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1. **Title:** IGNITION AND FORMALDEHYDE FORMATION IN DIMETHYL ETHER (DME) REACTING SPRAY UNDER VARIOUS EGR LEVELS

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Abstract

As an alternative fuel to diesel in compression-ignition (CI) engines, dimethyl ether (DME) has gained interest in combustion research due to its high cetane number for fast ignition and ultra-low emission of particulate matter. In this study, ignition and important intermediate species including formaldehyde are experimentally investigated in a constant-volume combustion vessel facility that includes a fuel injection system for spray-like behavior of liquid DME. Experiments of different oxygen concentrations simulating various levels of exhaust-gas recirculation (EGR) were performed to study its corresponding effect on the flame structure and emissions from DME combustion. Results from the experiment were then used to validate a 3-D CFD simulation using a detailed chemistry solver. Different stages of ignition, characterized by temperature profile and certain species (e.g., CH_2O for cool flame) after start of injection, are provided to conceptualize the DME combustion process under the effect of low-to-high oxygen ambient gas concentrations. Both simulations and experiments showed that there is a supporting link between CH_2O formation and low-temperature combustion prior to diffusion-controlled flame uniquely for DME. By studying the temperature and equivalence ratio dependence of the reacting spray at different O_2 levels, different stages of ignition along with the formation of CH_2O suggested that the start of the depletion of CH_2O can be used as an ignition indicator.

Keywords: DME; spray combustion; formaldehyde PLIF; ignition; CFD

1. Introduction

Dimethyl ether (DME) is a promising alternative fuel for diesel engines that produce ultra-low soot due to its lack of C-C bonding in the chemical structure [1, 2]. There are numerous studies on DME, establishing extensive data for fuel properties [3]; the kinetic mechanism and chemical pathway [4-6]; spray and combustion features in direct injection (DI) system [7, 8], and experiments in a combustion vessel using optical diagnostics for flame visualization [9, 10]. In most of these studies, the fast ignition characteristic of DME was demonstrated due to its higher cetane number compared to diesel [11]. Prior to ignition, certain chemical reactions during the mixing of fuel vapor and oxidizers play an important role in determining the flame structure (e.g. lift-off length) and the later emissions of soot and NO_x during the high temperature combustion process of diffusion flame [12, 13].

Exhaust-gas recirculation (EGR) is a well-known combustion concept with the benefit of reducing emissions by burning at a lower temperature and leaner in-cylinder fuel/air mixture [14]. Higher EGR levels generally delay the ignition timing by providing more time for the mixing of fuel and air prior to combustion. In this study, experiments were performed with DME reacting spray in a constant-volume combustion chamber at various oxygen concentrations imitating different EGR levels. Planar laser-induced fluorescence (PLIF) technique was used to capture the formation of CH_2O before, at, and after the time of ignition. Ignition delay from a photodiode measurement and the visualization of CH_2O from PLIF imaging were used to validate a CFD model using a detailed chemistry solver to further understand the relationship between formaldehyde and different stages of ignition. In a DME reaction mechanism, CH_2O plays an important role in the chemical pathway of fuel oxidation process: it is formed from methoxymethyl (CH_2OCH_3) decomposition [4] and is consumed later to form carbon dioxide through the basic combustion path ($\text{CH}_2\text{O} \rightarrow \text{HCO} \rightarrow \text{CO} \rightarrow \text{CO}_2$) [15]. The objective of this study is to: first, confirm the commonly known hypothesis that CH_2O is formed mostly prior to ignition delay, at

upstream region, before lift-off length for typical diesel combustion [12, 16], and second, conceptualize the ignition process of DME flame based on formation of CH_2O mainly with the support from simulated model.

2. Experimental and Numerical Setup

2.1. Combustion vessel and fuel injection system

Liquefied DME was delivered by a fuel injection system coupled with a single-hole nozzle injector ($D_0=180\text{ }\mu\text{m}$) of a hydraulically activated electronic unit injector (HEUI) [17]. The advantage of HEUI injector lays on the minimization of exposing DME fuel to the injector nozzle. This is because the low viscosity and lubricity of DME can potentially damage the moving parts of the fuel injection system. In some studies, a lubricity additive such as Lubrizol or Infineum R655 is often used to facilitate this issue with DME [1]. The injector was driven by two iPod coil power EFS drivers that control the opening and closing coil events corresponding to the start and the end of the injection event, respectively. In this study, the electrical injection duration was kept to 2.0 ms, and the injection pressure was 75 MPa.

