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Identification of Burning and Extinguishing Behaviour in Spray Flames with Spark Ignition

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Abstract

The Gaussian Mixture Model (GMM) is used to analyse Direct Numerical Simulation results for sprays which are ignited using spark ignition. The variables considered in the GMM are the reaction progress variable and its dissipation. It is found that a case which sustained a self-propagating flame produces a burning branch, where a strong flame front is developed, and an extinguishing branch, which contains droplets which are offset from the main spark energy. These branches are distinctly observed through the various clusters that are formed by the GMM. In contrast, cases which ignite but subsequently undergo global extinction do not produce clusters that are distinctly from the burning branch or extinguishing branch near the flame kernel. However, the clustering does display a strong extinguishing branch near the leading edge of the flame front.

Keywords: Direct Numerical Simulations, Spark Ignition, Spray Flames, Extinction, Gaussian Mixture Model

1. Introduction

Spark ignition for spray combustion is common in gas turbine engines while the automotive industry is adopting it as DISI (Direct-Injection Spark-Ignition) engine technology: an active research area [1–5]. Classic experiments showed that spray flames need more spark energy than equivalent gaseous mixtures to overcome the latent heat of vaporisation, with turbulence impacting negatively on ignition success [6, 7]. The behaviour is sensitive to the droplet size, with fine droplets able to sustain lean flames (when the equivalent gaseous flame cannot) because the gaseous distribution of fuel is more variable, producing local stoichiometric conditions [6].

This paper is the continuation of a sequence of investigations into the cause of extinction in spray flames [8–10]. It draws heavily on the findings of the most recent paper, where a quantitative measure distinguishing between burning and extinguishing flames was established. This paper will explore a different means of analysing the cases to describe the distinct behaviour of these two types of cases.

1.1 Simulations

Direct Numerical Simulations (DNS) of sprays using spark ignition are investigated; the simulations have been comprehensively described previously [10]. In summary, droplets are initially randomly distributed in pure air that is preheated to 500°C; the droplets are located in the central slab of the domain, with no droplets near the non-reflecting boundary conditions that allow the flame to exit the domain. A spark is activated in the middle of the droplet field and this paper analyses the field when the spark is deactivated.

The cases studied in Ref. [10] are investigated here (Table 1). The base case is chosen as one which successfully burns throughout the simulation (the flame front reaches the boundaries), while the remaining droplet cases are chosen to show progressively-increasing global extinction. Case BE burns throughout the simulation (the flame front propagates throughout), but extinction was about to commence when the simulation was stopped. The I cases ignited, but global extinction commenced soon after the spark was deactivated. The F cases did not ignite at all. The parameters that were varied to achieve these cases were the equivalence ratio Φ (which is the value within the droplet field if all the fuel was vapour), the square of the ratio of initial droplet diameter to the same quantity for the base case, and ratio of the initial turbulent kinetic energy to the same value for the base case. Having fewer droplets (reduced Φ) or larger droplets are well-known to reduce the flammability of the mixture. The increased turbulence in these simulations moves the flame kernel away from the spark, so the spark is less effective [10].

Table 1: DNS Cases investigated here. Columns are: equivalence ratio (Φ), the square of the ratio of initial droplet diameter to base case, and ratio of turbulent kinetic energy to base case. Case BE is Burning, but about to Extinguish; "I" means "ignited"; "F" means "failed to ignite".

Name	Φ	**Rel. Diam. Sq.**	k/k_b
Base	2.0	1	1
BE	1.7	1	1
I1	1.6	1	1
I2	2.0	1.5	1
F1	1.0	1	1
F2	1.0	1	8

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1.2 DNS data to be analysed

The reaction progress variable was calculated using

$$c = \frac{(1-Z)Y_{O,i} - Y_O}{(1-Z)Y_{O,i} - \max\left(0, \frac{Z_{st}-Z}{Z_{st}}\right)Y_{O,i}} \qquad (1)$$

where Z is the mixture fraction, Z_{st} the stoichiometric mixture fraction and $Y_{O,i}$ is the mass fraction of the oxidiser in the oxidiser stream. Also of interest is the dissipation of c:

$$N_{cc} = D\nabla c \cdot \nabla c \qquad (2)$$

with D the diffusivity. It has previously been shown that the joint-probability density function (jpdf) of these two quantities provides an indication of whether extinction is imminent [10]. This paper investigates another description of the behaviour, which provides another perspective on why the extinction occurs. To achieve this description, data mining is used to distinguish between the burning behaviour of successfully-propagating flames and extinguishing behaviour of isolated droplets.

