PILOT INJECTION OF DME FOR IGNITION OF NATURAL GAS AT DUAL FUEL ENGINE-LIKE CONDITIONS

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ABSTRACT–The ignition delay of a dual fuel system has been numerically investigated by adopting a constant volume chamber as a model problem simulating diesel engine relevant conditions. A detailed chemical kinetic mechanism, consisting of 28 species and 135 elementary reactions, of dimethyl ether (DME) with methane (CH_4) sub-mechanism has been used in conjunction with the multi-dimensional reactive flow KIVA-3V code to simulate the autoignition process. The start of ignition was defined as the moment when the maximum temperature in the combustion vessel reached to 1900 K with which a best agreement with existing experiment was achieved. Ignition delays of liquid DME injected into air at various high pressures and temperatures compared well with the existing experimental results in a combustion bomb. When a small quantity of liquid DME was injected into premixtures of CH_4/air, the ignition delay times of the dual fuel system are longer than that observed with DME only, especially at higher initial temperatures. The variation in the ignition delay between DME only and dual fuel case tend to be constant for lower initial temperatures. It was also found that the predicted values of the ignition delay in dual fuel operation are dependent on the concentration of the gaseous CH_4 in the chamber charge and less dependent on the injected mass of DME. Temperature and equivalence ratio contours of the combustion process showed that the ignition commonly starts in the boundary at which near stoichiometric mixtures could exists. Parametric studies are also conducted to show the effect of additive such as hydrogen peroxide in the ignition delay. Apart from accurate predictions of ignition delay, the coupling between multi-dimensional flow and multi-step chemistry is essential to reveal detailed features of the ignition process.

KEY WORDS : Natural gas, DME, Dual fuel engines, Autoignition, Ignition delay

1. INTRODUCTION

In an effort to develop relatively clean and efficient fuels, attention is being focused on various gaseous fuels. In particular, natural gas is thought to be one of the most attractive alternative fuels for internal combustion engines. Most combustion devices are adaptable to use gaseous fuels for power production. In particular, high compression ratio diesel engines are generally suitable when high thermal efficiency is desired. Experiments in a combustion bomb have shown that autoignition of natural gas under diesel-like conditions requires temperatures as high as 1100–1200 K (Naber *et al.*, 1994). This high temperature requirement mandates that either a high compression ratio (about 23:1) or a high intake air temperature should be used, both of which have negative effects on engine performance and durability. In diesel engine appli-

cations, poor ignition properties of CH_4, which is the primary constituent of natural gas, necessitate the use of an ignition source to initiate combustion and hence, dual fuel operation is required.

The dual fuel combustion system features essentially a homogeneous gas-air mixture compressed rapidly below its autoignition conditions and ignited by the injection of pilot liquid fuel near the top dead center. The amount of pilot liquid fuel, which is injected through the conventional diesel injection equipment, is in the order of 5–10 percent of the total energy consumption at full load (Karim, 1980; Nielsen *et al.*, 1987; Liu and Karim, 1995). The pilot self ignites and becomes the ignition source for the inducted charge to complete the combustion process.

Recently, DME attracts more attention as an alternative fuel for diesel engines and can be mass-produced from natural gas or coal using simple synthetic technologies. It can be stored and transported using existing propane facilities (Ho *et al.*, 2003; Hang *et al.*, 2003). The self-

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ignition temperature of DME is low and it has a shorter ignition delay than that of diesel fuel under same engine operation condition (Wakai *et al.*, 1998; Kajitani, 2004). The low self-ignition temperature and the oxygen content of 34.8% (by mass) are two major factors that characterize low soot and unburned hydrocarbon emissions of DME fueled engines.

DME has been used as an ignition enhancer for methanol fueled diesel engine (Golovitchev *et al.*, 1997). Investigations of DME as an ignition source in natural gas dual fuel engines are limited. Golovitchev and Chomiak (1998) reported in a preliminary numerical study that DME could be used as pilot fuel for dual fuel Application. They studied only the ignition of stoichiometric CH_4/air mixture in a constant volume bomb at a pressure of 50 bars and an initial temperature of 950 K. It is believed that more research is needed to study the capability of using liquid DME as an ignition source of CH_4/air mixtures. The aim of this study is to investigate numerically the autoignition delay and combustion characteristics of CH_4/air mixtures ignited by liquid DME under a wide range of initial conditions.

