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A Direct Numerical Simulation Investigation of Ignition at Diesel Relevant Conditions

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Abstract

A two-dimensional direct numerical simulation was performed with detailed dimethyl ether chemistry in isotropic turbulence to investigate the ignition behaviour in engine relevant conditions. Dimethyl ether was selected as the fuel because it exhibits two-stage ignition and a negative temperature coefficient of ignition delay times, similar to practical diesel fuels, while having a computationally tractable chemical mechanism. Distinct low and high temperature ignitions are observed which trigger deflagrations that transition to edge-flames, propagating along the stoichiomectric mixture fraction contour. The edge flames have a tetrabrachial (quadruple flame) structure consisting of a main tribrachial (triple) flame propagating into a fourth low temperature branch. Conditional statistics reveal a complex ignition process in which low temperature ignition, high temperature ignition, and propagating edge-flames all contribute to the transition to a fully-burning flame. The low temperature chemistry was observed to substantially affect the development of the main ignition. The results also suggest that partially premixed edge flames could play an important role during the ignition and flame stabilisation process in diesel engines.

Introduction

Autoignition in diesel engines occurs as a multi-stage process in a partially premixed environment. Experimental investigations of these conditions have produced conceptual models which are successful in describing the overall combustion processes [3]. However, due to the harsh environment of the diesel engine, it is very difficult to characterise some important thermochemical and turbulence-chemistry processes via experimental techniques alone.

Direct numerical simulation (DNS) provides an alternate avenue. By completely resolving all temporal and spatial scales of the chemistry and fluid mechanics, DNS offers a complete description of certain canonical configurations. In order to make the DNS computationally affordable, a number of simplifications must be taken. In the present DNS, the fluid mechanics was approximated while a relatively detailed chemical kinetic model was adopted.

In this study, a two-dimensional mixing layer of air and diluted dimethyl ether (DME), subject to decaying isotropic turbulence, was simulated. The ambient pressure was 40 atmospheres, the oxidiser temperature was 900 K, and the fuel temperature was 400 K. These conditions were selected so that the DME fuel was within the negative temperature coefficient regime [10].

DME was selected as the fuel as it has the smallest detailed mechanism while retaining the salient features of diesel fuel

such as a negative temperature coefficient regime and multistage ignition [10]. The mechanism used here contains 30 species and was used previously in studies of lifted laminar flames [8] and a temporally evolving jet [1]. The fuel stream was composed of 30% N₂ and 70% DME by volume. This level of dilution produced a stoichiomectric mixture fraction, Z_{st} , of 0.123 (Bilger's definition). At the conditions considered here, DME has a two stage ignition. The most reactive mixture fraction for the first stage of ignition, $Z_{mr,1}$, defined as the mixture fraction that leads to the shortest first stage ignition delay time, $\tau_{ig,1}$, occurs at 0.03 [8]. The most reactive mixture fraction for the main stage of ignition, Z_{mr} , defined as the mixture fraction that leads to the shortest main stage ignition delay time, τ_{ig} , occurs at 0.11 and $\tau_{ig} = 5.14x10^{-4}$ s [8]. The $Z_{mr,1}$ and Z_{mr} values are based on zero-dimensional, constant pressure simulations.

The simulation was performed using the program S3D [8, 1, 9, 2, 5, 4], which solves the fully compressible Navier-Stokes, conservation of energy, conservation of mass, and conservation of species equations. Spatial gradients are evaluated using an eight-order central differencing scheme and the time advancement employs a fourth-order, six-stage explicit Runge-Kutta method.

Configuration

The domain was two-dimensional and 3.6 mm by 3.6 mm in size, composed of a periodic direction, \hat{x} , and a non-periodic direction, \hat{y} , in which the composition varied across a mixing layer of $\sigma = 25 \ \mu$ m thickness from pure oxidiser at 900 K at the left boundary, to pure fuel at 400 K at the right boundary. The boundary conditions in the \hat{y} direction are non-reflecting outflow. The initial mixing layer was described by:

$$Z(y) = \frac{1}{2} \left(1 + \tanh\left(\frac{y - \frac{1}{2}(y_{max} - y_{min})}{\sigma}\right) \right)$$

which specified the mixture fraction, Z, profile. The temperature profile was determined from the fuel and oxidiser enthalpies and the mixture fraction profile.