The single-hole HEUI injector system was integrated into the current combustion vessel research facility [18, 19]. Baseline condition of the experiment consists of 18% O_2 ambient composition, and an ambient density of 14.8 kg/m^3 . The O_2 concentration was varied from baseline to imitate the effect of EGR. The ambient pressure was 3.8 MPa at the injection event for all conditions in this study. The initial ambient temperature of 900 K at injection was obtained by igniting a combustible mixture of C_2H_2 , H_2 , O_2 , and N_2 using an electrode. The test condition is summarized in Table 1.

Table 1 Summary of test condition

Parameter	Value
Fuel	DME
Nozzle Diameter (μm)	180
Injection Pressure (MPa)	75
Ambient Composition (% O_2)	21, 18, or 15
Ambient Temperature (K)	900
Ambient Pressure (MPa)	3.8
Ambient Density (kg/m^3)	14.8
Fuel Temperature (K)	383
Energizing Duration (ms)	2.0

2.2. Optical diagnostics

Formaldehyde (CH_2O) was excited at the wavelength of 355 nm by an Nd:YAG laser (Continuum Surelite III) with a 10 ns laser pulsewidth. A schematic of the optical setup is shown in Fig. 1 with the laser sheet directed toward the injector tip through the spray centerline. Similar studies have been performed to visualize CH_2O in spray combustion using the same excitation wavelength [12, 16, 20]. The species fluorescence was captured through an intensified CCD camera (DiCam Pro) at several timings ASOI to visualize the formation and consumption of CH_2O . The camera was equipped with a 105 mm UV lens f/4 (250-650 nm transmission) and 400 nm band-pass filter with 20 nm FWHM. The filter selection was found to obtain the formaldehyde signal effectively while avoiding elastically scattered light or reflection from the laser excitation. The camera gate was set at 200 ns covering the time when laser is activated and the final spatial resolution is 0.091 mm/pixel. A full view of the spray from the tip of the injector to the oppositely impinging wall was visualized.

Fig. 1: A schematic of experiments.

A photodiode (Thorlab DET36A) was also used to detect the time of ignition. The photodiode is not sensitive to liquid scattering signal as confirmed from the recorded signal over time. The actual start of injection was found by using a High Speed camera detecting the first liquid signal that exits the injector nozzle. The ignition delay was calculated as the time difference between the start of actual injection to photodiode signal rise.

2.3. CFD simulation setup

The actual diameter of the injector nozzle was measured using scanning electron microscope (SEM) imaging and was determined to be $174.2 \mu\text{m}$. The rate of injection (ROI) was measured experimentally using the Bosch tube technique [21]. The total injected mass at 75 MPa and 2.36 ms (actual duration) was 15.16 mg. A simplified version of the ROI was generated using an ROI profile generator developed by Payri et al. [22] with input conditions of injection pressure, nozzle size, discharge coefficient, injection duration, and fuel density. This ROI profile, as shown in Fig. 2 with experimental measurement, was used as the input in the CFD simulation.

Fig. 2: Measured and numerical rate of injection.

In this study, CONVERGE [23] was selected as the CFD simulation tool that is capable of using adaptive mesh refinement (AMR) to automatically generate grid based on sub-grid gradients of certain parameters, for this case, temperature and velocity. The finest grid is 0.125 mm with a base grid size of 2 mm. The selected grid size was considered to be appropriate and robust for validating both non-reacting and reacting spray, as suggested by Senecal et al. [24] for currently selected Reynolds-Average Navier-Stokes (RANS) Re-normalization Group (RNG) k - ϵ turbulence model. A Lagrangian spray “blob” injection model of Reitz and Diwakar [25] with subsequent breakup and atomization of liquid blobs model of Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) [26] with no break-up length were used in the simulation. Additionally, No Time Counter (NTC) collision method of Schmidt and Rutland [27] is included in the simulation to model droplet collision with linear increase in computational cost at higher number of spray parcels. The SAGE detailed chemistry solver [28] which is a well-mixed reactor based model running on CHEMKIN-format of chemical kinetic inputs was used with the consideration of all species and reactions.

