



Full Length Article

Structure of tetrabrachial flames in non-premixed autoigniting dimethyl ether/air mixtures

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ABSTRACT

Structures of tetrabrachial flames in two-stage autoigniting dimethyl ether (DME)/air mixture under diesel engine relevant conditions are investigated by direct numerical simulation. Three cases with different initial turbulent integral length scales are studied. Results show that the first stage of autoignition initiates in lean mixtures, and subsequently develops into a diffusion-supported cool flame propagating into rich mixtures; the second-stage autoignition features spatially distributed kernels in fuel-rich mixtures, followed by hybrid autoignition/tetrabrachial flames. The detailed chemical structures of the tetrabrachial flames are analyzed in terms of reactant concentrations and the reaction rate profiles. The cool flame branch is dominated by low temperature reactions, while the other branches are mainly involved in high temperature oxidation of the remaining fuel and intermediate species. The excess DME is consumed in the premixed flame branches and decomposed into more stable fuels including H₂, CH₄ and CO in the trailing diffusion flame, where H₂ and CO are mainly oxidized by intermediate species OH and O. The structures and reaction rates in the tetrabrachial flame exhibit significant asymmetry, which is more distinct in the mixture fraction-temperature phase space. Effects of turbulence on the timing and location of two-stage ignition are then studied. In this study, turbulence tends to advance ignition compared with laminar cases, while the first high-temperature ignition time is similar for the three cases with different initial turbulence integral length scales.

1. Introduction

Autoignition of fuel-air mixtures in a turbulent flow is a complex problem of great theoretical interest and also relevant to practical combustors, where ignition occurs after fuel injection in a high-pressure and high-temperature environment. A two-stage autoignition has been observed under conventional diesel engine conditions, involving pre-ignition reactions due to low-temperature chemistry (LTC), followed by the main ignition due to high-temperature chemistry (HTC) [1]. Conceptual models of diesel combustion, based on observations in optically accessible engines and chambers, have not yet been conclusively demonstrated [2,3]. Experimental observations still have limitations in simultaneous measurement of multiple parameters [4,5], especially in a combusting environment.

Tibrachial flames (also known as triple flames) present to facilitate the flame propagation during nonuniform ignition [6–8]. Domingo et al. [7] showed that tibrachial flame structures played a key role in the propagation of ignition along stoichiometric contours. Echehki et al. [8] detected the formation of tibrachial flames during the autoignition

of non-homogeneous mixtures of hydrogen in heated air. The tibrachial flame structure also provides a mechanism for partially premixed flame stabilization that may be present in lifted jet flames [9]. The stabilization, propagation, and instability of tibrachial flames in non-autoignitive conditions have been reviewed by Chung [10], and they further studied the tibrachial flames in autoignited conditions [11,12]. Practical hydrocarbon-based fuels generally have two-stage ignition process, and may exhibit the negative temperature coefficient (NTC) phenomena in the intermediate temperature regime [13]. The ignition characteristics of nonpremixed flames can be fundamentally affected by NTC effects, especially at elevated pressures. A transition from tibrachial to polybrachial flame structure has been found in partially premixed laminar DME/air jet flame, with various temperatures of the oxidizer [14]. The multibrachial flame structures are also observed by Deng et al. [15,16] in laminar DME/air coflow flames, and further investigations into the controlling chemistry are conducted based on Chemical Explosive Mode Analysis. Krisman et al. [17] have also reported that the edge flame in a two-stage igniting turbulent mixing layer has a hybrid structure consisting of a tetrabrachial flame.

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Nomenclature		turb	turbulent
Da	Damköhler number	ign	ignition
l	length scale (m)	st	stoichiometric
r	radius (m)	Od	zero dimensional
Re	Reynolds number	<i>Abbreviation</i>	
T	temperature (K)	CF	cool flame
t	time (s)	DME	dimethyl ether
u	velocity (m/s)	DF	diffusion flame
Y_k	mass fraction of species k	HTC	high-temperature chemistry
ξ	mixture fraction	HRR	heat release rate
χ	scalar dissipation rate	HIK	high-temperature ignition kernel
τ	ignition delay time (s)	LPF	lean premixed flame
δ	thickness of mixing layer (m)	LTC	low-temperature chemistry
<i>Subscript</i>		NTC	negative temperature coefficient
mr	most reactive	RPF	rich premixed flame

However, no detailed chemical structures have yet been analyzed.

