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Influence of scalar dissipation on flame success in turbulent sprays with spark ignition

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ABSTRACT

A Direct Numerical Simulation (DNS) study is performed to determine a quantitative indicator of imminent global extinction in spray flames ignited by a spark. The cases under consideration have Group Combustion numbers sufficiently small that each droplet has an individual flame form around it, which subsequently merge. The structure of the flames is examined, including identification of non-premixed behaviour in the core of the flame and premixed flame fronts except in the presence of droplets, which cause strong non-premixed behaviour. The reaction progress variable c is studied and its dissipation rate is identified as being a key indicator of whether a flame will globally extinguish after being ignited by the spark. Specifically, immediately after the spark is deactivated, the volume containing the end of the flame front and hot products is studied in detail with respect to c. For successful flames, it is observed that regions of zero dissipation of c were predominantly restricted to the highest reaction progress variable ($c > 0.98$), with zero probability within the range $0.95 < c < 0.98$ and low probability within $0.9 < c < 0.95$. In contrast, cases which subsequently extinguished had substantial probability of zero dissipation for $0.95 < c < 0.98$. This region was a secondary structure separate from the main flame kernel that was unable to evaporate sufficient liquid to create a self-sustaining flame and therefore contributed to the subsequent quenching of the flame. In the successfully-burning case under consideration, this region was part of the main flame structure. The low reaction rate contributed to a thickened flame structure near the hot core, which reduced the heat transfer to the flame front and prevented effective evaporation and preheating of the fluid ahead of the flame front. Calculation of the conditional probability of c for its dissipation rate being zero could provide a quantitative measure to determine whether a flame is likely to extinguish within a relatively short timeframe. This is equivalent to detecting that, for every value of $0.9 < c < 1$, there are volumes of significant size where the value of c is uniform. Note that a successful flame must have a volume of substantial size with $c = 1$. From a practical perspective, if each individual flame kernel is monitored, then extinction is imminent if secondary structures of incomplete reactions are present when the spark ceases adding energy.

1. Introduction

Spray combustion using spark ignition is a technique commonly used in gas turbines and is being introduced into the automotive industry through the DISI (Direct-Injection Spark-Ignition) engine technology: a focus of research interest [1–5]. Classical experiments determined that the minimum spark energy required to successfully ignite droplet-laden mixtures is greater than equivalent gaseous mixtures and that turbulence can reduce ignition success [6,7]. Spray systems with fine droplets can ignite more easily than gaseous systems at lean equivalence ratios (Φ) because the discrete gaseous field caused by sprays can produce stoichiometric conditions locally [6]. This complexity in the gaseous scalar field [8] produces larger gradients than in single-phase systems, therefore the scalar dissipation field is more variable, and this results in additional challenges for modelling two-phase systems [9,10].

Direct Numerical Simulations (DNS) provide a tool for investigating these complexities while potentially providing models that can be useful for full-scale simulations [10]. However, this approach is currently limited because of the computational effort required to fully resolve the liquid phase. Two scales of simulations are generally employed: small-scale with full resolution and only a small number of droplets; and larger scale with the droplets modelled as particles smaller than the grid scale. In the latter (the approach used in this paper), the droplets are considered to be point sources of mass, momentum and energy, without resolving

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the gas in the droplet boundary layer. Some of these investigations have studied non-premixed flames, mixing, autoignition and soot formation [11–20]. Fully-resolved modelling, utilising simplifications of the geometry, has previously been performed [21,22], while examples of fully-resolved DNS include non-reacting cases [23–27] and reacting cases [28–30]. Recently [29], it was found that self-similar behaviour is predicted well by the Amplitude Mapping Closure (AMC) model [31] and first-order Conditional Moment Closure (CMC) [31] can be utilised. The use of CMC to model sprays has been advocated elsewhere [8,9,15,18,19,31]. A model for the mixture-fraction probability density function (pdf) was also suggested [29] that may be more applicable than the β-function pdf.

A series of experiments, where the flame was stabilised by a bluff-body, have been conducted to determine the probability of successful combustion as a function of spark location. For both gaseous non-premixed [32] and spray [33] conditions, the probability of successful combustion was found to be a strong function of the location of the spark with respect to the flow field. In particular, because of the bluff-body stabilisation, it is better to locate the spark within a region of recirculation where the droplet size is relatively small and mean equivalence ratio is within the flammability limits. These conclusions have also been drawn from LES-pdf (Large Eddy Simulations using pdf modelling for the sub-grid scalar mixing) of spark-ignition of sprays in an aircraft gas turbine [34]. An extrapolation of these results to a jet flame would suggest that the spark needs to be sufficiently far downstream of the exit for droplet breakup to be well-advanced but not so far that the mixture is too dilute to sustain a flame. It has been observed in DNS studies of homogeneous flows using single-step [35,36] and detailed [37] chemistry that the success of flame ignition is directly related to the spark's ability to evaporate sufficient fuel to promote sustained combustion. It is possible to create a successful flame even if the spray does not directly encounter the spark provided the heat transfers sufficiently quickly to the droplets [33,36]. The flame propagation mechanisms have also been investigated using detailed chemistry [38].

