Simulations of droplet combustion for gas turbine conditions

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Abstract

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1. Introduction

The chemical complexity of spray combustion combined with its usefulness in aviation transport makes the investigation and understanding of its behaviour in complex combustion systems, including gas turbines, essential. Gas turbine development is typically concerned with NO_x emission reduction lean burn technologies in which liquid fuel is injected as a fine spray to encourage rapid evaporation and mixing with the surrounding air flow. Although injection systems are designed to ensure full pre-vaporization of the spray before it enters the combustion region, complete evaporation at all operating conditions may not be possible [1]. The autoignition of surviving droplets and presence of primarily single droplet flames, among other less common combustion regimes [2, 3], significantly affect combustor NO_x and soot emissions [4].

Such systems may be improved by investigating single droplet behaviour in the autoignition combustion regime characterised by extensive reactant dilution and preheat, typically through the mixing of reactants with hot combustion products. This regime, in which dilution limits the peak flame temperature and, in turn, the formation of NO_x , is known as the Moderate or Intense Low Oxygen Dilution (MILD) regime [5]. MILD combustion systems have been studied both experimentally [6–10] and numerically [11–14]. These studies reported an absence of sudden extinction behaviour even at very high strain rates [6, 7], a reduction in NO emission [8, 13], and a widening of the flame heat release region [11–13]. Systems which are diluted and preheated simultaneously through the mixing of reactants with hot combustion products should be of particular relevance to MILD regime studies as they closely mimic the recirculation often found in applied combustion devices.

Considering the impact of droplet combustion on emission levels in gas turbine combustors based on the lean burn technology and the potential for MILD processes in the aviation industry in both recirculation and staged combustors, work must be done to understand practical fuels autoigniting and burning with oxidisers mixed with hot combustion products at pressures relevant to gas turbine conditions. Although single droplet evaporation and combustion have been studied [15, 16], there is need to further investigate droplet ignition phenomenon and combustion behaviour with multi-component fuels under realistic conditions with varying oxidiser characteristics and droplet diameters, as discussed in Ref. [17],

This work aims to investigate kerosene surrogate single droplet evaporation and autoignition behaviour with vitiated air oxidiser as a function of droplet diameter and dilution conditions relevant to gas turbine combustion. It focuses on an analysis of single droplet flame structure in mixture fraction space, highlighting the limitations of conventional flamelet models as tools to model spray combustion systems, and aims to offer insight into system parameters relevant for gas turbine design such as residence time, droplet diameter, and dilution.

2. Method

In this work, the behaviour of a kerosene droplet in vitiated air at a pressure of 11 bar was analysed. Chemical reactions were modelled using a detailed kinetic mechanism developed for kerosene surrogate by Dagaut and Cathonnet [18, 19] with 209 species, 1673 reversible reactions, and reaction rates recommended for 10 bar. According to this mechanism, the fuel was modelled as a surrogate of three components, with the following molar composition [18]: 74% n-decane ($\text{N-C}_{10}\text{H}_{22}$), 15% n-propylbenzene ($\text{PH-C}_3\text{H}_7$), and 11% n-propylcyclohexane ($\text{CY-C}_9\text{H}_{18}$). First, a premixed gaseous flame with equivalence ratio $\phi = 0.6$ and reactants at 600 K, using air as oxidiser and kerosene surrogate as fuel, was run to produce hot combustion products. The vitiated air, used as oxidiser in all the following computations, was obtained by adiabatically mixing such hot

combustion products with air at 600 K, as in Fig. 1. A dilution variable ζ , defined as the mass fraction of hot combustion products in the vitiated air, was introduced to describe the level of vitiation so that $\zeta = 0$ and $\zeta = 1$ correspond respectively to undiluted air and pure hot combustion products. Enthalpy remains constant during this mixing process and the final mixture temperature was determined by the enthalpy and the species mass fractions. The temperature and composition of the vitiated air as a function of ζ are summarized in Table 1.