2. MODEL FORMULATION

The numerical modeling in this study is based on the KIVA-3V code (Amesden, 1997) with modifications in chemical model. The standard chemistry model in KIVA-3V is based on rather simple numerical scheme and relies on global reaction mechanisms, which make it inappropriate for ignition delay studies. The code treats in different ways fast chemical reactions, which are assumed to be in equilibrium, and slow reactions, which proceed kinetically, although a detailed chemical mechanism accounting for trimolecular collision processes with different chaperon efficiencies was not incorporated. For this reason, a more advanced chemistry solver accounting for the multi-step chemical mechanism developed by Golovitchev and Nordin (1999) is adopted in this study. This solver was specially designed to handle detailed kinetics chemistry in an efficient way and has been validated on ignition delay data. A detailed chemical kinetic mechanism (Golovitchev and Chomiak, 1998), consisting of 28 species and 135 elementary reactions, of DME with CH_4 sub-mechanism was adopted.

The ignition and combustion of the CH_4/air mixtures initiated by the injection of a small amount of liquid DME at diesel–like conditions was numerically studied using a constant volume combustion chamber. The combustion chamber is assumed to be cylindrical with a diameter of 30 mm and length of 80 mm. The computational mesh used in the simulation was uniformly distributed in both axial and radial directions with a grid size of $\delta x = 1$ mm and $\delta r = 0.5$ mm. DME spray was injected

through a single hole (0.2 mm in diameter) from the top of the combustion chamber along the symmetry axis. The injection profile of the injected spray was a square wave with a total injection period of 2 ms. The initial droplet temperature was 323 K and the chamber walls were assumed to be adiabatic.

3. RESULTS AND DISCUSSION

Several definitions of ignition delay times have been reported in the literatures. Each researcher selected a definition independently. For example, in the SENKIN code (Lutz *et al.*, 1988), the moment of ignition for a homogeneous mixture study is defined when the temperature exceeds the initial temperature by the prescribed value of 400 K. Rente *et al.* (2001) defined it as the moment when the temperature averaged over the combustion chamber exceeded the initial value by 1%. In the study of Khalil *et al.* (1996), a value of 2% rise in the average pressure over the initial pressure has been chosen. In our case, the start of ignition was defined as the moment when the maximum temperature in the combustion vessel reached to 1900 K with which a best agreement with experiment was achieved.

The ignition delays of both homogeneous stoichiometric CH_4/air and DME/air mixtures were first calculated using SENKIN with the constant volume option using GRI-3.0 mechanism (Smith *et al.*) together with DME mechanism (Curran *et al.*, 2000). The results were compared with the calculated data of a stoichiometric mixture containing 90% CH_4 and 10% DME at a pressure of 4.1 MPa and various initial temperatures as shown in Figure 1. It can be seen that the application of DME as an ignition improver for CH_4/air indicates that a small amounts of DME can substantially reduce the ignition delays of the
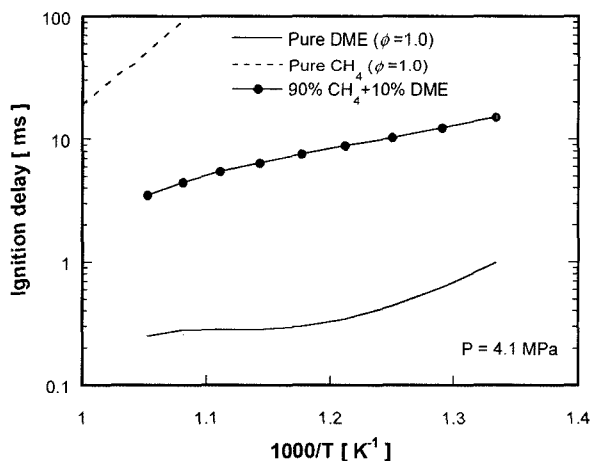

