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Numerical analysis of carbon monoxide, formaldehyde and unburned methanol emissions with ozone addition from a direct-injection spark-ignition methanol engine

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ABSTRACT

Numerical simulations were performed to assess the relationship between carbon monoxide (CO) and formaldehyde and unburned methanol-unregulated emissions in cylinders and a tailpipe with ozone (O_3) addition from a direct-injection spark-ignition methanol engine. This simulation study was performed during cold-start and steady-state modes with O_3 addition of 3000 and 7000 ppm. The initial phase of produced CO and formaldehyde is advanced significantly with O_3 addition, but the initial phase of produced unburned methanol had little impact. 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. When the exhaust valve opened, CO, formaldehyde and unburned methanol emissions with 7000 ppm O_3 addition for the cold-start mode are 15.3%, 52% and 70% lower than those without O_3 addition, respectively. CO, formaldehyde and unburned methanol emissions with 7000 ppm O_3 addition for the steady-state mode are 52.6%, 28% and 28% lower than those without O_3 addition, respectively.

1. Introduction

The demand for fossil-fuels substitution has become increasingly urgent for energy security and environmental protection [1,2]. Recently, much attention has been given to the development of cleaner alternative fuels to reduce air pollution and to reduce the dependence on fossil fuels [3]. Methanol is considered to be one of the most favorable fuels for future engines because it can be produced from coal, natural gas and biomass with a relatively low cost [4]. Methanol has many desirable characteristics to improve combustion and emission behaviors; these include a high octane number, a high laminar flame speed, an excellent antiknock performance and a high latent heat of vaporization. The drawbacks of using methanol, such as the cold-start difficulties from a low vapor pressure and a high vaporization latent heat at low ambient temperature, and more toxic formaldehyde and unburned methanol emissions, make it difficult in vehicle applications [5,6]. Plasma-produced ozone-assisted combustion is a promising technology to improve engine performance, increase lean burn flame, reduce emissions and enhance low-temperature fuel oxidation and processing [7].

Many effects have been devoted to study regulated and unregulated emissions of alternative-fuel engines. Zhou et al. [8] investigated the combustion, performance and regulated and unregulated emissions of a diesel engine with hydrogen addition. They found that the BSCO and BS(HCHO) decreased with an increasing engine load at a low and medium engine load, and vice versa at a high engine load. Zhang et al. [9] studied the regulated and unregulated emissions of diesel/methanol compound combustion engines with and without a diesel oxidation catalyst. Carbon monoxide (CO), formaldehyde and unburned methanol

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Table 1
Information of model components.

Type	Model
Turbulence	k-zeta-f
Evaporation	Dukowicz
Breakup	Huh/Gosman
Ignition	Spherical selection module
Material composition and reaction mechanism	General gas phase reaction module

emissions increased with an increasing fumigation ratio without a diesel oxidation catalyst. Cheung et al. [10] studied the regulated and unregulated emissions from a diesel engine that was fueled with biodiesel and biodiesel blended with methanol. They reported that, in general, CO emissions decreased with an increase in engine load from 0.2 to 0.7 MPa. However, CO emissions increased with an increase in engine load from 0.08 to 0.2 MPa for each fuel. Formaldehyde emissions reached the highest level at a medium engine load for each fuel. For blended fuels with methanol, the unburned methanol emissions decreased as the engine load increased from 0.08 to 0.55 MPa, but they increased slightly from 0.55 to 0.7 MPa. Zhang et al. [11] investigated experimentally the regulated and unregulated emissions from a diesel engine that was fueled with Euro V diesel fuel and fumigation methanol. They found that CO, formaldehyde and unburned methanol decrease with an increase in engine load. Agarwal et al. [12] compared CO and formaldehyde emissions from a biodiesel and methanol blend and reported that CO emissions decreased with an increase in engine load below 75% and increased with an increasing engine load above 75%. Wang et al. [13] studied the effect of misfire on regulated and unregulated emissions from a methanol-fueled vehicle and they reported that CO and formaldehyde emissions increased with an increasing misfire rate. Qu et al. [14] investigated regulated and unregulated emissions from a direct-injection spark-ignition (DISI) methanol engine under homogenous combustion and a light load and their experimental results showed that formaldehyde and unburned methanol emissions showed opposite tendencies with variations in the methanol-injection timing, ignition timing, excess air ratio and intake air temperature. When the methanol-injection timing was retarded, the CO and unburned methanol emissions increased. With an advancing ignition timing, the CO increased slightly and the unburned methanol emissions increased rapidly. By using a lean mixture, the CO and formaldehyde emissions decrease rapidly. Agarwal et al. [15] measured unregulated emissions from a gasohol (gasoline–alcohol blend) and found that ethanol-based gasohols emitted more acetaldehyde and higher alcohol emissions resulted from higher-alcohol-proportion gasohols.

