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Simulations of droplet combustion under gas turbine conditions

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ABSTRACT

In various applications with recirculation, liquid droplets can be immersed in gases that may have a wide range of possible compositions, from pure air to hot combustion products. In order to gain fundamental understanding of the behaviour of individual droplets in vitiated air, numerical simulations of kerosene single droplet evaporation, autoignition, and combustion in conditions relevant to gas turbines have been performed. The droplet autoignition behaviour has been analysed in both physical and mixture fraction space for a wide range of vitiated air compositions and initial droplet diameters. Results show that the autoignition time delay decreases with increasing level of dilution with hot combustion products and decreasing initial droplet diameter. Chemistry is confined up to a radius of almost 10 initial droplet diameters and the location of autoignition is influenced by both the initial droplet diameter and the level of dilution. The time evolution of species in the gaseous phase after autoignition shows similar trends for all the diameters and dilution levels investigated here with the peak of temperature and OH mass fraction moving towards the droplet surface as a consequence of the balance between fuel production and consumption. In mixture fraction space, the location of the peaks of temperature and OH mass fraction after autoignition do not change in time whereas other intermediate species such as CH_2O and pyrolysis products still exhibit a quite variable behaviour. The long-time flame structure has been compared with gaseous laminar counterflow simulations and, although qualitatively similar, the flame structure in the two configurations has differences with implications for flamelet combustion models used in spray combustion. The droplet evaporation, autoignition, and combustion behaviour has been summarized through a regime diagram showing the evaporation and autoignition time delays as a function of both initial droplet diameter and vitiated air dilution. This allows the identification of different states in the droplet combustion scenario and the introduction of critical values of dilution and initial droplet diameter beyond which single droplet rather than cloud combustion can occur, which can be exploited in the design of lean burn gas turbine combustion systems. The approach presented here can be easily extended to other conditions and fuels allowing the generation of regime diagrams for various operating conditions.

1. Introduction

In a conventional spray flame of relevance to technological practice in stationary combustion systems, the spray is injected in close proximity to a recirculation zone that helps stabilise the flame. Therefore, the droplets are found in gases with a wide range of possible compositions, spanning air to fully-burnt combustion products. This is schematically demonstrated in Fig. 1 where the scenario of a typical aero-engine injection configuration based on the airblast concept [1] is shown. The fuel is injected in the form of a liquid film and the swirling air that flows on the two sides of the atomizing lip determines both the film atomization and the formation of the recirculation zone in the primary combustion region providing flame stabilisation. Due to the highly unsteady nature of the atomization process and the high level of velocity fluctuations induced by the swirling flows, droplets can be transported inside the recirculation zone or at the shear layer, being therefore exposed to hot combustion products with different levels of dilution. A similar scenario also applies to configurations based on pressure atomizers, typically used in pilot stages. Depending on the droplet's history (size, temperature, ambience), a droplet-scale flame may be ignited or the fuel may burn in a cloud, i.e. a predominantly non-premixed flame with fuel supplied from droplet evaporation [2]. Both these options suggest that combustion occurs at a mixture fraction close to the stoichiometric value, and hence the formation of NO_x is not minimal [3]. Technologies that try to avoid droplet-scale or stoichiometric reaction zones offer a way of burning with a low reaction zone temperature so that NO_x is

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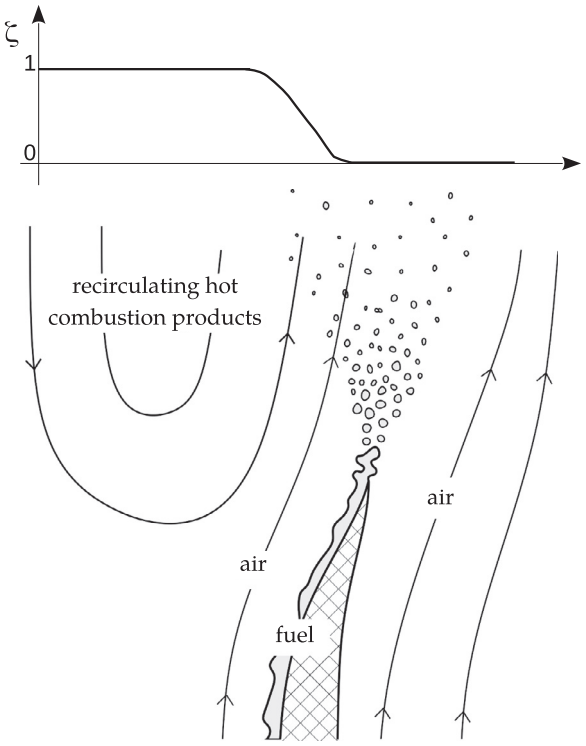

Fig. 1. Droplet injection scenario in a typical aero-engine combustor.

minimised. Hence, the Lean Premixed Prevaporised (LPP) concept (e.g. [4,5]), or "Lean Burn" as it is often denoted, is receiving attention from gas turbine and industrial burner manufacturers. In this concept, the spray is injected early on so that significant evaporation occurs before the flame, and hence the flame may be made lean [6–8]. To make this idea work, the evaporation time, autoignition time, residence time, but also droplet path (in the sense of composition of gases it encounters) must be such as to preclude the development of a droplet-scale flame and to promote full evaporation upstream of the flame.