The mechanism used in the simulation was a reduced mechanism for DME (45 species, 249 reactions) developed from detailed mechanism by Cung et al. [29] (originally, 260 species and 1039 reactions).

Ignition delay calculated using both reduced and detailed mechanism were well correlated with experimental data by Pfahl [30]. The reducing mechanism method is based on direct relation graph with error propagation (DRGEP) using Reaction Workbench utility [31] and compared with original detailed mechanism over a number of parameters (ambient density, temperature, oxygen concentration) with no significant difference in the prediction of ignition delay. Important species and reactions are kept in the final reduced mechanism: (1) CH_3OCH_3 (dimethyl ether), CH_3OCH_2 (methoxymethyl radical), $\text{CH}_3\text{OCH}_2\text{O}_2$ (methoxymethyl-peroxy radical), $\text{CH}_2\text{OCH}_2\text{O}_2\text{H}$ (hydroperoxymethoxymethyl radical), $\text{O}_2\text{CH}_2\text{OCH}_2\text{O}_2\text{H}$ (peroxy-methoxymethyl-hydroperoxide radical) and $\text{HO}_2\text{CH}_2\text{OCHO}$ (hydroperoxy-methylformate) [32]; (2) soot precursors including C_2H_2 (acetylene), C_2H_4 (ethylene) [1], with similarly selected soot precursor and soot indicator from ref [33] of C_6H_6 (benzene), and $\text{C}_{16}\text{H}_{10}$ (pyrene); and (3) the NO_x formation species including NO , NO_2 , N_2 . The combination of the detailed chemistry solver (SAGE) for reaction rate calculation, CFD transport equation solver, and a well-validated mechanism provides an efficient tool for modeling combustion including ignition.

3. Results and Discussion

A comparison of ignition delays from experiments and CFD simulations for three different O_2 levels is shown in Fig. 3. Note that, prior to performing combustive case in CFD simulation, non-reacting spray simulations were well-validated with liquid/vapor penetrations profiles from a separate experiment (Mie/Schlieren hybrid imaging) of different ambient temperatures (750 K, 900 K, and 1100 K) for non-reacting condition (0% O_2 , similar other parameters as described in Table 1) [29]. The ignition delay in the simulation was defined as the time when the temperature of any cell is above 2000 K, while experimental ignition is defined by the very initial rise of photodiode signal. Overall, the time of ignition is shortened by increasing the amount of oxygen content. The difference between the actual and

simulated ignition delays are relatively small (0.01 ms in average). This shows that the simulation provides good prediction for the ignition event in DME reacting spray at the given conditions.

Fig. 3: Ignition delay from experiment and simulation at various O₂ concentrations.

A side-by-side comparison of the PLIF and CFD formaldehyde formation regions over varying times ASOI is shown in Fig. 4 for 18% O₂. Here CFD simulation predicts the trend of CH₂O formation fairly well compared to experimental images (false color with same range level of legend). There is a $\pm 10 \mu\text{s}$ time difference between simulation and experimental images. This is due to the defined time interval for exporting 3D outputs in CFD simulation. It can be seen that CH₂O is mostly formed upstream near the nozzle region with higher concentrations along the spray centerline. In simulation, CH₂O is formed initially in the periphery of the spray, but this was not illustrated in PLIF images. Since the RANS model simplified the dynamic structure of the spray compared to LES model [34, 35], it seems to underpredict turbulence within the spray centerline where the low temperature reactions to form CH₂O may take place. However, other experiments showed that CH₂O does form at the radial periphery of the spray initially rather than at the core [12, 16]. This could be due to the different conditions of ambient oxygen levels, injection strategies (injection pressure, duration, nozzle diameter, etc.), and even differences in the reaction pathway from fuel to fuel that would result in the different structure of CH₂O, especially at its initial formation. The simulated ignition delay was 0.745 ms (6% higher than the experiment).