A Passot-Pouquet turbulence spectrum [7] was superimposed at the initial time. The proscribed turbulence had a Damkhöler number, Da, of 0.4, defined as $Da = t_{eddy}/\tau_{ig}$, where t_{eddy} is the characteristic eddy time defined as $t_{eddy} = L_t/u'$, and L_t is the integral length scale equal to 1×10^{-4} m and u' is the turbulent velocity fluctuation equal to 0.486 ms^{-1} . This Da was selected to match the approximate Da at the location of ignition in representative conditions [6]. The turbulence was tapered to zero for the regions near the \hat{y} boundaries, for numerical stability. The initial vorticity field is presented in Fig. 1.



Figure 1: Magnitude of vorticity at the initial condition. The vorticity is tapered to zero near the outflow boundaries in the \hat{y} direction for numerical stability.

The simulation was solved on a mesh which was uniform in the \hat{x} direction and stretched in the \hat{y} direction, with a fine-mesh region in the middle 1.8 mm, centered about the mixing layer. At the initial condition, the fine-mesh region had a resolution of 2.5 μ m in both directions. The simulation was advanced at this resolution with a time step size of 4 ns from the initial condition to just before the high temperature ignition. At this point the domain was re-meshed to produce a resolution of 1.25 μ m in both directions in the fine-mesh region, which was required to resolve some high temperature intermediate species. The solution was then advanced to the end with a time step of 1.5 ns.

Results

Figure 2 contains four instantaneous views of a 1.2 by 1.2 mm window, which show the ignition dynamics progressing in nondimensional time, $t^* = t/t_{eddy}$, where t is the physical time. The colour shading represents the heat release rate. The solid black line represents the Z_{st} contour. The black dashed line represents the contour of methoxymethyl-peroxy radical (CH₃OCH₂O₂) mass fraction equal to $5x10^{-4}$. Species CH₃OCH₂O₂ is formed via the low temperature chemistry kinetics and the selected threshold indicates regions of low temperature heat release. The white dashed line represents the contour of hydroxyl radical OH mass fraction equal to $5x10^{-3}$. Species OH is formed via high temperature kinetics and the selected threshold indicates regions of burning stoichiometric mixture.

At $t^*=1.3$, multiple low temperature ignition kernels developed at lean mixture fractions (to the left of the Z_{st} line). By $t^*=2.5$, the low temperature kernels developed at all locations in the \hat{x} direction. The region of low temperature chemistry had also propagated into rich mixture fractions (to the right of the Z_{st} line). The low temperature chemistry continued to move into richer mixture fractions, and by $t^*=3.2$ the first high temperature ignition kernel had formed. The kernel formed between the Z_{st} line and the region of peak low temperature chemistry. From this time the kernel rapidly expanded towards richer and leaner mixture fractions and multiple additional ignition kernels formed (not shown here). By $t^*=4.1$, several ignition kernels had expanded across the Z_{st} line. When this occurred, edge flames were formed, centered on the Z_{st} line, which propagated in each direction along the Z_{st} contour. At $t^*=4.1$, multiple edge flames existed which had a main tribrachial (triple flame) structure, propagating into regions of low temperature chemistry, which formed a fourth "upstream" branch. As the simulation continued from this point, the edge flames propagated along the Z_{st} line until all regions of Z_{st} were fully-burning. Concurrently, the region of low temperature chemistry continued to propagate into increasingly rich mixture fractions.

To understand this complex ignition, a conditional probability density function (PDF) of temperature was created. Figure 3 shows the PDF of temperature, conditioned on Z at the instants in time corresponding to Fig. 2. At $t^*=1.3$, the initiation of the low temperature chemistry is observed as a peak at a very lean mixture fraction. By $t^*=2.5$, the low temperature chemistry expanded to a broad region in mixture fraction space, forming a distinct branch. By $t^*=3.2$, the first high temperature ignition kernels are apparent as the new high temperature branch forming at Z=0.3. From $t^*=3.2$ to $t^*=4.1$, repeated high temperature ignitions consume the low temperature branch about Z=0.3. The propagation of edge flames established a strong high temperature branch. At very high Z, the low temperature branch is still observed at the end of the simulation.

Figure 3 reveals the evolution of a bimodal temperature distribution in mixture fraction space. To further investigate this behaviour, Reynolds averages were calculated for the heat release rate (HRR) and Favre averages for the low temperature species $CH_3OCH_2O_2$ and high temperature species OH mass fractions, conditioned on Z. Reynolds average quantities are denoted by an overline. Favre average quantities are denoted by $\langle \rangle$ notation.

