

DETAILED NUMERICAL SIMULATIONS OF THE AUTOIGNITION-AFFECTED STABILIZATION OF LAMINAR NONPREMIXED DME/AIR COFLOW FLAMES AT ELEVATED PRESSURE

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ABSTRACT

The structure and stabilization mechanism of laminar nonpremixed autoignitive DME/air coflow flames were investigated at elevated pressure and coflow temperatures, with constant jet and coflow velocities, using detailed numerical simulations. The heat release rate and species profiles were examined for each case. Further investigation with Chemical Explosive Mode Analysis (CEMA) and Lagrangian Flamelet Analysis (LFA) were performed to identify the controlling chemistry and elucidate the dominant combustion mode and stabilization mechanism. At 700 to 900 K, autoignition was observed to be the dominant stabilization mechanism, and NTC chemistry determines the stabilization point in mixture fraction space. Moreover, the coupling between the autoignition process and premixed flame propagation results in a multibrachial structure. Conversely, at 1100 K, the kinematic balance between the premixed flame propagation velocity and the incoming flow velocity becomes the dominant stabilization mechanism, and the classical triple flame structure was observed. Extended stabilization regimes, in terms of increasing boundary temperature, are therefore identified, including blow-off, purely kinetically stabilized, autoignition-propagation-coupled stabilized, purely kinematically stabilized, and burner stabilized regimes.

COMPUTATIONAL DETAILS

The flow configuration is an axisymmetric DME stream at 300 K in a heated coflow of air (700, 800, 900, and 1100 K) at 30 atmospheres. Uniform inlet velocities of 3.2 m/s were specified for both fuel and air streams and kept the same for all the cases to establish lifted flames.

Dimethyl ether was chosen in this work, for it is a clean biofuel and one of the smallest hydrocarbons exhibiting NTC behavior. The present computations were conducted using a skeletal mechanism of 39 species from Bansal *et al.* (2011), including both low and high temperature oxidation pathways, which was reduced from the well validated detailed mechanism of Zhao *et al.* (2008).

THERMAL STRUCTURE

To visualize the flame structures, the heat release rate profiles for the four cases are shown in Fig. 1. Qualitatively, the most upstream point on the largest heat release contour

(the leading point), colored by red, will be referred to as the stabilization point.

COMPUTATIONAL DIAGNOSTICS AND ANALYSIS

The above heat release rate profiles demonstrate the thermal structure of the reacting fronts at different boundary temperatures. However, more detailed computational diagnostics and analysis are needed to further demonstrate the controlling chemistry and the stabilization mechanism.

Chemical Explosive Mode Analysis

Chemical Explosive Mode Analysis (CEMA, Lu *et al.* (2010); Shan *et al.* (2012)) was conducted to identify the controlling chemistry in these complex reacting flows. For each case, the local species concentrations and temperature were sampled along the Z_{st} , $Z = 0.2$, and $Z = 0.3$ iso-contours, as marked in Fig. 1, and processed by CEMA to demonstrate the evolution of the dominant reactions.

For the three lower coflow temperature cases, following the Z_{st} iso-contour, the dominant chain branching reaction shifts from $H_2O_2 + M \rightleftharpoons OH + OH + M$ to $H + O_2 \rightleftharpoons O + OH$, indicating that the combustion mode shifts from autoignition to flame propagation. The nature of the tribrachial structure (around Z_{st}) at 700 – 900 K is therefore identified: an autoignition assisted premixed flame front.

CEMA conducted along the $Z = 0.2$ iso-contour, which crosses the rich heat release front in the 800 and 900 K cases, shows different chemical mode evolution. The H_2O_2 chain branching reaction is always the dominant reaction. Therefore, this heat release front is dominated by autoignition chemistry rather than flame chemistry and is considered as an autoignition front.

On the contrary, for the 1100 K, the hydrogen peroxide chain branching reaction is not very important for all the sampled locations. Since the hydrogen peroxide reaction is the crucial chain branching reaction for the autoignition process, it is concluded that the 1100 K case is less affected by autoignition chemistry than the lower boundary temperature cases.