2. Data Mining Method

The Gaussian Mixture Model (GMM) is a density-based method used to find clusters of arbitrary shape [11]. A cluster is defined to be a collection of data points which are considered to have similar properties and are thereby classified to belong to a group (with a total of M groups). Each group contains data points which are close together in space. The data points from a different group can be considered to have different properties.

The derivation follows Ref. [12]. A GMM is a weighted sum of component Gaussian densities given by the equation

$$P(\mathbf{x}|\lambda) = \sum_{i=1}^{M} w_i g(\mathbf{x}|\mu_i, \Sigma_i) \qquad (3)$$

where $\mathbf{x}$ is an n-dimensional continuous-valued data vector; w_i are the mixture weights; $g(\mathbf{x}|\mu_i,\Sigma_i)$ are the component Gaussian densities (clusters), which are n-dimensional Gaussian functions; M is the number of clusters; μ_i is the mean vector; and Σ_i is the covariance matrix. This mixture distribution has the constraints

$$0 \le w_i \le 1 \quad \text{and} \quad \sum_{i=1}^{M} w_i = 1 \qquad (4)$$

The complete Gaussian Mixture Model is parameterised by the mean vectors, covariance matrices and mixture weights from all component densities:

$$\lambda = \{w_i, \mu_i, \Sigma_i\} \qquad (5)$$

A maximum-likelihood estimation is used to find λ.

3. Results and Discussion

The reaction progress variable and its dissipation are the quantities to be considered in the GMM, hence $n = 2$. For this paper, $M = 20$ was chosen. The nodes with $c < 0.02$ were excluded to reduce processing effort. These nodes account for the vast majority of data and the nodes of interest here have $c > 0.9$.

The cluster plots for the Base case and case BE are shown in Figs. 1 and 2 respectively. For $0 < c < 0.3$, the behaviour is similar, with multiple clusters in the leading edge of the flame front. The behaviour for $0.3 < c < 0.7$ is substantially different. For the Base case, there is a very large, dominant cluster for the highest values of N_{cc}, which is overwhelmed in case BE by the clusters which are on the shoulders and penetrate closer to $c = 0.5$ than in the Base case. This uppermost cluster was identified as belonging to a burning branch [10], which has a high probability in the Base case, i.e. a large region of space takes these values. The extinguishing branch for $0.3 < c < 0.7$ is also more segmented in case BE than the Base case. This large number of clusters in case BE is probably due to multiple flame fronts being created around individual droplets (see Fig. 23(b) [10]), while the Base case produced a large, strong flame kernel.

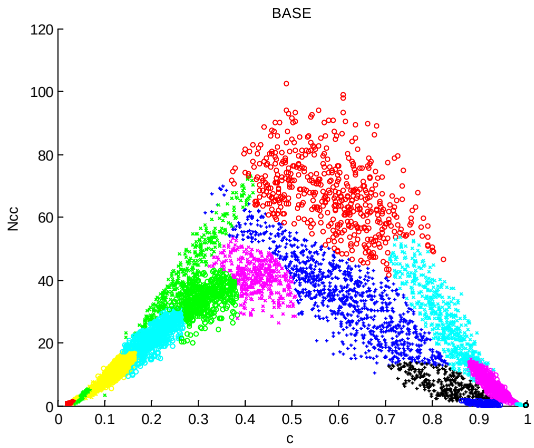

Figure 1: Cluster plot of N_{cc} vs c for Base case. The colours are randomly chosen to distinguish between clusters and cannot be matched to other cases.

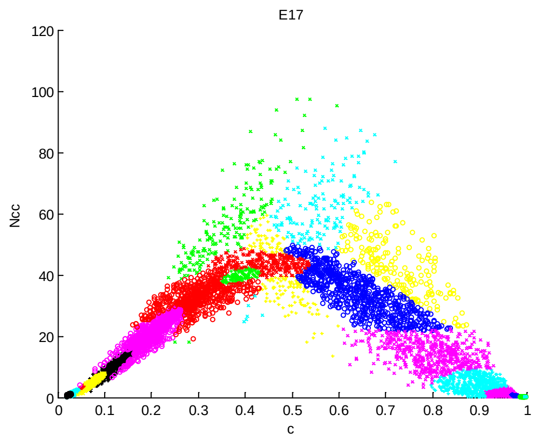

Figure 2: Cluster plot of N_{cc} vs c for case BE.