Figure 1. Computed ignition delay times with temperature for homogeneous mixture of CH_4/air/DME.

stoichiometric CH_4/air mixture. The ignition delay, however, is still longer than that of DME/air mixture by an order of magnitude. The ignition delay is ranged from 3.5 to 7.6 ms for mixture containing 90% CH_4 and 10% DME as compared to 0.25 to 0.3 ms for pure DME at a temperature ranged from 950 to 850 K (the most applicable temperature range in diesel engines). For DI diesel engines, autoignition of a mixture of fuel and air must occur within less than 2 ms (Agarwal and Assanis, 1998) after the start of injection. Therefore, the application of DME as an ignition improver for natural gas is not suitable at the conditions examined. An alternative method is to use DME as an ignition source by injecting a small quantity of liquid DME into a homogeneous mixture of CH_4/air. The numerical results will be discussed in the following section.

3.1. Liquid DME as Ignition Source

The ignition of CH_4/air mixtures in an inhomogeneous system initiated by the injection of a small amount of liquid DME (10 mg) at diesel–like conditions was then numerically investigated. The measured values of ignition delay of DME spray from Wakai et al. (1998) were used to validate the model and the detailed chemical kinetic mechanism. The calculations were done with an initial temperature range of 750 to 950 K for two different levels of initial pressures of 2.1 MPa and 4.1 MPa similar to that used in the experiment.

Figure 2 shows the comparison of the calculated ignition delay times, plotted in an Arrhenius diagram, of a DME spray injected into either air or mixture of CH_4/air ($\phi = 0.6$) for the initial pressures of 2.1 MPa and 4.1 MPa, along with the experimental data of Wakai et al. (1998). A reasonable agreement was achieved between calculated and measured ignition delays of DME spray injected into air. The ignition delay of dual fuel setup operation is extended from that observed with DME only operation, especially at higher initial temperatures and lower initial pressure. The variation in the ignition delay between DME only and dual fuel case tend to be similar for lower temperatures which can be easily confirmed when the slopes and values of both curves are compared.

It is well known that the ignition delay period of a liquid fuel is divided into two parts. The first part is the so called physical delay which is the time required for heat transfer, fuel evaporation, fuel-air mixing, and, finally establishment of a combustible gaseous mixture whose temperature meets the requirement for auto-ignition (Ho et al., 2003). The remaining part of the delay is the chemical part, which is associated with the progress of the oxidation reactions of the fuel towards ignition, inflammation and the exothermic release of energy. Fuel evaporation is the actual physical stage of ignition delay because fuel evaporation takes place simultaneously with
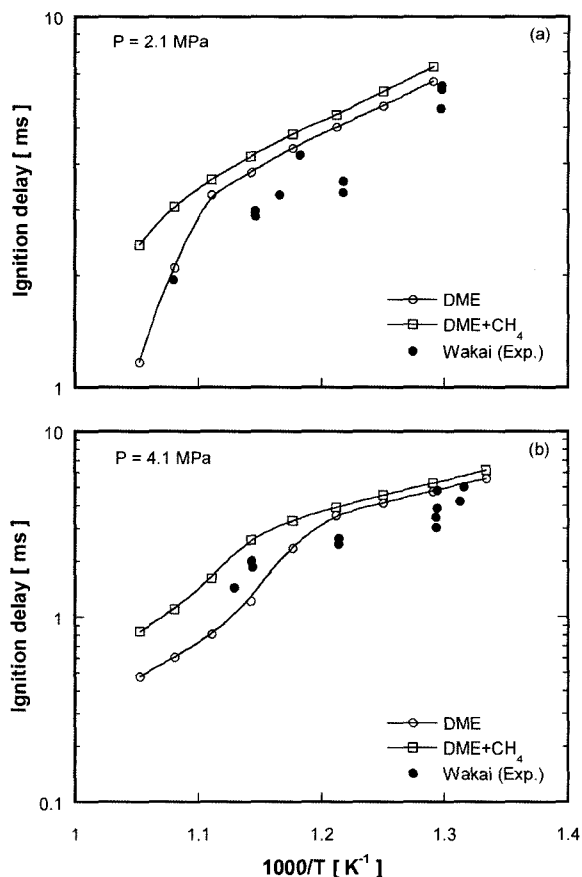