In the present investigation, two configurations were considered. The first, which will be referred to as the *single droplet* configuration, is representative of a case in which an isolated droplet burns in a stagnant oxidiser in the absence of any convective motion. By assuming the droplet is spherically symmetric, physical space may be simplified to include only the radial coordinate. The liquid droplet was modelled as a three-component fuel, replicating the kerosene surrogate composition considered in the chemical mechanism, and an equilibrium assumption was used at the droplet surface in order to compute the fuel vapour mass fraction at the droplet surface. The single droplet case was investigated using the code described and validated in Ref. [20] modified to include multi-component liquid droplets [21]. The physical properties of the three components of the kerosene surrogates were modelled using data and correlations reported in Refs. [22, 23]. Further details can be found in Refs. [20, 24, 25]. The initial temperature of the droplet, $T_{droplet}$, was set to 400 K in all the performed computations and the droplet initial diameter d_0 was varied in order to analyse the effect of droplet dimension on autoignition and combustion properties. The values of d_0 discussed here range from 200 μm to 10 μm to include typical droplet sizes in gas turbine applications, although most of the discussion presented here refers to the $d_0 = 100\mu\text{m}$ case. The vitiated air composition and temperature was imposed at the droplet far field boundary. These results are compared to steady gaseous flames, described below, a long time after ignition such that the resulting flame structures may be considered near-steady state.

The second configuration studied in this work is a steady, gaseous, laminar, non-premixed, counterflow flame, referred to as the *gaseous* configuration, with kerosene surrogate as fuel and vitiated air at different dilution levels as oxidiser at a constant rate of strain, A . The temperature of the fuel was set to match the temperature profile of the droplet case influenced by heat and mass transfer phenomena at the droplet surface, as discussed in Section 3.2. Gaseous solutions are representative of typical flame structures resulting from flamelet approaches. These solutions are compared to single droplet combustion flame structures in mixture fraction space [26], ξ , space. Gaseous counterflow flames were directly computed in mixture fraction space whereas for the single droplet cases the mixture fraction was computed from the spatial distribution of species [20]. Counterflow and premixed flame calculations were performed with the software COSILAB[®] [27].

3. Results and Discussion

3.1. Droplet autoignition behaviour

The autoignition behaviour of a droplet in vitiated air strongly depends on the dilution, ζ . Figure 4 shows the time evolution of the maximum temperature of the gas surrounding the droplet in both reacting and non-reacting cases for $\zeta = 0.3, 0.6$, and 0.9 and $d_0 = 100\mu\text{m}$. Non-reacting cases are calculated by simulating the single droplet case without allowing a reaction to occur. The ignition time delay, defined here as the time at which gas temperature becomes higher than 2000 K (similar to the criterion used in [20] for hot flames), increases with the level of dilution due to increasing oxidiser temperature. Figure 5, right, shows the time evolution of the droplet diameter. Evident through the non-reacting and reacting cases, total evaporation time decreases with increasing dilution due to the high temperature of highly diluted oxidiser. It is interesting

to note that the presence of a flame around the droplet increases the evaporation rate, as already observed in early studies (e.g. [15]). For low values of ζ , the autoignition time delay is relatively high, resulting in a two-stage evaporation clearly shown by the change of the slope of the d^2/d_0^2 line at the time corresponding to the autoignition event. The presence of a flame around the droplet changes the properties and structure of the droplet near field, and classical evaporation models used in CFD (e.g. [28]) cannot be applied when autoignition occurs. Figure 5, left, shows the time evolution of the mixture fraction at the droplet surface which represents the maximum value of the mixture fraction in the gas phase surrounding the droplet [20]. The increase in time of the mixture fraction at the droplet surface is related to the increase of droplet temperature which enhances the fuel vapour saturation mass fraction until an equilibrium between heat and mass transfer is reached (only possible for very large droplets). Again, the sudden change of the mixture fraction, clearly visible for the case $\zeta = 0.3$, is related to the occurrence of autoignition. It should be noted that in all the cases investigated in this work the droplet temperature was always below the boiling temperature of each fuel component at the operating pressure. This lead to a maximum value of mixture fraction lower than one.

3.2. Flame structure

Scalar dissipation (N , left) and temperature (T , right) profiles in ξ -space resulting from single droplet and steady gaseous flames with diluted oxidiser are shown in Fig. 6. Single droplet flame structures presented here are near-steady state, sampled long time after autoignition, showing only small time dependent changes associated with decreasing droplet diameter. Gaseous flames with $A = 1000 \text{ s}^{-1}$ were selected for comparison with $d_0 = 100 \text{ }\mu\text{m}$ single droplet solutions because their scalar dissipation rate, N , approaches a similar peak value, as shown in Fig. 6, left. The peak single droplet N is at a leaner ξ than that of gaseous cases because of the shift in rich ξ discussed in Section 3.1. Dilution, ζ , has little effect on N , suggesting that mixing characteristics are independent of vitiation level. The lean composition of the hot product diluent in this study implies that the diffusion characteristics of the oxidiser are dominated by the behaviour of N_2 for all ζ .