In Fig. 4 plots for $\overline{\text{HRR}|Z}$, $\langle Y_{\text{OH}}|Z\rangle$, and $\langle Y_{\text{CH}_3\text{OCH}_2\text{O}_2}|Z\rangle$ are presented at points in time corresponding to the previous figures. At $t^*=1.3$, the profiles of HRR |Z| and $\langle Y_{CH_2OCH_2O_2}|Z\rangle$ are well-correlated, supporting the notion that the ignition is initiated by low temperature chemistry pathways. By $t^*=2.5$, the region of low temperature chemistry has broadened in mixture fraction space, with the peak values of both $\langle Y_{CH_3OCH_2O_2}|Z\rangle$ and $\overline{\text{HRR}|Z}$ moving into very rich values. At $t^*=3.2$, the $\langle Y_{\rm CH_3OCH_2O_2}|Z\rangle$ peak continued to move towards richer Z, but the $\overline{\text{HRR}|Z}$ profile has developed a prominent peak about Z=0.3. This peak corresponds to the onset of the main ignition event, and its location in Z-space is effectively the most reactive mixture fraction, but differs substantially from the τ_{mr} obtained from zero-dimensional simulations. By $t^*=4.1$, the $\overline{\text{HRR}|Z}$ profile has two distinct peaks. The primary peak is centered about the stoichiometric mixture fraction and is coincident with the $\langle Y_{\rm OH}|Z\rangle$ profile. This peak is the high temperature branch and is associated with the propagating edge flames and the trailing diffusion flames on the Z_{st} contour. A secondary peak exists at very rich mixture fractions and is associated with the profile of $\langle Y_{CH_2OCH_2O_2} | Z \rangle$. This peak is the low temperature branch, which continues to exist as a significant feature long after the high temperature ignition and deflagrations were initiated.

Conclusions

A two-dimensional DNS simulation of dimethyl ether ignition was conducted at diesel engine relevant conditions. The configuration consisted of a mixing layer superimposed with a spectrum of decaying isotropic turbulence with a Damkhöler number of 0.4 selected to be commensurate with typical ignition conditions [6]. At the selected oxidiser temperature of 900 K and pressure of 40 atmospheres, the dimethyl ether fuel was within the negative temperature coefficient regime.

A complex ignition process was observed. The first stage of ignition was initiated via multiple kernels of low temperature chemistry in lean mixtures after about one eddy-time. These kernels then rapidly spread throughout the domain in the periodic direction and slowly propagated in the non-periodic direction towards increasingly rich mixture fractions.



Figure 2: Instantaneous view of 1.2 by 1.2 mm window at four points in time. The colour shading represents heat release rate, the solid black line represents the Z_{st} contour, the black dashed line represents the threshold of $CH_3OCH_2O_2$ mass fraction equal to $5x10^{-4}$, and the white dashed line represents the threshold of OH mass fraction equal to $5x10^{-3}$.



Figure 3: Conditional probability density functions of temperature, conditioned upon mixture fraction, at four points in time.



Figure 4: Instantaneous Favre averaged profiles, conditioned on mixture fraction. Hear release rate (solid blue line, left yaxis), OH mass fraction (dot-dashed green line, right y-axis) and CH₃OCH₂O₂ mass fraction (dashed red line, right y-axis).

By 3.2 eddy-times, the first high temperature ignition kernels were observed, located at very rich mixture fractions of 0.3. These kernels then rapidly expanded into rich and lean mixtures, establishing edge-flames where they encountered the stoichiometric mixture fraction contour. The edge-flames were observed to have a main tribrachial (triple flame) structure and an additional low temperature chemistry branch ahead of the tribrachial flame, making the edge-flame structures tetrabrachial (quadruple flames). This finding is consistent with a previous study of lifted, laminar dimethyl ether flames which observed additional branches in edge-flames at negative temperature coefficient conditions.

The results suggest that at engine-relevant conditions edgeflames may play an important role in the ignition and stabilisation process. This has implications for modeling of diesel combustion since the edge-flames impose their own time and length scales, and require that diffusion and conduction processes are correctly represented.

The two-stage ignition observed suggests that the low temperature chemistry is important in determining the location and timing of the high temperature ignition. The high temperature ignition was initiated from regions with a mixture fraction of 0.3, much higher than the most reactive mixture fraction of 0.11 obtained from zero-dimensional simulations at identical thermo-chemical conditions [8]. The authors propose that this discrepancy is due to effect of the low temperature chemistry. As the low temperature chemistry propagates in mixture fraction space, it alters the ignition delay behaviour of the rich mixture, leading to an effective most reactive mixture fraction much richer than the nominal value. This behaviour could have implications for practical diesel combustion, as the degree of low temperature heat release and its interactions with turbulence may influence the location of the ignition kernels in mixture fraction space.

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