As shown in both the simulation and experiment, CH_2O appeared to start diminishing after ignition. This vanishing phenomenon of CH_2O has been pointed out in other literatures for the diesel combustion [13, 36]. In Ref. [13], it was mentioned that CH_2O is a common species that appears during the first stage of ignition where the low temperature reaction takes place. As temperature increases, certain concentrations of OH are released by the decomposition of H_2O_2 , and OHs are immediately oxidized with other unburned hydrocarbon (UHC). Specifically, in the DME kinetic mechanism, the reaction of OH and CH_2O is one of the most important reactions via $\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{HCO} + \text{H}_2\text{O}$ [4, 15]. Wang et al. [4] also pointed out that both CH_3 , H, and HO_2 contribute to the consumption of CH_2O to form HCO in their chemical pathway analysis of DME reaction with air at lean and rich conditions. This chemical conversion is similar to what Musculus et al. [13] described as an indicator of the second stage of ignition. At the time of 875 μs in the simulation, a void region appears near the front stream of the CH_2O formation. This seems to limit the extension of CH_2O prior to $X/D = 250$. CH_2O is eventually diminished as seen between ~ 2.1 to 2.9 μs . Note that the injection of fuel in both experiment and simulation has already finished at 2.36 ms ASOI. It is reasonable that CH_2O is near complete extinction as no further parent fuel is supplied to initiate chemical reactions as described in Ref. [4] through this reaction path: $\text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_3\text{OCH}_2 \rightarrow \text{CH}_2\text{O}$.

Fig. 4: Time-elapsd CH₂O from PLIF images (top) and simulation (bottom) at 18% O₂.

To further illustrate the formation and consumption of CH₂O, the global mass formation profiles of various species are shown in Fig. 5 together with the normalized temperature and heat release rate (HRR).

Fig. 5: Species evolution from CFD simulation at 18% O₂.

As temperature gradually increases before 0.745 ms, CH₂O is produced abundantly, and almost simultaneously with CH₃OCH₂ (produced via H-abstraction from DME) which again confirms good correlation between these two species from the reaction step: $\text{CH}_3\text{OCH}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{CH}_3$. As temperature rises significantly and maximum HRR occurs at the time of ignition, CH₂O production reaches peak value and starts to decrease. At the same time, OH is formed, indicating a transition to the high temperature combustion process. OH is known to later consume CH₂O through H-abstraction to form HCO [4, 13]. It can also be seen that there are slow and fast reactions for each species to reach its peak value. The fast reaction would probably be related to HCO with a sudden release of the species when a large amount of heat release is present. In summary, the formation of formaldehyde marks the initial stage of ignition where low temperature oxidation of DME takes places. Its production drop may be used as an indicator for the on-set high-temperature combustion process where the release of OH radicals is commonly known for the oxidation of unburned hydrocarbons.

Going beyond the oxygen concentration conditions performed in the experiment, a more dilute ambient environment was simulated in CFD model for 12% and 9 % O_2 . Ignition still occurs even at these conditions but with lower peak temperatures and longer ignition delays as expected by the effect of more diluents, however, it results in somewhat different stages of ignition as shown in temperature profile in Fig. 6. It can be seen that as O_2 level is reduced, the combustion duration lengthens because ignition is delayed due to the slower chemical kinetics resulting from the lack of oxygen entrainment. Therefore, for the same amount of fuel injected, it would take more time to consume all the hydrocarbons. The negative temperature coefficient (NTC) regime can also be seen at different oxygen levels with a longer NTC period at lower oxygen levels where HRR continues to decrease despite the temperature still increasing.

Fig. 6: Simulated temperature (top) and HRR (bottom) at each O_2 concentration.

The importance of CH_2O and OH as indicators of different ignition stages is considered at different oxygen levels in Fig. 7. While the early stage of ignition process can be defined by the formation of formaldehyde, it is believed that the consumption of formaldehyde should be used as an indicator of hot ignition instead of the release of OH . As shown in Fig. 7, the time difference between the peak of CH_2O and rise of OH increases as the oxygen level is decreased. The defining ignition delay proposed by

temperature ($T_{\text{cell}} > 2000 \text{ K}$), CH_2O peak, and OH rise are shown in Fig. 8 over various oxygen concentrations to compare with each other.

Fig. 7: CH₂O (top) and OH (bottom) formation over simulation time at each O₂ concentration.