All droplet and gaseous dilution cases have typical temperature profiles in ξ -space, shown in Fig. 6, right. Note that, as discussed in Section 3.1, the rich mixture fraction, ξ_{fuel} , of the droplet case is not equal to 1 and the corresponding temperature, $T_{droplet}$, is higher than the initial droplet temperature, $T_{droplet,i} = 400 \text{ K}$, due to the liquid-vapour equilibrium at the droplet surface. These heat and mass transfer phenomena at the droplet surface lead to an increase in $T_{droplet}$, resulting in differences in fuel temperature compared with gaseous cases set to the same initial condition, shown as $\zeta = 0.9$, $T_{fuel} = 520 \text{ K}$ on the right of Fig. 6. Both changes in $T_{droplet}$ and ξ_{fuel} lead to a disagreement between droplet and gaseous flame structure and suggest that modifications to fuel boundary conditions need to be considered when simulating liquid fuel systems with gaseous configurations. In order to account for the liquid-vapour equilibrium effects on $T_{droplet}$, gaseous simulations should be set to a lower T_{fuel} to match single droplet temperature profiles with more accuracy. The gaseous cases in this work have a $T_{fuel} = 280 \text{ K}$ in order to minimize differences in temperature at rich mixture fractions. Although gaseous kerosene at such a low temperature is not physically feasible, this adjustment is necessary for the comparison of gaseous and liquid combustion simulations.

Increased dilution level, ζ , is noticeable when considering the increasing oxidiser temperature of single droplet and gaseous cases. Increased hot product dilution also causes the peak temperature to shift to leaner ξ , a result discussed previously [11, 12, 14]. Single droplet and gaseous flame behaviour as a function of varying dilution agree well; an expected result considering the two

configurations differ only in fuel state which predominately affects flames structure at at richer ξ . Small discrepancies in temperature profile to the right of the peak temperature are expected considering differences N .

Although no significant changes in peak temperature arise from increasing dilution, heat release rate, HRR, shown in Fig. 7 is strongly affected by ζ . Diluted HRR profiles show a positive, thin HRR near the maximum temperature and a double pyrolysis region at richer ξ . The positive HRR region in ξ -space is thin and heavily influenced by oxidiser O_2 content, as observed in Ref. [13, 14], with higher levels of dilution resulting in lower HRRs. The larger peaks of HRR observable in gaseous results is due to the larger values of N at very lean ξ . The increasingly large mismatch of single droplet and gaseous results in ξ -space at richer ξ is due to the shift of single droplet ξ_{fuel} discussed previously. The double pyrolysis HRR region on the rich side of the peak HRR, a typical feature of simulations involving this chemical mechanism [18, 29], may be explained through an analysis of intermediate species and pyrolysis products shown in Fig. 8.

The top left and middle plots in Fig. 8 show the kerosene surrogate and O_2 mass fractions in ξ -space, respectively. The kerosene surrogate mass fractions at the richest ξ in the single droplet results differs from that of the gaseous case, again a result of the mass and heat transfer effects at the surface of the droplet. Because of this discrepancy, despite efforts to match the rich temperature profile regions, the gaseous configuration cannot accurately predict the pyrolysis and intermediate species behaviour of a single droplet flame. This causes the kerosene surrogate and O_2 are consumed at a leaner ξ than in the gaseous case, while increased levels of dilution also cause a shift in the flame zone to a leaner ξ due to the reduced oxidiser O_2 content. The peak of OH in ξ -space also shift to ξ with increasing dilution, although the entirety of OH in ξ -space remains thin, an important consideration for MILD experimental investigations [14]. A comparison between gaseous and single droplet CH_2O , CO_2 , and H_2O shows little differences between the two, with the exception of CO_2 , and only a slight dependency on ζ . The consumption of the kerosene surrogate and production of intermediate hydrocarbons (Fig. 8, bottom two rows) corresponds well with the richest pyrolysis region in the HRR profile of each case. The consumption of these intermediate hydrocarbons, such as CH_4 , C_2H_2 , C_2H_4 , C_2H_6 , C_6H_6 , aligns with the leaner pyrolysis region in ξ -space in the HRR profile of each case. Discrepancies in peak levels of intermediate hydrocarbons in single droplet and gaseous cases are due to differences in N and T profiles. In complex pyrolysis processes, even small changes in temperature can significantly affect product concentrations.

