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Numerical analysis on original emissions for a spark ignition methanol engine based on detailed chemical kinetics

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ABSTRACT

Nowadays, in order to meet the various emission regulations and improve the atmospheric environment, methanol has been used as a clean fuel to replace conventional fuels for engines. In this study, original emissions under various engine operating conditions are simulated, and the effects of different spark timings, engine speeds, mixture concentrations and combustion chamber shapes for emissions in a SI methanol engine are studied based on LES (large eddy simulation) with detailed chemical kinetics. A methanol reaction mechanism including 84-reactions, 21-species is used to simulate the methanol combustion. The results showed that carbon monoxide (CO) emission could be decreased by retarding ignition timing or increasing engine compression ratio. The formaldehyde (CH_2O) had two effects, which were production and consumption. The produced formaldehyde was consumed quickly in the later stages of the combustion process, so the residual formaldehyde was very little after combustion. With the increase of equivalence ratio, the carbon monoxide emission was gradually increased, when the equivalence ratio was less than 0.9, the produced carbon monoxide was gradually decreased, and almost approached zero in lean conditions. It was difficult to improve the carbon monoxide emission for the present SI (spark ignition) methanol engine by optimizing the combustion chamber shape.

1. Introduction

As the atmospheric environment pollution is more and more serious today, the various emission regulations have been made by many countries so as to improve the atmospheric environment. It is generally accepted that auto-mobile emission is one of the main sources of atmospheric pollution. Therefore, it is an effective method to improve the atmospheric environment by reducing vehicle emissions. Furthermore, with the reserves of these conventional oil resources such as gasoline and diesel are being rapidly depleted, so many alternative resources such as natural gas, hydrogen and methanol need to be developed to replace conventional fuels (for instance, gasoline or diesel) for internal combustion engines [1–4].

Among various alternative resources, there are many advantages to the development of methanol fuel to replace the conventional oils. Methanol is a colorless, pure substance, and it can be produced from many resources such as biomass, natural gas or coal etc [5–8]. The basic properties of methanol fuel, diesel fuel and gasoline fuel are illustrated in Table 1. It can be seen that high octane rating allows a significant increase in the engine compression ratio, and the high vaporization heat value can increase the volumetric efficiency [9].

Many researches on engine emissions have been done by various researchers. Surawski et al. [10] investigated the ethanol impacts on emissions in a compression ignition engine. It was found that as the addition of ethanol, the emissions of $PM_{2.5}$ (fine particulate matter) and NO (nitric oxide) could be decreased, but the emissions of HC (hydrocarbon) and CO were increased. Rakopoulos et al. [11] studied the emissions of diesel/diethyl ether blends in a diesel engine. It was found that as the addition of diesel/diethyl ether blends, the emissions of CO and NO_x could be decreased, but the un-burnt HC emission was increased. Poompipatpong and Cheenkachorn [12] investigated the compression ratio impacts on the emissions in a natural gas engine. It was found that the total HC emission could be increased by increasing compression ratio. Huang et al. [13] studied the HC emissions in a SI engine by

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Table 1
The properties of methanol, gasoline and diesel.

Fuel property	Methanol	Gasoline	Diesel
Formula	CH_3OH	C5-12	C10-26
Molecular weight (g/mol)	32	95–120	180–200
Oxygen content	50%	0	0
Stoichiometric air/fuel ratio	6.45	14.6	14.5
Low calorific value (MJ/kg)	19.66	44.5	42.5
High calorific value (MJ/kg)	22.3	46.6	45.8
Freezing point (°C)	−98	−57	−1 ~ −4
Boiling point (°C)	64.8	30–220	175–360
Flash point (°C)	11	−45	55
Auto-ignition temperature (°C)	465	228–470	220–260
Research octane number	108.7	80–98	
Motor octane number	88.6	81–84	
Cetane number	3	0–10	40–55
flammability limits (vol)	6.7–36	1.47–7.6	1.85–8.2
specific heat (20 °C) (kJ/kg · K)	2.55	2.3	1.9
latent heat (kJ/kg)	1109	310	270
Viscosity (20 °C) (cP)	0.6	0.29	3.9

using gasoline-oxygenate blends. It was found that compared with the neat gasoline, the HC emissions could be decreased through blend oxygenated fuels in gasoline. Zheng et al. [14] studied the impacts of nitrogen dilution on the premixed combustion by using an extended methanol reaction mechanism. It was found that the emissions of formaldehyde and NO_x were decreased simultaneously through the nitrogen addition. Yilmaz [15] investigated methanol/biodiesel/diesel and ethanol/biodiesel/diesel impacts on emissions in a diesel engine. It was found that compared with the ethanol blends, methanol blends were more effective to decrease the emissions of CO and HC. Muralidharan et al. [16] studied the bio-diesel emissions in a variable compression ratio engine. It was found that the HC emission was higher at higher loads excepted for B20 (biodiesel: diesel = 1:4) blends, and the NO emission was higher at lower loads excepted for B40 (biodiesel: diesel = 2:3) blends.