Figure 2. ignition delay times with temperature for DME injected into air or into CH_4/air mixture ($\phi = 0.6$). Comparison of predictions and experimental data. (a) P = 2.1 MPa and (b) P = 4.1 MPa.

atomization. At higher temperatures, favorable conditions are provided for fuel droplet evaporation and hence mixing of fuel vapor with hot environment is enhanced as well as the chemical processes that bring about ignition. In case of dual fuel operation at high initial temperatures, the evaporated fuel is expected to diffuse rapidly into the surrounding CH_4/air mixture and the existence of the gaseous fuel with air may inhibit the preignition processes of the injected fuel compared with air only.

The Arrhenius diagram in Figure 2 can be divided into two regimes. The first one is the part at which the ignition delay is less than 2 ms (injection duration) and the other part for ignition delays more than 2 ms. It can be seen that the slops of the two curves of ignition delays (DME only and DME + CH_4) are nearly parallel at the upper part (after termination of fuel injection). It is expected that injecting more fuel will assist in the formation of combustible mixtures and hence reducing the ignition delay at higher initial temperatures.

In general, the extension of the ignition delay in a dual

fuel operation has been observed before (Karim, 1980; Nielsen *et al.*, 1987; Liu and Karim, 1995; Khalil *et al.*, 1996; Karim *et al.*, 1991) and has been referred to either the reduction in the oxygen concentration as a result of the displacement of some of the air by the fumigated gaseous fuel or a thermal effect; introducing gaseous fuel into the combustion chamber changed the specific heat of the compressed mixture, which is functions of temperature and pressure, causing gas temperature decrease (Nielsen *et al.*, 1987). Karim *et al.* (1991) suggested that the preignition reaction activity of the gaseous fuel-air charge during compression contributes significantly to the observed extension of the ignition delay in dual fuel operation.

Figure 3 shows the effect of gaseous fuel-air equivalence ratio on the ignition delay. It can be seen that the ignition delay increases gradually with the gas admission for all initial temperatures examined. This result may support the contribution effect of the reduction in the oxygen concentration. Our results are somewhat different from that obtained by Karim *et al.* (1991) in which they found that the ignition delay increases gradually with the increased admission of the gaseous fuel up to a detectable maximum value and then drops to a minimum just prior to reaching the stoichiometric ratio and then increases again as excessively rich mixtures are employed. It must be noted that in our study, the effect of preignition reactions prior to DME injection is not considered since our calculations started when injection start, although there may be some preignition reactions during injection. Also, it is noted that in all previous works of dual fuel operation, the pilot fuel was a diesel fuel while in our study, the pilot fuel is DME. Therefore, it is expected that the type of a pilot fuel may also affect the degree of extension in ignition delay. It can be seen that the ignition
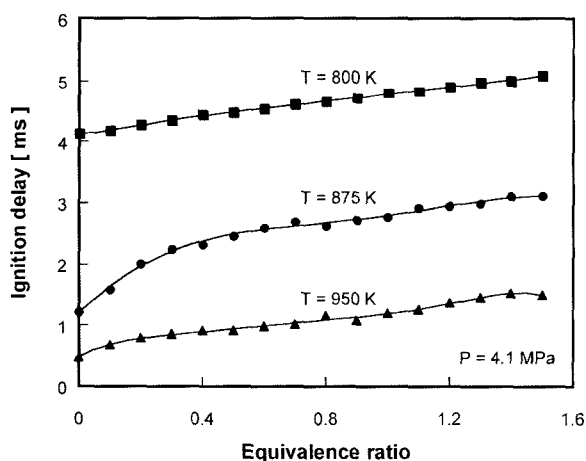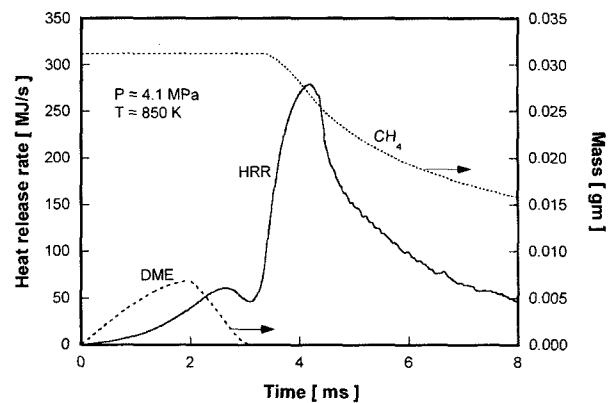