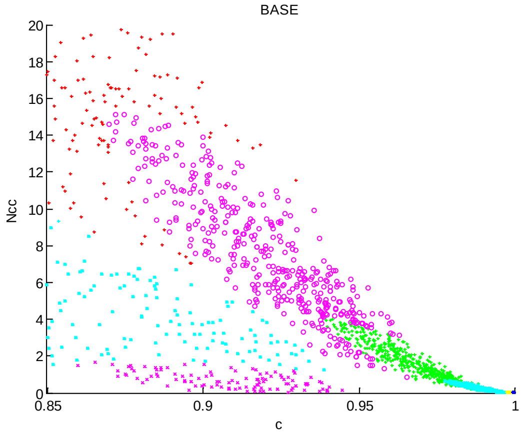

Figure 3: Zoomed-in image of Fig. 1.

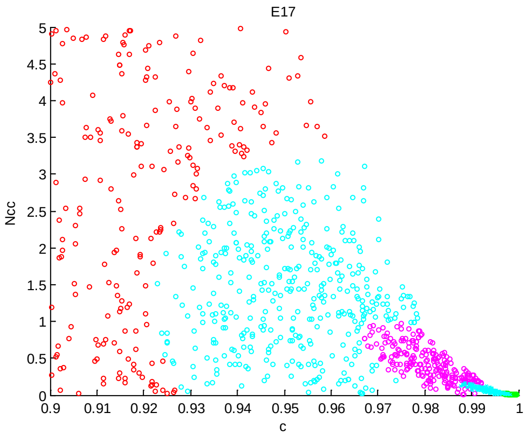

Figure 4: Zoomed-in image of Fig. 2.

For the region closest to the flame kernel ($c > 0.7$), the clustering is completely different. In the Base case, the separation of clusters is parallel to the edges of the data, while in case BE, the separation is essentially for constant N_{cc}. In the successfully-burning Base case, this behaviour is caused by a large, stable flame kernel which supports the burning branch, while some droplets are separated from the flame kernel and produce the extinguishing branch. In case BE, the primary flame kernel is not sufficiently strong to support combustion, so there is no clear distinction between that region and the region around separated droplets.

To investigate this further, Figs. 3 and 4 zoom in on the highest values of c in Figs. 1 and 2. The separation of the clustering in the Base case is fundamentally caused by the burning branch being fed by the strong flame kernel at $c = 1$, while the extinguishing branch is sourced by incomplete combustion from isolated droplets. This completely different behaviour produced the findings of Ref. [10]. It is interesting that the burning branch contains multiple clusters for $c > 0.98$. By contrast, the clustering for case BE is only separated radially from $c = 1$: the flame kernel is insufficiently strong to produce self-sustaining flame fronts which could be considered a burning branch.

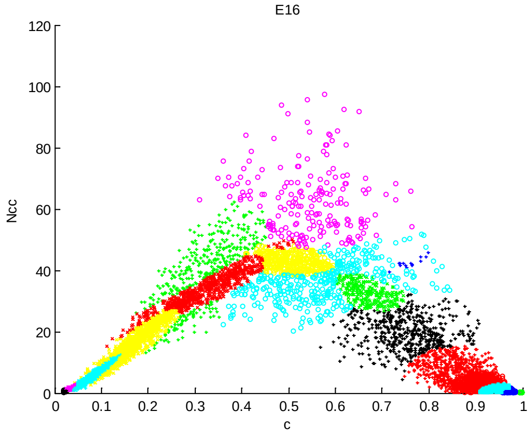

Figure 5: Cluster plot of N_{cc} vs c for case I1.

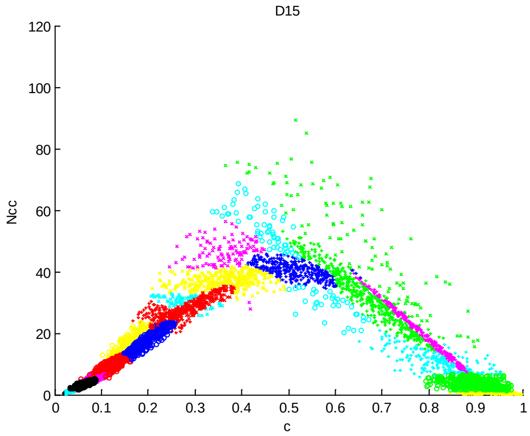

Figure 6: Cluster plot of N_{cc} vs c for case I2.