As can be seen from the previous analysis, it can be found that most of the studies have been focusing on blends, synthetic fuels, or conventional gasoline and diesel fuels [17–20], where the emission mechanism of methanol/air mixture have not been fully studied. For instance, the produced intermediate radicals and species (for instance, the mass fraction and reaction rate etc) have not been fully studied. The study of the emission mechanism is the core scientific engineering technology issue for the development of the spark ignition methanol engine, and the findings can provide adequate theoretical guidance to the development of the spark ignition methanol engine. Therefore, it is necessary to study the emission mechanism during combustion.

In this paper, emissions were studied based on LES coupled with methanol chemical kinetics (84-reaction, 21-species) in a developed spark ignition methanol engine. The adopted methanol mechanism was validated through many experimental tests [21]. The results from this study should be valuable in explaining the emission mechanism of methanol fuel during combustion.

Table 2
Engine specifications and conditions.

Engine type	Methanol 4100 series
Engine configuration	Inline four-cylinder, four-stroke, turbocharged and intercooled
Bore (mm)	100
Stroke (mm)	127
Compression ratio	17.5
Displacement (L)	3.99
Chamber shape	ω shape
Chamber diameter (mm)	54.0
Chamber depth (mm)	18.0
Combustion mode	Intake port injection, spark ignition
Rated power (kW)	83
Maximum torque (N·m)	410
Maximum speed (r/min)	2600
Fuel	Methanol

2. Modeling methodology

2.1. LES models

It is important to choose the turbulence model in the study, and the calculated results are different when using different turbulence models. In recent years, LES method is widely used to analyze the turbulent flow in various research fields [22–24]. It is a spatial average of turbulence pulsation (or turbulent vortex), that is, the large-scale vortex and small-scale vortex are separated through some kind of filter functions, and the large-scale vortex is simulated directly, and the small-scale vortex is simulated by using sub-models. Compared with the conventional Reynolds averaged Navier Stokes models, LES has more advantages, for instance, it can simulate the large turbulent structures and strongly separated flows.

The governing equation of LES in this study is:

$$\frac{\partial\left(\overline{u_i}\right)}{\partial t}+\frac{\partial\left(\overline{u_i u_j}\right)}{\partial x_j}=-\frac{1}{\rho}\frac{\partial\overline{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\nu\frac{\partial\overline{u_i}}{\partial x_j}-\left(\underbrace{\overline{u_i u_j}-\overline{u_i}\,\overline{u_j}}_{\tau_{ij}}\right)\right] \tag{1}$$

The equation of sub-grid scale stress tensor is:

$$\tau_{ij}-\frac{1}{3}\tau_{kk}=-2\upsilon_{SGS}S_{ij} \tag{2}$$

The sub-grid scale viscosity is:

$$\upsilon_{SGS}=\left(C_s f\Delta\right)^2|S| \tag{3}$$

where $C_s = 0.1$; $\Delta = (Vol)^{1/3}$, Vol is the volume of calculated cell; $|S| = (2S_{ij}S_{ij})^{1/2}$; $f = 1-exp(y^{+}/25)$.

2.2. Engine model

The specifications of spark ignition methanol engine are listed in Table 2. The methanol engine is modified from a conventional four cylinders, four stroke, and direct injection diesel engine. The spray pattern is changed from the original direct injection mode into the intake port injection mode. Because the cetane number of methanol is very low (the cetane number is only 3), it is difficult to adopt compression ignition combustion mode, so the spark ignition mode is applied in the developed methanol engine. The developed new methanol engine is a four cylinders engine. So, four spark plugs and four injectors are added to the developed methanol engine. The combustion chamber shape is not changed, which is also the ω type.

The simulation is calculated between intake valve closing and exhaust valve opening. The simulated boundary conditions and initial conditions are obtained from the experimental results as well as the calculated results from the one-dimensional (1-D) engine simulation model. The 1-D engine simulation model is established through the GT-Power, and the established 1-D engine simulation model is shown in Fig. 1 [25,26]. The three-dimensional (3-D) simulations are calculated through the CFD (computational