Figure 4. Variation of calculated heat release rate (HRR) and mass of DME and CH_4 with time for dual fuel operation ($\phi = 0.6$).

delay of dual fuel operation is slightly longer than that of DME only as shown in Figure 2.

Figure 4 shows the mass concentrations of both DME and CH_4 for a dual fuel operation and the corresponding heat release rate (HRR) with time exhibiting a distinct two stages of oxidation. The first stage is mainly dominated by the DME kinetics at a low-intermediate temperature range without any noticeable oxidation of CH_4. During this period, fast depletion of some of the injected DME takes place rapidly accompanied by the characteristic heat release rate profile. This followed by a second period where the CH_4 depletion begins to take place at a higher temperature level. A similar result has been obtained by Khalil *et al.* (1996).

To illustrate the ignition scenario, temperature distributions at various times in the combustion chamber for T_i = 850 K, P_i = 4.1 MPa and ϕ = 0.6 are shown in Figure 5. The regions of higher temperature in the periphery of the

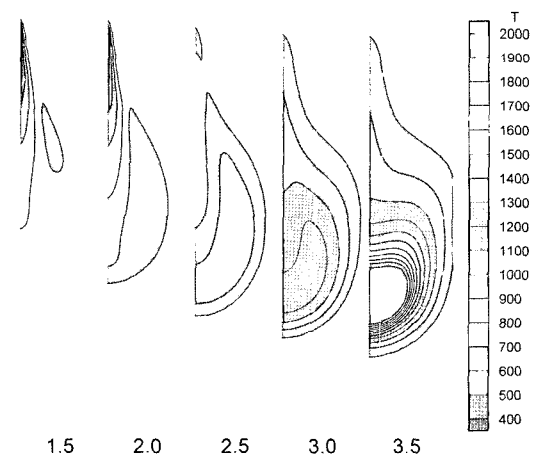Figure 3. Computed ignition delay times over the whole range of equivalence ratio of CH_4/air mixtures ignited by DME injection. P = 4.1 MPa.

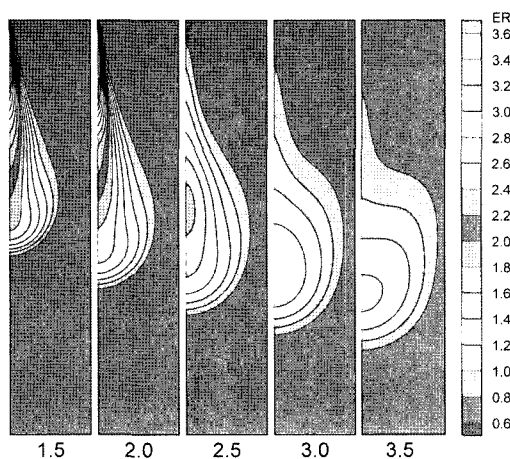Figure 5. Calculated temperature distribution at different times for dual fuel operation. T = 850 K and P = 4.1 MPa.

Figure 6. Calculated equivalence ratio distribution at different times for dual fuel operation. T = 850 K and P = 4.1 MPa.

spray are clearly seen in the course of the early ignition stages. It can be seen that the ignition commonly starts in the boundary of the mixing-flow region where droplet sizes are small and a favorable conditions are provided for droplet evaporation and mixing of DME vapor with hot environment (air or CH_4/air mixture). The corresponding equivalence ratio distributions at the same conditions of Figure 5 are presented in Figure 6. Because of the limited air entrainment into the jet core, the jet core is fuel rich and low temperature; thus, the start of ignition in the jet core is inhibited.

Figure 7 shows the variation of ignition delay times with the injected mass of DME at various ambient temperatures. It can be seen that, at a fixed ambient temperature, the ignition delay decreases slightly with the increase in the injected mass. It is clear that even a small
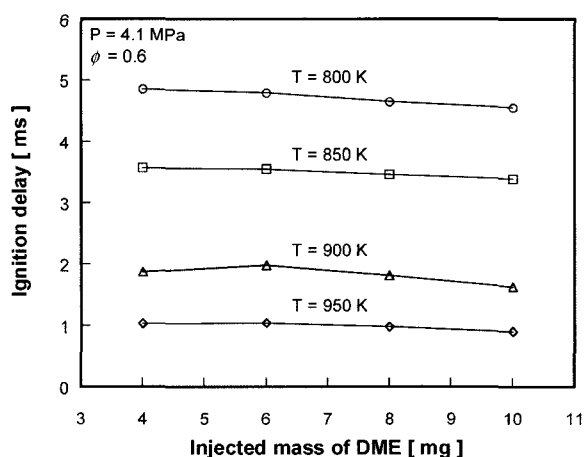

Figure 7. Effect of the injected mass of DME on the ignition delay at various ambient temperatures for dual fuel operation.

quantity of DME (4 mg) is sufficient to ignite a lean mixture of CH_4/air (ϕ = 0.6) without any noticeable increase in the ignition delay as compared with higher injection rate.

3.2. Hydrogen Peroxide as Ignition Improver

The effect of additives in promoting autoignition of CH_4 at high temperatures has been examined before (Karim et al., 1991; Zamansky and Borisov, 1992; Golovitchev et al., 1996). Systematic data on the effect of stable additives, higher hydrocarbon fuels, and free radicals on CH_4 autoignition are summarized by Zamansky and Borisov (1992). According to their findings, the best promoters are additives which are able to increase the radical concentration without disappearing during the induction period. The use of formaldehyde as an additive in reducing ignition delay of dual fuel engines running with CH_4 was investigated numerically by Karim et al. (1991).

Golovitchev et al. (1996) investigated the effectiveness of hydrogen peroxide (H_2O_2) in promoting the autoignition of CH_4 at conditions of interest for supersonic combustion. Using a time dependent model, with no spatial variation, they found that replacing 5–10% (volumetric) of the fuel with H_2O_2 shortens the ignition delay by over one order of magnitude for all the conditions examined in their work. The effect of promotion was particularly pronounced at temperatures below 1500 K.

Since the effect of H_2O_2 was so dramatic, its effect on the ignition delay of a CH_4 dual fuel engines was studied in the present investigation. Two mixtures were studied: 99% CH_4 plus 1% H_2O_2 and 95% CH_4 plus 5% H_2O_2 by replacing some of existing CH_4 in a mixture of CH_4/air (ϕ = 0.6) with the desired percentage of H_2O_2. The calculations were done at an initial ambient pressure of 4.1 MPa and various initial temperatures. The same quantity of DME (10 mg) was injected into the selected two mixtures as ignition source.

Figure 8 shows the variation of the calculated ignition delay times for a DME spray injected into either a mixture of CH_4/air (ϕ = 0.6) or a two other mixtures with addition of H_2O_2 for an ambient pressures of 4.1 MPa. Some curves plotted in Figure 2 are reproduced in Figure 7 for a better evaluation of H_2O_2 efficiency. It is interesting to note the presence of relatively small concentration of H_2O_2 (1% by volume of CH_4) assists markedly the reactions so that the ignition takes place earlier and hence, the addition of just 1% of H_2O_2 reduces the ignition delay substantially, especially at higher ambient temperatures. For example, at ambient temperature of 850 K, addition of only 1% H_2O_2 reduces the ignition delay to one third than the corresponding value without H_2O_2 addition. These results are similar to the results obtained by Glovitchev et al. (1996). A corresponding decrease in delay of CH_4 dual fuel system by temperature alone would require an
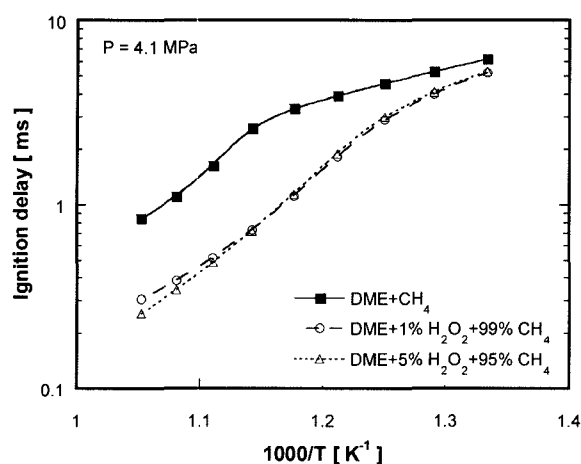
Figure 8. Calculated ignition delay with temperature of CH_4/air (ϕ =0.6) and two blends with H_2O_2.

increase of about 75 K. This saving in ambient temperature is substantial and could be used to mitigate the high compression ratio requirement in a compression ignition natural gas engine.

It is also seen that the blend with 5% H_2O_2 doesn't show any appreciable decrease in the delay over the blend with 1% H_2O_2. Although not shown, due to the action of H_2O_2, there is virtually no drop in pressure in the initial stages (compared with calculations without the addition of H_2O_2), i.e. the induction period has been reduced significantly. This is consistent with the results obtained before (Agarwal and Assanis, 1998). The reason why H_2O_2 acts as such an effective ignition promoter is that in the early stages of ignition, it rapidly decomposes via the reaction H_2O_2 + M $\Leftrightarrow$ OH + OH + M and thus H_2O_2 serves as the major radical source (Golovitchev et al., 1996). The practical advantage of H_2O_2 as a free radical promoter is its stability. It can be quickly transported into the flame and after rapid decomposition it releases free radicals as the key location of the ignition process.

4. CONCLUDING REMARKS

The ignition delay times of a dual fuel setup (liquid DME injected into mixtures of CH_4/air) are numerically simulated using a multi-dimensional reactive flow KIVA-3V code with a detailed chemical kinetic mechanism consisting of 28 species and 135 elementary reactions of DME with CH_4 sub-mechanism. The detailed kinetic mechanism was first tested to evaluate its predictive capability by comparing the calculated DME ignition delay with the measured data available in the literature under typical compression ignition conditions of pressure and temperature. Comparison of the predicted ignition delay with

experiments yielded good agreement. The start of ignition was defined as the moment when the maximum temperature in the combustion vessel reached to 1900 K with which a best agreement with experiment was achieved. When a small quantity of liquid DME (4–10 mg) is injected into pre-mixtures of CH_4/air, the ignition delay times of dual fuel setup were longer than that of observed with DME only, especially at higher initial temperatures. The variation in the ignition delay between DME only and dual fuel case tend to be constant for lower initial temperatures. It was found also that the ignition delay times increase gradually with the increased admission of the gaseous fuel. This result may support the contribution effect of the reduction in the oxygen concentration due to air replacement by CH_4. Temperature and equivalence ratio contours of the combustion process show that the ignition commonly starts in the boundary at which a near stoichiometric mixture exists.

The influence of additives like H_2O_2 in reducing the ignition delay period of CH_4 was also studied. The addition of small amounts of H_2O_2 (about 1% by volume), in particular, was found to reduce the ignition delay substantially. The enhanced reactivity of CH_4 in the presence of small amounts of more reactive species like H_2O_2 could be used in natural gas engines to alleviate the high temperature requirements.

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