At an O₂ level of 15% or higher, there is negligible difference in ignition delay defined by these parameters. However, as the O₂ level is decreased below 15%, the difference in predicting ignition delay between CH₂O-approach and others becomes larger. The shortest ignition delay is defined by CH₂O peak. Note that for 9% O₂ case, the peak temperature is below 2000 K, therefore the ignition defined by cell temperature of over 2000 K cannot be determined. Note that the temperature at the ignition time defined by peak CH₂O for 9 and 12% O₂ cases is about 1400 K, which is considerably high to indicate the start of ignition.

Fig. 8: Computed ignition delay over O₂ concentration based on temperature, CH₂O, and OH.

To further confirm the hypothesis of ignition timing by formation of CH₂O spatially, different contour images of CH₂O and OH are shown in Fig. 9 along with the temperature and equivalence ratio (or “Phi”)

scatter plots from all simulated cases. Phi-T plots are a very important tool where ignition can be easily recognized by period of high temperature and locally fuel rich region. The plots in Fig. 9 are arranged to represent the pre, at and post ignition times for the varying O_2 cases. Each point in the Phi-T scattering plot represents a point in the computational domain. This type of scattering plot gives information about equivalence ratio of the ignited computation cell and the intensity of reactivity based on the temperature rise. Basing on the Phi-T scatter plots, the reactivity of the sprays is reduced when O_2 concentration reduces from 21% to 9% with the peak temperature at the time of ignition reducing from 2600 to 1450 K. However, the equivalence ratio at ignition time is almost similar for all the cases simulated ($\Phi_{\text{ignition}} \sim 1.65$).

Additional information about the behavior of ignition can be obtained by relating CH_2O and OH species contours together. In the case with higher ambient oxygen levels, the generation of ignition kernels takes place at multiple spots, randomly, but within CH_2O region. Nonetheless, at lower ambient oxygen level cases in which the fuel-air mixture is given longer time to react due to less favorable conditions for ignition. Consequently, with longer time to reach homogeneity, ignition appears as a lump rather than the disjointed ignition spots as in a higher oxygen level case. As a general note with respect to Fig. 9, it can be seen that the depletion of formaldehyde prior to an ignition event creates a void spot that are quickly filled with the formation of OH. Thus the depletion of formaldehyde or an increase in OH can be generally considered as an estimate to the ignition delay.

Fig. 9: Phi-Temperature scatter and contour plots of CH₂O and OH from simulation.

4. Conclusions

Correlation of formaldehyde (CH₂O) to the ignition process in DME reacting spray was investigated in both experiment and simulation. Fluorescence of CH₂O excited by a 355 nm laser wavelength was captured at different ASOIs over separate runs to provide a temporal and spatial view of its progression and recession. It was confirmed that the general concept of diesel combustion can be applied to DME combustion, meaning that CH₂O appears abundantly in low temperature combustion process. CH₂O starts depleting when temperature increases significantly, usually known as the time of ignition, or ignition delay. A validated CFD simulation predicted this phenomenon very well. Different stages of

ignition were described by the profiles of: CH_2O (low temperature combustion or 1st stage of ignition), and OH (2nd stage of ignition characterized by high temperature diffusion flame). CH_2O is seen upstream near nozzle and is extended up to the flame lift-off location where OH is present. By studying the effect of ambient oxygen levels on DME combustion, ignition process was reviewed by temperature profile, CH_2O , and OH. Regardless of which criteria was being considered, it was shown that ignition delay increases as the oxygen concentration reduces. However, at the lower oxygen concentrations, indication of ignition was shown to be more reliable by the formation of CH_2O . It was seen that CH_2O was formed initially during 1st stage ignition, and its depletion marks an important stage where high temperature combustion is initiated as shown in the reactivity of fuel/air mixture in Phi-T scatter or overall temperature profile. OH is formed around the time of CH_2O depletion indicating the start of 2nd stage ignition where high temperature reactions are present. However, this is not clearly observed in the cases of lower oxygen concentration as the initial formation of OH appears at longer time after CH_2O is consumed. The temperature at the time of CH_2O depletion was already high (~ 1400 K) suggesting that the CH_2O profile can be a reliable source for understanding the ignition process. Overall, the results of this study provide information on single or two stage behavior of the ignition in DME reacting spray with the general suggestion on the use of CH_2O (its depletion) as a marker for ignition from low-to-high oxygen ambient conditions. With the growing research in combustion using laser diagnostic, it is prominence that the ignition process can be defined more accurately by the profile of CH_2O .

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