The locations of the peak values of intermediate species in ξ -space are shown in Fig. 9. Intermediate hydrocarbons, Fig. 9, left, tend to peak at leaner ξ in single droplet flames (solid markers) than gaseous flames (open markers) due to the leaner single droplet fuel ξ . A light dependence on dilution shows that, with increasing ζ , peak values shift to leaner ξ for both both simulations as expected considering the lower O_2 content of diluted oxidiser and corresponding shift of the flame zone to leaner ξ . Figure 9, right, shows that the peak locations of flame zone and hot product species such as OH, CH_2O , H_2O , and CO_2 also shift to a leaner ξ with increasing ζ . However, little discrepancy in peak location between single droplet and gaseous simulations is apparent. This suggests that flame structure characteristics at richer ξ are more heavily influenced by discrepancies between single droplet and gaseous simulations, as expected considering these discrepancies occur at the fuel boundary.

3.3. Implications for gas turbine applications

Droplet evaporation and autoignition times from single droplet simulations allow for the definition of critical boundaries separating states in the droplet life as functions of the vitiated air dilution. The behaviour of an isolated droplet, $d_0 = 100 \mu m$, in vitiated air may be summarized

with plot in Fig. 10. The solid line shows the total evaporation time without autoignition and was obtained through non-reacting simulations. The dashed line is the ignition delay time which exponentially decays as ζ increases, primarily due to the increase in temperature of the air-hot combustion products mixture. The point of intersection between the evaporation and autoignition time delay corresponds to a critical value of dilution below which no droplet autoignition can occur. For values of ζ below this critical value, the evaporation time is smaller than the autoignition delay time and the droplet evaporates before a flame can ignite around it. Once the droplet has completely evaporated, autoignition can still occur in the gaseous mixture (for this reason, the autoignition line has been extended above the total evaporation line in an approximation). The dotted line shows the total evaporation time after autoignition. As discussed in Section 3.1, the presence of a flame around the droplet increases the evaporation rate, reducing the total evaporation time. Note that this critical line is asymptotic and for high ζ , the total evaporation time of the burning droplet is approximately constant. This asymptotic behaviour corresponds to small autoignition delay times where the total evaporation time is primarily controlled by the temperature of the flame generated around the droplet.

Different states of droplet behaviour can be bounded and described by these lines. The region below the evaporation and autoignition lines (lined region in Fig. 10), corresponds to droplet evaporation and gaseous mixing without a flame around the droplet. The region between the evaporation and the approximated gaseous autoignition line (blank region) we have gaseous mixing in the absence of a droplet. The region defined by the droplet autoignition and total time after autoignition (shaded region) corresponding to the single droplet combustion with a flame generated around the droplet. Once the liquid fuel is completely evaporated, single phase gaseous combustion occurs (dotted area).

Figure 10, which describes dilution and time dependent states for a single initial droplet diameter, may be extended to understand the effect of droplet size on evaporation and autoignition behaviour under diluted conditions in Fig. 11. Considering the small effect of the heat up period during the first stages of evaporation on the total evaporation time, results are plotted with time scaled with the square of the initial droplet diameter, causing the evaporation lines for all the diameters to overlap (slight deviations exist only for small values of ζ where the heat period has a stronger influence on evaporation time). If the classical d^2 -law, $d^2 = d_0^2 - Kt$, is used to describe the evaporation, a reasonable approximation for $\zeta > 0.2$ as can be deduced from Fig. 5, the value of the inverse of the scaled total evaporation time corresponds to K . This value increases with ζ due to the temperature dependence of transport properties. By decreasing the d_0 , the critical point defining the minimum ζ at which droplet autoignition occurs increases. This is consistent with the observation that smaller droplet systems tend to resist autoignition due to their high scalar dissipation rates [20]. Considering dilution, this corresponds to the existence of a minimum diameter below which no autoignition occurs for each value of ζ . The minimum diameter increases with ζ (temperature of the vitiated air), consistent with results reported in Ref. [20] where the critical diameter for various air preheat conditions were investigated.