Fuel droplets immersed in hot combustion products is also a scenario relevant for another combustion technology, related to the MILD (Moderate or Intense Low-Oxygen Dilution) combustion concept [9], where the fuel and the air are injected though high-velocity jets so that significant mixing with the recirculating hot combustion products occurs. This leads to low peak flame temperatures, limiting the production of NO_x, and encourages long residence times, reducing CO and UHC emissions [7]. Most MILD combustion studies focus on gaseous jets in vitiated co- or cross-flows [10–12] or the development of MILD gaseous gas turbine combustion concepts [13–16]. Sprays in hot combustion products have received less attention so far from the perspective of constructing a MILD combustion gas turbine system, but some fundamental experimental studies [17,18,19] discuss the emergence of single-droplet or group combustion in configurations where a spray is interacting with hot products.

The canonical problem of a single isolated droplet evaporation, autoignition and quasi-steady combustion helps identify the timescales of the various processes involved in the above, from both a practical and a fundamental perspective. However, a systematic estimation of these timescales, for a range of possible ambient gas compositions and temperature, and using detailed simulation approaches, is not available at present [20]. This work focuses in particular at kerosene and gas turbine conditions, but the type of calculations presented here can be done for any condition, ambience or fuel.

A further motivation for studying the single-droplet combustion problem is to explore whether the species profiles, especially when plotted *vs.* mixture fraction, are similar to what one would expect from a gaseous flame. Flame structures derived from laminar gaseous flame configurations are often used in spray combustion calculations based on flamelet approaches (e.g. [21–23]). However, there is evidence that the presence of droplets may have a strong impact on the local structure of the flame [24–28] making the predictions based on the pure gaseous flames possibly inaccurate. The structure of spray flamelets is not only determined by the mixture fraction and its scalar dissipation rate, as in typical counterflow gaseous laminar diffusion flames, but also by the initial droplet size and velocity [29,30]. In particular, as also recently pointed out in [31,32], droplet evaporation plays a key role in the characterization of the spray flame structure, as well as in the flame–vortex interaction [33], leading to significant differences compared to the corresponding gaseous flame. For these reasons, the use of flamelet approaches with evaporation effects included has been suggested [31,34]. Spray flame structure in mixture fraction space is also relevant for methods based on the solution of quantities conditioned on the mixture fraction, such as the Conditional Moment Closure (CMC) model [35]. The importance of including the spray evaporation terms in the equations describing the evolution of conditional quantities has already been highlighted in many studies [36–38]. However, there is still need to further investigate the effect of the spray on the probability density function of the mixture faction and the boundary conditions to be applied on the fuel side in mixture fraction space. The shape of the scalar dissipation rate in mixture fraction space is also another crucial aspect in CMC modelling due to the important effect that it has in the prediction of flame extinction. Therefore, exploring the solutions of the single droplet combustion in a mixture fraction context [39,40] helps identify whether flamelet-based pre-calculated flame structures can be accurate enough for cases characterized by the presence of single droplet flames and further investigate the behaviour of relevant quantities, such as scalar dissipation rate and fuel characteristics at the droplet surface, for advanced combustion models.

The specific objectives of this paper are: (i) analyse the autoignition and combustion behaviour of a single kerosene droplet in vitiated air at conditions relevant for gas turbine applications, with focus on the effect of hot combustion product dilution and initial droplet diameter; (ii) compare the flame structure in mixture fraction space resulting from the single droplet combustion with the one derived from the gaseous counterflow flame configuration; (iii) characterize the droplet behaviour in vitiated air in terms of characteristic time delays, such as autoignition, evaporation and residence time, distinguishing different regimes on the basis of the vitiated air dilution and initial droplet diameter; (iv) highlight the relevance of such parameter for gas turbine applications. This paper extends the preliminary calculations presented in [41], that were performed only for a single initial droplet diameter, to a wide range of droplet diameters and discusses further the individual processes leading to a suggestion of a regime diagram for LPP combustor operation. The rest of the paper is organised as follows. In Section 2 the numerical methods used in the present investigation are introduced. Results are presented and discussed in Section 3: the droplet autoignition behaviour for different compositions of the vitiated air and different initial droplet diameters is analysed followed by the comparison of the quasi-steady flame structure resulting from droplet combustion calculations with the gaseous counterflow flame solution. The droplet combustion and evaporation behaviour in vitiated air is finally summarized by means of a state diagram which reports the droplet characteristic timescales (such as autoignition delay time and total evaporation time) as a function of the vitiated air dilution and initial droplet diameter. The relevance of such parameters in the