The cluster plot for case I1 (Fig. 5) shows similar behaviour to case BE in the vicinity of $c = 1$ in that the clusters do not separate into burning and extinguishing branches. The more immediate extinction in case I1 can be heralded by the lack of any distinct burning branch cluster except for the few nodes with the highest values of N_{cc}. At lower values of c in case I1, there is an intense series of narrow clusters that overlays broader clusters. This is caused by the predominance of droplets which have not sustained flames (the narrow clusters), with a small number of droplets which have produced reasonable flames that have insufficient energy to sustain the entire field.

Case I2 (Fig. 6) continues this trend, with a very strong extinguishing branch overlaying weakly-burning clusters at lower values of c and no clear separation of burning and extinguishing branches at the highest values of c. A distinct feature of this case is the thin cluster present in $0.6 < c < 0.9$, which, when compared to Fig. 1, is in the middle of the extinguishing branch. This case has a very small flame kernel (Fig. 23(e) [10]), with a substantial, very lean secondary structure and a tiny tertiary flame kernel around a single droplet. It is likely that the thin cluster is caused by the substantial secondary structure which cannot sustain combustion due to insufficient fuel.

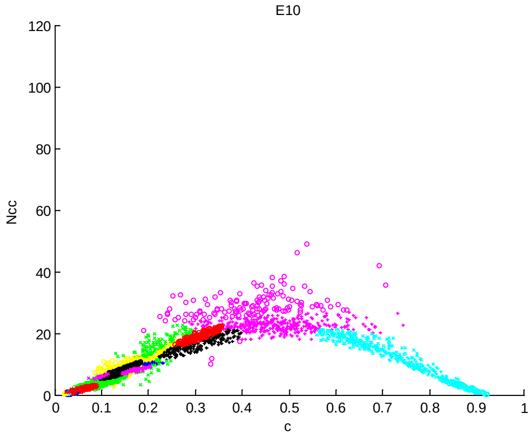

Figure 7: Cluster plot of N_{cc} vs c for case F1.

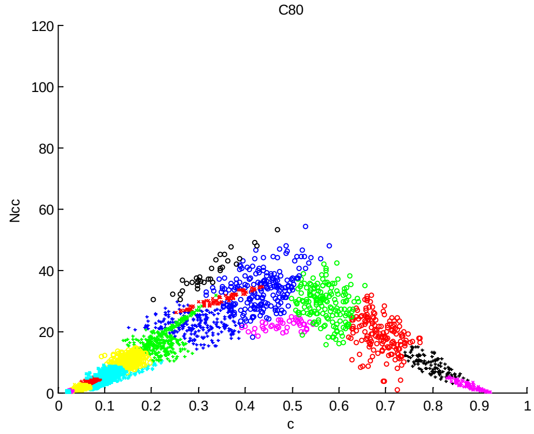

Figure 8: Cluster plot of N_{cc} vs c for case F2.

Case F1 (Fig. 7) does not show a burning branch because this case fails to ignite. There is weak scatter for $c \approx 0.5$ due to the discrete nature of the droplet field. This discrete nature also produces parallel clusters for lower values of c; the large number of such clusters is probably due to the high value of M given that there are only two clusters for $c > 0.4$.

The higher turbulence in case F2 significantly distorts the field, thereby producing a few clusters for the highest values of c as well as a number of very thin clusters for $0.3 < c < 0.5$ (Fig. 8). The primary mechanism by which the turbulence suppresses ignition is to push the heated region away from the centre of the spark, thereby preventing sufficient time for ignition to commence.

4. Conclusions

A data mining tool, the Gaussian Mixture Model, has been used to analyse Direct Numerical Simulation results for a spray which is ignited using a spark. It has been found that the case with a self-sustaining propagating flame produces clustering which distinctly shows a burning and extinguishing branch for values of the reaction progress variable above 0.4. In contrast, cases which extinguished did not produce similarly-distinct clusters.

The clustering method identified that for cases where extinction is imminent, a strong extinguishing branch is visible for values of reaction progress variable lower than 0.5. This distinction was not apparent when considering the joint-probability density functions [10].

Future work will consider the sensitivity of the method to the number of clusters M and compare a wider range of simulation parameters to confirm that the identified trends are observed for the different types of behaviour.

5. Acknowledgments

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6. References

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