Zhen et al. [16] analyzed the original emissions for a spark-ignition methanol engine numerically in cylinder-based detailed chemical kinetics. They found that CO emissions could be decreased in the cylinder by retarding the ignition timing or by increasing the engine-compression ratio. The produced formaldehyde was consumed rapidly during the later stage of the combustion process, and minimal residual formaldehyde remained after combustion. Zhang et al. [17] proposed a detailed oxidation mechanism to predict formaldehyde emissions from a methanol–gasoline spark-ignition engine. Low-temperature methanol oxidation at the end of the intake process occurs in the cylinder, and some formaldehyde was generated, which increased with an increasing methanol blend. After the start of the mixture combustion, cylinder formaldehyde was generated rapidly and it decreased by rapid oxidation. Liu et al. [18] studied formaldehyde and unburned methanol emissions numerically from a DISI methanol engine under cold-start and steady-state operating conditions, and found that formaldehyde and unburned methanol emissions increase rapidly when the overall equivalence ratio is less than 0.4. Formaldehyde and unburned methanol emissions are very low when the overall equivalence ratio is larger than 0.4. A rapid decrease results from oxidation at the corresponding position of the maximum cylinder temperature, after which formaldehyde is generated rapidly for any operating conditions.

Much previous research has focused mainly on the combustion, regulated and unregulated emissions of methanol, gasoline–methanol blends, gasoline–ethanol blends and gasoline–-other fuel blends in spark-ignition engines [19–27], with little work

Table 2
O_3 chemical kinetics sub-mechanism.

No.	Chemical reaction	$K = AT^b\exp(-E/RT)$		
		A	b	E
1	$O_3 + H\langle = \rangle O_2 + OH$	8.43E+13	0	934
2	$O_3 + O \langle = \rangle O_2 + O_2$	4.82E+12	0	4094
3	$O_3 + OH \langle = \rangle O_2 + HO_2$	1.85E+11	0	831
4	$O_3 + HO_2 \langle = \rangle O_2 + OH + O_2$	6.02E+09	0	938
5	$O_3 + H_2O \langle = \rangle O_2 + H_2O_2$	6.62E+01	0	0
6	$O_3 + CH_3 \langle = \rangle O_2 + CH_3O$	3.07E+12	0	417
7	$O_3 + NO \langle = \rangle O_2 + NO_2$	8.43E+11	0	2603
8	$O_3 + N \langle = \rangle O_2 + NO$	6.03E+07	0	0
9	$O_3 + H \langle = \rangle O + HO_2$	4.52E+11	0	0
10	$O_3 + H_2 \langle = \rangle OH + HO_2$	6.00E+10	0	19840
11	$O_3 + CH_4 \langle = \rangle CH_3O + HO_2$	8.13E+10	0	15280
12	$O_3 + N_2 = \rangle O_2 + O + N_2$	4.00E+14	0	22667
13	$O_2 + O + N_2 = \rangle O_3 + N_2$	1.60E+14	−0.4	−1391
14	$O_3 + O_2 = \rangle O_2 + O + O_2$	1.54E+15	0	23064
15	$O_2 + O + O_2 = \rangle O_3 + O_2$	3.26E+19	−2.1	0
16	$O_3 + O_3 = \rangle O_2 + O + O_3$	4.40E+14	0	23064
17	$O_2 + O + O_3 = \rangle O_3 + O_3$	1.67E+15	−0.5	−1391

Table 3
Engine specifications.

Bore (mm)	130
Stroke (mm)	150
Displacement (L)	1.99
Compression ratio	16:1
Rated power/speed (kW/rpm)	18.3/2000
Number of nozzle holes	7
Diameter of nozzle hole (mm)	0.45

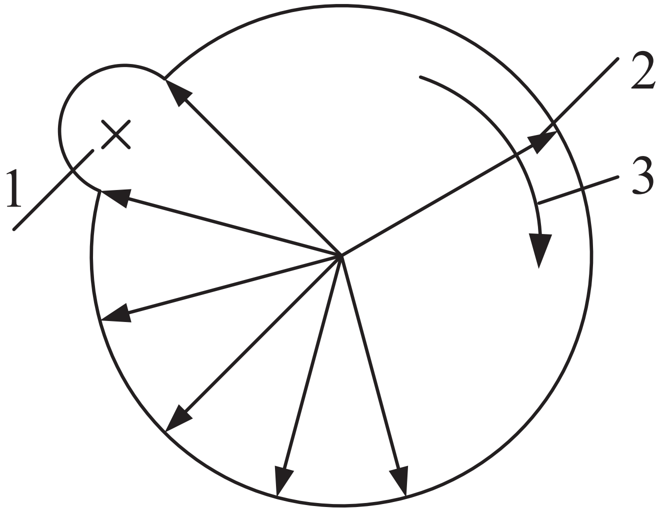

Fig. 1. Injector spray-line distribution.