The total evaporation time after autoignition asymptotically tends to the same value of scaled time at high values of ζ for all droplet diameters. Note that this plot is expressed in scaled time and that the physical time corresponding to a given value along the y -axis increases with the initial droplet diameter. This means that although all droplets are represented by the same evaporation line in the scaled plot, the total time for evaporation increases with the droplet diameter.

Figures 10 and 11 contain useful information for gas turbine applications and spray simulations. Dilution level, ζ , may be representative to a specific region inside a combustion chamber, ranging from a pure air stream to a recirculation zone or staged combustor containing hot combustion

products. The total evaporation time associated with a droplet size offers an initial indication of the total time required to vaporise the fuel (this time could be lower in the case of relative motion between the droplet and the surrounding medium) and, along with the mixing time, is an essential consideration in the design of combustors based on lean burn technology with intense mixing requirements upstream of the primary flame region. The autoignition line defines the conditions at which single droplet combustion might occur. It should be noted that this study considers the simplified case of a droplet in a quiescent medium and that the formation of a flame around a droplet requires stability consideration depending on the droplet relative velocity and turbulence level, as also observed in Ref. [15]. On the basis of these considerations, the autoignition critical line discussed in this work may be interpreted as a necessary condition for the single droplet burning mode at different of the gaseous phase compositions.

4. Conclusions

Kerosene droplet evaporation and autoignition in vitiated oxidiser at conditions relevant to gas turbine applications as a function of initial droplet diameter and dilution have been numerically investigated.

The flame structure of single droplet flames long after autoignition are compared with a steady, gaseous, laminar, non-premixed, kerosene surrogate-vitiated air counterflow flame. Although qualitatively similar, single droplet and gaseous flame structures differ in pyrolysis behaviour and fuel consumption primarily due to discrepancies in scalar dissipation rate and the fuel boundary. The lack of agreement between single droplet and gaseous flames have implications for liquid fuel systems simulated with combustion models based on the mixture fraction approach. The flame structure generated by droplet evaporation and autoignition is strongly influenced by the conditions at the droplet surface and, in order to properly simulate and understand flame behaviour, an accurate reproduction of conditions at the saturation mixture fraction is necessary.

Different states during the lifetime of the droplet have been identified based on their dependence on droplet size and oxidiser dilution level. Autoignition time decreases with increasing dilution due to the high temperatures of vitiated air, allowing for the presence of isolated burning droplets in a given region of the reacting field. It is possible to identify, for each value of dilution, a critical initial droplet diameter below which no autoignition will occur. This critical diameter decreases with increasing dilution.

Evaporation time is affected by the presence of a flame around the droplet, leading to a decrease of evaporation time after autoignition. It is interesting to note that, in the cases with autoignition, the dependency of evaporation time on dilution behaves asymptotically. This corresponds to conditions with very small autoignition delay times where the droplet experiences the presence of a burning flame throughout evaporation. **STRONG CONCLUSIONS DISCUSSING GAS TURBINE IMPLICATIONS AND DESIGN.**

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Fig. 1. Adiabatic mixing of hot combustion products and fresh air at 600 K to define the dilution variable, ζ .

Table 1
Oxidiser conditions

ζ	T_{ox} [K]	Y_{O_2}	Y_{OH}	Y_{H_2O}	Y_{CO_2}
0.3	1001	0.1905	1.05×10^{-4}	0.015	0.036
0.6	1402	0.148	2.10×10^{-4}	0.030	0.072
0.9	1803	0.106	3.15×10^{-4}	0.045	0.108

Fig. 2. –

Fig. 3. –

Fig. 4. –

Fig. 5. –

Fig. 6. Scalar dissipation rate, N , left, and temperature, T , right, profiles in ξ -space as a function of dilution, ζ , from single droplet (thin lines) and gaseous (bold lines) simulations.

Fig. 7. Heat release rate profiles in ξ -space as a function of dilution, ζ , from single droplet (thin lines) and gaseous (bold lines) simulations.

Fig. 8. Intermediate species mass fractions, Y_i , in ξ -space as a function of dilution, ζ , from single droplet (thin lines) and gaseous (bold lines) simulations.

Fig. 9. Location of peak values of intermediate species mass fractions in ξ -space from single droplet (solid markers) and gaseous (open markers) combustion cases as a function of dilution, ζ .

Fig. 10. Single droplet state diagram as a function of dilution ($d_0 = 100 \mu m$).

Fig. 11. Single droplet state diagrams as a function of dilution, ζ , for various initial droplet diameters, d_0 .

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