occurrence of very high Karlovitz number values, which have a detrimental effect on the ignition performance of the combustor. This non-linear effect does not appear when only Reynolds-averaged spray properties are considered otherwise in the original model. In fact, the stochastically obtained values of flame speed and Karlovitz number differed significantly from their values obtained from mean flow variables. This also illustrates, for example, why in the proposed model the propagation of flame particles can be verified in regions of extremely high Ka values, or even in regions with a mean equivalence ratio below the lean flammable limit. Moreover, successful ignition events were characterized by the propagation of flame particles to a rich and high-turbulence region just downstream of the spray cone, followed by ignition of the whole combustor, while ignition failure events were marked by quenching of flame particles immediately after the spark or, simply, their advection downstream the combustor.

Overall, using the modified SPINTHIR model, i.e. accounting for the fuel fluctuations due to the spray, resulted in lower values of ignition probability for the combustor studied when compared to results where a single, time-averaged cell equivalence ratio value was considered. For the lowest injection SMD case considered ($50\text{ }\mu\text{m}$), increasing the spark diameter in the model from 10 to 20 mm resulted in suppression of events where quenching of the flame particles in the model was observed immediately following the spark, thus leading to higher ignition probability values. The same trend was not observed for higher injection SMDs ($75\text{--}100\text{ }\mu\text{m}$). Although for these cases, increasing the spark size resulted in an initially larger volume occupied by the flame particles, their

Figure 10. Ignition progress factor in terms of time after the spark for conditions with $d_{32}=50, 75, 100 \mu\text{m}$, $d_{\text{spark}}=10, 16, 20 \text{ mm}$.

Figure 11. Resulting (a) probability of generating a flame in the combustor and (b) probability of ignition for conditions in Fig. 10.

subsequent growth and propagation was not significant to achieve ignition. This effect was likely observed due to an overall reduction of the flammable area of the combustor due to the fuel fluctuation model. Further work is needed on the ignition model to better predict ignition at conditions of poor fuel atomization, for example, considering other approaches as a dependency between individual ignition attempts, building up of vapor fuel in the combustor, as well as temperature increase of the combustor with failed attempts.

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Appendix - Rosin-Rammler distribution parameters

The purpose of this Appendix is to show how the parameters of the modified Rosin-Rammler distribution, X and q , are related to d_{10} and d_{32} , which are readily available from the CFD simulation.

First, consider the regular Rosin-Rammler distribution where with the following cumulative volume density function,

$$Q(d) = 1 - \exp \left[- \left(\frac{d}{X} \right)^q \right] \quad (12)$$

with $X > 0$, $q > 0$. Then the volume distribution is

$$f_Q(d) = \frac{dQ}{dd} = \frac{q}{X} \left(\frac{d}{X} \right)^{q-1} \exp \left[- \left(\frac{d}{X} \right)^q \right] \quad (13)$$

We note the definition of the gamma function:

$$\Gamma(n) = \int_0^\infty t^{n-1} \exp(-t) dt \quad (14)$$

Integrating f_Q by substituting $u = (d/X)^q$ leads to

$$\int_0^\infty d^k f_Q(d) dd = X^k \Gamma \left(\frac{k}{q} + 1 \right) \quad (15)$$

Figure 12. Rosin-Rammler: relations diagram for d_{10} and d_{32} in terms of Rosin-Rammler distribution parameters X and q .

Since the number distribution is defined as $f_N(d) = f_Q(d)/d^3$, for instance, for d_{10} one has $k = -2$ and -3 for the numerator and denominator. It follows that

$$d_{10} = X \frac{\Gamma(1 - 2/q)}{\Gamma(1 - 3/q)}, \quad d_{32} = X \frac{1}{\Gamma(1 - 1/q)}. \quad (16)$$

The relations diagram for d_{10} and d_{32} in terms of Rosin-Rammler distribution parameters X and q is shown in Fig. 12.

Second, for the modified Rosin-Rammler volume distribution (Eq. 8) the relationship between X and q , and d_{10} and d_{32} is determined numerically.