Lagrangian Flamelet Analysis

To elucidate the role of autoignition for the current flow configuration, unsteady flamelet analysis (Pitsch *et al.*

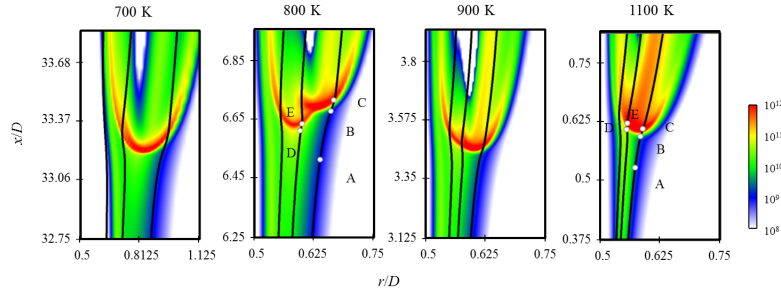


Figure 1. Heat release rate [$\text{J/m}^3\text{-s}$] profiles. The iso-contours of Z_{st} , $Z = 0.2$, and $Z = 0.3$ are outlined from right to left in solid lines, respectively. The CEMA sampling points at 800 and 1100 K are marked along the iso-contours.

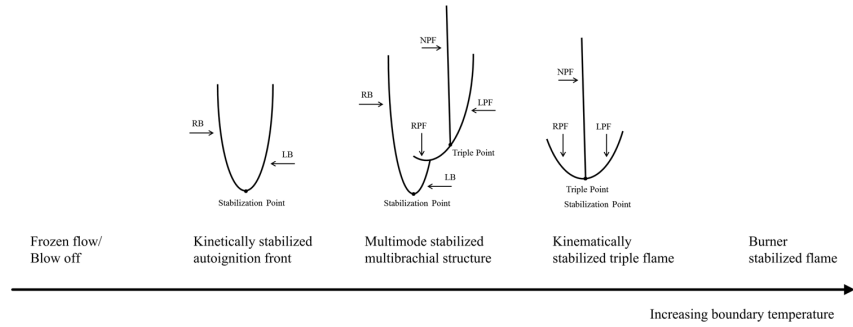


Figure 2. Extended regimes of the stabilization mechanism as coflow boundary temperature increases.

(1998)) was conducted to account for diffusion parallel to mixture fraction gradients, and comparisons with the two-dimensional computations can then demonstrate the dominant stabilization mechanism.

The 700 – 900 K cases show good agreement between the flamelet profile with the time history of the two-dimensional computation, indicating that the thermal structure is stabilized by inhomogeneous autoignition.

On the contrary, for the 1100 K case, the ignition delay time computed with the one-dimensional flamelet assumption is significantly longer than the two-dimensional counterpart, indicating that autoignition is less important to the stabilization mechanism and that transport processes along the mixture fraction iso-contours must be important.

STABILIZATION MECHANISM

In the current study, two fundamental stabilization mechanisms are relevant: the *kinetic* stabilization mechanism, due to the balance between the autoignition delay time and flow residence time, and the *kinematic* stabilization mechanism, due to the balance between the premixed flame propagation velocity and the local flow velocity.

In this stratified composition and temperature field, autoignition and flame propagation are coupled through thermal and radical interactions, for the accumulation of the upstream radicals and heat release from autoignition accelerate the flame propagation velocity. The flame also transfers heat and radicals through back diffusion processes to the upstream, which could also facilitate autoignition.

Based on the understanding obtained from the current study, further extension of the stabilization regime can be made, as shown in Fig. 2. For sufficiently high inlet ve-

locity, as the boundary temperature increases from the cold case, frozen flow is first achieved, where the mixture is nonautoignitive, and even the flame generated by an external ignition source will blow off. When the mixture can be autoignited, the *kinetically* stabilized autoignition front gradually transits to a *kinematically* stabilized classical triple flame, where the premixed flame front propagation velocity balances the local incoming flow velocity. The triple flame will eventually become attached when the boundary temperature is sufficiently high, and the flame speed is sufficiently fast.

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