Turbulence has been observed to affect the location and timing of autoignition in the mixing layer [18,19]. Experimental and numerical studies of single stage autoignition of non-premixed mixture in turbulent inhomogeneous flows at atmospheric conditions have revealed that autoignition kernels appear first at locations around most reactive mixture fraction ξ_{mr} [18,20–23], along with the lowest scalar dissipation rate χ . This has been confirmed in direct numerical simulation (DNS) studies with detailed chemical and transport models both in two- and three- dimensional turbulence [23,24]. Several DNS studies have been devoted to the investigation of ignition under diesel engine-relevant conditions with appropriate simplified assumptions. Yao et al. [25] investigated hydrogen/air autoignition in turbulent mixing layer at elevated pressures up to 30 atm and found that autoignition occurred at the most reactive mixture fraction isosurfaces. Borghesi et al. [26] conducted DNS of autoigniting n-heptane sparse spray at 24 bar with reduced chemistry. The doubly conditioned statistics revealed a two-stage autoignition. DNS of an igniting turbulent mixing layer of DME-air mixture was performed by Krisman et al. [17,27]. They found that ξ_{mr} calculated from the homogeneous reactor is not sufficient to predict the location of the second stage autoignition. This is also proved in a further 3D DNS of a temporally evolving planar jet of n-heptane at 40 atm with global chemistry by Krisman et al. [28].

Despite considerable progress made regarding two-stage autoignition, a complete clarification of the structure of the polybrachial flames is still lacking. Further detailed information on turbulence effects on two-stage autoignition would enhance our understanding of the underlying physical processes. The present DNS study considers ignition of a DME pocket in turbulent air at 40 atm within the NTC regime. The main objectives of the present work are to demonstrate the chemical structures of the tetrabrachial flames, as well as turbulent effects on ignition timing and locations in the DME/air mixture.

2. Configuration and numerical methods

The computational domain is sketched in Fig. 1, with a pocket of low temperature (400 K) pure DME exposed in high temperature air (composed of 21% O_2 and 79% N_2 , 900 K). The square two-dimensional domain has a size of 3.2 mm by 3.2 mm, and the radius of the fuel pocket is initialized as $r_0 = 0.8$ mm. The system has a pressure of 40 atm. The initial composition and temperature vary across a mixing layer with a specified hyperbolic tangent mixture fraction profile which is described as $\xi(r) = \left(1 + \tanh\left(\frac{r_0 - r}{\delta}\right)\right)/2$, where $\delta = 40$ μ m is the initial thickness of the mixing layer. Initial fuel and air profiles are set according to the mixing line while all other species are initially set to

zero.

Periodic boundary conditions are employed at all boundaries, to mimic the constant volume configuration. The Passot-Pouquet isotropic kinetic energy spectrum [17] is employed to generate the initial turbulent velocity field: $E(k) = \frac{32}{3} \sqrt{\frac{2}{\pi}} \frac{u'^2}{k_e} \left(\frac{k}{k_e}\right)^4 \exp\left[-2\left(\frac{k}{k_e}\right)^2\right]$, where k is the wave number, the subscript e is for the most energetic wave number, and u' is the root mean square (RMS) velocity. The generated velocity is then superimposed on the stationary mean flow field as the initial condition. The prescribed turbulence varies with the integral length scale l_t , while the initial RMS turbulent velocity fluctuations remain the same and are set equal to 0.5 m/s. The initial l_t equals 0.1, 0.2, and 0.4 mm for cases 1, 2 and 3, respectively. l_t is the only varied parameter for the three cases studied. The corresponding Damköhler numbers (Da) are 0.57, 1.14 and 2.28, where Da is defined as $Da = \tau_{turb} / \tau_{(\xi=\xi_{mr,0d})}$, τ_{turb} is the eddy time defined as $\tau_{turb} = l_t / u'$, $\tau_{(\xi=\xi_{mr,0d})}$ is the ignition delay time of the most reactive mixture measured in a homogeneous reactor, which is also used for non-dimensionalization of time t ($t^* = t / \tau_{(\xi=\xi_{mr,0d})}$).

The full compressible Navier-Stokes equations, species and energy conservation equations for a reacting gas mixture are solved with an in-house DNS code. A fourth-order explicit Runge-Kutta method for time integration and an eighth-order central differencing scheme for spatial discretization are used with a tenth-order filter for removing spurious

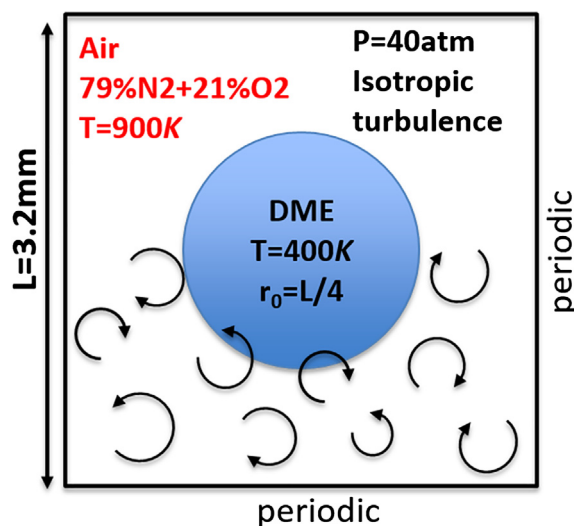


Fig. 1. Schematic of the computational configuration.

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