Much of the work has focussed on the nature of successful ignition and flame propagation, but little understanding has been gleaned as to whether the cause of failure stems from poor kernel establishment, propagation or stabilisation [9]. To address this, the author has identified qualitative *a posteriori* [35] and qualitative *a priori* [39] indicators for whether global extinction will occur, but neither study was able to identify a quantitative control measure that could be used to avert extinction. The current study addresses this issue with analysis of the reactive scalar's dissipation rate that yields a quantitative indicator that distinguishes *a priori* whether a flame will undergo global extinction in the near future. Unlike the indicator based on the mixture fraction scalar dissipation rate [39], the current results are not immediately transferable to gaseous cases because the mechanism that is observed is due to the discrete nature of the spray field. The conditions that are simulated in the current study—spark ignition of fine, relatively-sparse droplets—could occur in a number of situations, such as: at the edge of spray streams, a significant distance from the injector or in overall lean sprays (which can be rich close to the injector).

2. Modelling

A three-dimensional compressible DNS code called SENGA [40] was used for this study. The code is non-dimensionalised, with the normalising parameters being: the width of the domain L; the laminar flame speed at the stoichiometric condition, S_L; the unburned gas density, ρ_0; the unburned gas temperature, $\widehat{T}_0$; and the specific heat of the unburned gas, $c_{P,0}$. The computational domain is a cube of width $L = 21l_F$, where the characteristic laminar flame thickness is

$$l_F = D/S_L \tag{1}$$

and D is the unburned gas diffusivity. Partially non-reflecting boundary conditions [41] are used for the x-direction, while the y- and z-dimensions are considered to be periodic. The first- and second-order spatial derivatives are computed using 10th-order central-difference schemes, which reduce to 2nd-order one-sided derivatives at the non-reflecting boundaries. A third-order, low-storage Runge–Kutta scheme [42] is used for time advancement. A pseudo-spectral method [43] is used to generate the initial velocity field using the Batchelor–Townsend spectrum [44]. The velocity field is considered to be homogeneous and decaying. The droplets were initially distributed uniformly in space throughout the y- and z-directions and in the central half of the x-direction. The remaining quarter of the volume between each side of the droplet region and the partially non-reflecting boundaries was taken to be pure air because the boundary conditions for droplets entering the computational domain through these boundaries are difficult to specify. The gaseous phase was initialised to be pure air throughout the domain and both phases were set to a constant temperature.

2.1. Chemical modelling

A single-step irreversible chemical mechanism is used [45]

$$\text{Fuel} + s\ \text{Oxidizer} \rightarrow (1+s)\text{Products}, \tag{2}$$

where s is the mass of oxidiser per unit of mass of fuel at stoichiometric conditions. The consumption rate of fuel is given by an Arrhenius-type expression:

$$W_F = B^* \rho Y_F Y_O \exp\left[-\frac{\beta(1-T)}{1-\alpha(1-T)}\right] \tag{3}$$

where Y_F and Y_O are the fuel and oxidiser mass fractions respectively. The non-dimensionalised temperature is

$$T = \frac{\widehat{T} - \widehat{T}_0}{\widehat{T}_{\text{ad}} - \widehat{T}_0} \tag{4}$$

with $\widehat{T}_{\text{ad}}$ the adiabatic flame temperature at the stoichiometric condition. Here β is the Zel'dovich number, given by

$$\beta = \frac{E_a\left(\widehat{T}_{\text{ad}} - \widehat{T}_0\right)}{R_u \widehat{T}_{\text{ad}}^2}. \tag{5}$$

The activation energy is E_a, while R_u is the universal ideal gas constant. In Eq. (3), α is a heat release parameter given by

$$\alpha = \frac{\tau}{1+\tau} \tag{6}$$

$$\tau = \frac{\widehat{T}_{\text{ad}} - \widehat{T}_0}{\widehat{T}_0}, \tag{7}$$

while B^* is

$$B^* = B\exp(-\beta/\alpha), \tag{8}$$

with B the pre-exponential factor.

The mixture fraction is defined to be [46]

$$Z = \frac{Y_F - Y_O/s + Y_{O,i}/s}{Y_{F,i} + Y_{O,i}/s}, \tag{9}$$

where $Y_{F,i}$ is the fuel mass fraction in its inlet stream, while $Y_{O,i}$ is the oxidiser mass fraction in its inlet stream. The fuel simulated in the current case is n-heptane in the form of liquid droplets, injected into air. For the present conditions, the following values can be obtained: