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Numerical study of plasma produced ozone assisted combustion in a direct injection spark ignition methanol engine

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ABSTRACT

Numerical simulations were performed to better assess the effect of plasma produced ozone assisted combustion. The effects of ozone (O_3) addition from 0 to 7000 ppm in the intake manifold on cylinder pressure history, ignition delay, cylinder temperature history, and formaldehyde unburned methanol emission of a direct injection spark ignition (DISI) methanol engine during cold start and steady state conditions were simulated using computational fluid dynamics to couple the methanol chemical and kinetics reaction mechanisms. The model results show that the maximum cylinder pressure increases with increasing O_3 addition for cold start and steady state modes. O_3 addition can also significantly reduce ignition delay. Two maximum heat release rate peaks occurred with O_3 addition for cold start and steady state modes. The effect of O_3 addition on combustion processes of DISI methanol engines was significantly greater for cold start than steady state mode, particularly with higher O_3 concentrations. The effects on formation and oxidation of formaldehyde were greater than for unburned methanol, and the effects on formation and oxidation of formaldehyde were also significantly greater for cold start than steady state mode.

1. Introduction

Concerning energy security and environmental protection, the demand for substitute of fossil fuels has become increasingly urgent [1]. Therefore, there is strong motivation in looking for alternative fuels for different applications, such as motor vehicles [2]. Methanol has many desirable characteristics in improving combustion and emissions behaviors: high octane number, high laminar flame speed, indicating an excellent antiknock performance, high latent heat of vaporization, etc. Therefore, methanol is considered to be one of the most favorable fuels for engines of the future since it can be produced from coal, nature gas, and biomass with relatively low cost [3]. However, the drawback of the use of methanol such as the cold start difficulties due to low vapor pressure and high vaporization latent heat at low ambient temperature and more toxic formaldehyde and unburned methanol emissions make it difficult on the vehicle application [4,5]. Many measures for improving cold start combustion and formaldehyde and unburned emissions of methanol engines have been taken [6–10]. The control of combustion and formaldehyde and unburned methanol emissions has become the hotspots in the field of vehicle used methanol engines in recent years [11–14].

Plasma assisted combustion is a promising technology to control ignition, improve engine performance, increase lean burn flame stability, and enhance low temperature fuel oxidation under a wide range of conditions [15,16]. Plasma generates many species and excited states (such as ozone (O_3), etc.) [17,18]. O_3 has very long lifetime, approximately 3 days at room temperature, 1.5 h at 400 K, and 1.5 s at 500 K [15]. O_3 is one of the longer lived active species produced by electrical discharges in air [19] and has sufficient lifetime to be transported to the flame region to enhance fuel oxidation [20]. Wang et al. [19] investigated the effect of O_3 additive on the enhancement of the burning velocity for premixed methane-air flames, and found that O_3 addition can enhance flame

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propagation through kinetic and thermal effects under adiabatic conditions. Gao et al. [20] also studied the effect of O_3 addition on laminar flame speed, and found that the stoichiometric flame speed was increased by 8.3% for CH_4, and 7.7% for C_3H_8 with 6334 ppm O_3 addition. Pinazzi et al. [21] evaluated the potential of O_3 to overcome the low load limitations of direct-injection gasoline compression ignition engines, and shown that even small O_3 concentrations seeded in the intake manifold produced significantly advanced combustion phasing. Ombrello et al. [17] investigated plasma produced O_3 effects on flame propagation speeds experimentally using $C_3H_8/O_2/N_2$ mixtures, and found that O_3 can improve flame propagation speed due to decomposition of O_3 into atomic oxygen, and reported 8% increase in flame propagation speed for 1260 ppm O_3 addition. Foucher et al. [22] also showed that the rate of product of O atoms by O_3 decomposition during the compression stroke could be a mean to control, cycle to cycle, two stage ignition fuels in homogeneous charge compression ignition engines. Halter et al. [23] studied the effects of O_3 on methane combustion by experiment and detailed kinetic modeling, and confirmed that O_3 mostly affects methane combustion through its initial decomposition yielding O atoms.

As one of the strongest oxidizers, O_3 always enhances combustion processes because it can be transported to the preheat zone, then decompose to release O atoms which accelerate reactions by attacking fuel molecules [17,20]. Liang et al. [24] investigated the identical experimental platform for $H_2/CO/N_2$/air premixed combustion, and found that burning velocities increased 18.74% (maximum) at 0.7 equivalence ratio with 8500 ppm O_3 addition. Weng et al. [25] measured formaldehyde concentration profiles with O_3 addition in CH_4/air premixed combustion with CH_2O-PLIF, and found that formaldehyde concentration in Bunsen type laminar flame increased 58.5% for fuel-rich conditions and only 15.5% for stoichiometric conditions with 4500 ppm O_3 addition. The significant formaldehyde production increase was ascribed to the low-temperature (approximately 500 K) flame region when O_3 was seeded into the flame. Yamada et al. [26] reported the effects of methanol and O_3 as ignition control additives to the homogeneous charge compression ignition (HCCI) process of dimethyl ether (DME) engines. Masurier et al. [27] studied the effects of different oxidizing chemical species (O_3, nitric oxide, and nitrogen dioxide) which can modify the chemical kinetic on HCCI combustion. Schönborn et al. [28] described the ignition control of HCCI combustion through adaptation of the fuel molecular structure by reaction with O_3. Mohammadi et al. [29] studied combustion control in natural gas PCCI (premixed charge compression ignition) engines with O_3 added to the intake gas, and detailed chemical kinetic study indicated that reaction of O_3 with natural gas mixture at the early stage of the compression stroke produces species that played important roles in the natural gas ignition through the promotion of OH formation. Masurier et al. [30] investigated the effects of O_3 on HCCI combustion of three alcohol fuels, and found that O_3 can improve the HCCI combustion process and increase its concentration results in an advance of the combustion phasing. Gong et al. [31] reported the relationship between CO and formaldehyde and unburned methanol-unregulated emissions in cylinders and a tailpipe with O_3 addition from a direct injection spark ignition (DISI) methanol engine, and found the effects of O_3 addition on the formation and oxidation of CO, formaldehyde and unburned methanol are lower for the steady state compared with the cold start mode. The effects of O_3 addition on CO, formaldehyde and unburned methanol production and consumption in the cylinder are formaldehyde > CO > unburned methanol. CO, formaldehyde and unburned methanol emissions decrease with increasing O_3 addition.

Previous research regarding O_3 addition effects on combustion have concentrated on HCCI and PCCI engines, with little work on DISI methanol engines [32–34]. There is increasing interest in formation and oxidation of unregulated emissions in-cylinder for DISI methanol engines. However, there has been little research on formation and oxidation of unregulated emissions in-cylinder with O_3 addition for DISI methanol engines under transient and steady states. Therefore, the aim of this paper was to numerically study the effects of plasma produced O_3 addition on combustion, formaldehyde and unburned methanol emissions in DISI methanol engines for cold start and steady state conditions. The novelty of this study is trying to clarify the effect of O_3 addition on formation and oxidation of formaldehyde and unburned methanol unregulated emissions from a DISI methanol engine during cold start and steady state operating conditions. Hence, the contribution of this study is to obtain the relationship among combustion, formaldehyde and unburned methanol emissions with O_3 addition under cold start and steady state operation conditions from a methanol engines. The study outcomes will advance understanding of combustion, formation and oxidation of formaldehyde, unburned methanol emissions in-cylinder with O_3 addition, and methods to control formaldehyde and unburned methanol emissions for DISI methanol engines.

2. Modeling methodology

2.1. Numerical models

Many mathematical models are provided within the AVL-fire software describing turbulence, spray, spark ignition, and combustion [35]. The k-zeta-f model was chosen for the turbulence model in the current investigation, considering calculation results from the model show good agreement with experiments [36,37], and minimize calculation overhead. Dukowicz and Huh/Gosman models were used for evaporation and breakup, respectively. This model can be described in detail fuel burst into oil droplets from the nozzle into the cylinder under turbulence and high temperature and high pressure air flow, large volume of oil droplets break into a lot of small volume of oil droplets, and oil droplets with oil droplets, air and cylinder wall interaction. A spherical selection module replaced the spark plug in the computational domain. The initial fire nuclei of this model are spherical, and Ignition timing, ignition duration and ignition energy are customizable by the user. Spark timing is 14°crank angle before top dead center (CABTDC), the ignition duration is 0.03 ms, and the ignition energy is given by Ref. [38]:

$$E_{\min} = \pi d^2 \frac{\lambda_{av}(T_b - T_u)}{S_{av}} \quad (1)$$

where $E_{\min}$ is the minimum ignition energy (mJ), d is initial fire core diameter (mm), T_b is temperature of combustion gas (K), T_u is the temperature of unburned gas (K), λ_{av} is the average heat transfer coefficient at temperature from T_u to T_b, and S_{av} is average burning rate at temperature from T_u to T_b (m/s).

A general gas phase reaction module was defined from the material composition, and a reaction mechanism model simulated the combustion process. This is more conducive to the analysis formaldehyde and unburned methanol emissions of methanol engine.

Simulation calculations using AVL-fire were coupled with the chemical kinetics mechanism of methanol oxidation, considering 21 species and 91 reactions [39,40], and a supplementary 23 steps O_3 chemical kinetics sub-mechanism was developed and employed, as shown in Table 1 [17,30,41–50]. The adopted