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Full Length Article

Characteristics of evolution of in-cylinder soot particle size and number density in a diesel engine

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ABSTRACT

Particulate matter (PM) emission from diesel engines has been a critical issue due to its environmental impact. The soot size and number density inside the cylinder can severely affect the size and mass of PM emission emitted from the diesel exhaust pipe. In the present study, the temporal and spatial variations of the mean and instantaneous in-cylinder soot size and number density in a single cylinder direct injection diesel engine have been simulated numerically at different operating conditions, injection system parameters, fuel types and piston bowl geometry using AVL-FIRE code. The results show that the engine load has great effects on the mean soot particle size and number density with crank angle while the engine speed and the fuel injection system parameters have no obvious effects on them. It is observed that there is an obvious shift to larger particles at higher load. The mean soot number densities firstly increase with the increase of loads, but decrease at later crank angle. The in-cylinder soot size distribution shows a unimodal shape at different crank angle under all operating conditions. The soot particle numbers are concentrated from the start of combustion to 40 °CA after top dead center (ATDC). The spatial soot particle size distribution in the combustion chamber is closely related to engine load, impinging angle and airflow motion. The piston bowl diameter has large effect on the mean soot size and number density during the latter phase of the expansion stroke. The results also indicate that both in-cylinder mean soot size and number from biodiesel-diesel blends are affected not only by the oxygen content, but also engine operating conditions.

1. Introduction

Diesel engines are still widely employed in transportation and power generation because of their high thermal efficiency, reliability and excellent fuel economy. However, PM emission from diesel engines is one of the main sources of environment pollutants [1]. Particle emissions not only have negative effects on environment but also are toxic to human health. Fine particles can lead to such diseases as respiratory disease, cardiovascular disease and nervous system [2]. It is found that particle toxicity increases with decreasing of its size [3]. Particle emission regulations become more stringent in many countries. Besides the particle mass concentration standard, the particle number (PN) concentration standard was also established in the Euro 5 and Euro 6 emission regulations for light-duty diesel vehicles [4]. Controlling PM emissions are still a dominant research point in development of the diesel engine technology.

Diesel particle filters (DPF), as effective after-treatment devices, are being used in diesel engines to reduce PM emissions. Periodical regeneration behavior of DPF mainly depends on PM oxidative reactivity, which is closely related to PM size and nanostructure properties [5]. Therefore, particle size and PN concentration can represent a critical issue particularly for diesel engines owing to their effect on human health and DPF regeneration.

In the past, many researchers have performed studies to characterize the particle size distribution (PSD). These studies agree that PSD for conventional diesel combustion (CDC) show a bimodal shape, with nucleation (mobility diameter $<$ 50 nm) and accumulation mode (diameter $>$ 50 nm) particles [6]. Tsolakis [7] found that the diesel engine fueled with rapeseed methyl ester emitted particles below 90 nm. Sarvi et al. [8] did large-scale diesel engine experiments and reported the particles between 5 and 250 nm.

Recently, the PSD for diesel engines was concerned under advanced combustion modes, such as partially premixed charge compression ignition (PCCI) [9,10], low temperature combustion (LTC) [11–13], reactivity controlled compression ignition (RCCI) [14–16]. These combustion modes have merits such as the simultaneous reduction potential

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of the exhaust emission and the high thermal efficiency, but the control of the ignition timing and the limited power output involve great challenges. To optimize the combustion process, some necessary measurements were taken such as the adjustment of injection parameters and use of oxygenated fuels. Labecki et al. [17] studied the effects of fuel injection parameters on exhaust soot particle size distribution in diesel engines. They confirmed that the effect of fuel injection timings on the particle number concentration was not clear. Li et al. [18] found that early or late injection at moderate exhaust gas recirculation (EGR) resulted in a simultaneous reduction in soot with accumulation mode. Wei et al. [19] investigated the effects of injection timing on combustion and emissions in a diesel engine fueled with 2,5-dimethylfuran-diesel blends. They reported that injection timing had a distinct effect on PSDs due to different combustion characteristics. Multiple injection strategies are also used to investigate to PSDs. Li et al. [20] reported that the pilot-main injection case could greatly increase the number and mass of particles with the diameter above 100 nm while the main-post injection could reduce them. Jain et al. [12] carried out the experiments at different main-injecting timings, pilot-injection timings and EGR rates. They found that particulate number concentration was the minimum and average particulate size was the maximum at start of pilot injection timing of 40 °CA before top dead center (BTDC). However, the influences of the spray cone angle and hole diameter on particle number and size are not widely reported. Besides, several alternative fuels were used to investigate the PSDs of diesel engines, such as biodiesel [21–24] and alcohols [25–27].

As stated above, diesel exhaust particle number concentration and size at different combustion modes, injection parameters and fuels, have been reviewed in previous research. Furthermore, there is increasing concern regarding the relationship between the particle number and particle size. However, the above mentioned studies were not able to distinguish among in-cylinder mean soot size and number density with crank angle, their instantaneous spatial distribution and statistic PSD. Because of the high-pressure and high-temperature environment, a little work on in-cylinder diesel soot size has been conducted [28–31]. Based on these facts, the objective of this study is to character the evolution of in-cylinder soot size and number under different conditions including operating conditions, injection, nozzle parameters, fuel type and piston bowl geometry. The article's major importance is to provide a better understanding of the behavior of in-cylinder soot particles in a diesel engine combustion chamber and optimization suggestion on reducing soot formation.

2. Model setup and validation

In this paper, the AVL-FIRE CFD tool is used to simulate the combustion process and soot formation in a diesel engine. The engine main parameters are listed in Table 1. Since the piston bowl has a four-hole injector, the computation uses a 90 deg. sector mesh with a single nozzle, shown in Fig. 1. The total number of mesh cells for every computational case is more than 34,000.

Table 1
Main parameters of diesel engine.

Item	Parameters
Number of cylinders	1
Bore × stroke (mm)	86 × 70
Compression ratio	19
Displacement (L)	0.406
Rate power (kW)	5.7
Rate speed (r/min)	3000
Intake valve opening (deg ATDC)	−8.5
Intake valve closing (deg ABDC[a])	44.5
Exhaust valve opening (deg ABDC[a])	−55.5
Exhaust valve closing (deg ATDC)	8.5

[a] ABDC: After Bottom Dead Centre.

This model mainly computes those processes when the intake and exhaust valves are closed. The k-zeta-f model, a four-equation turbulence model, is employed and is more accurate than the k-epsilon model. The hybrid KH-RT model is used to simulate the secondary break-up of droplets. The Dukowicz model is used to describe droplet heat-up and evaporation. The ECFM-3Z (3-zones extended coherent flame model) model is used for premixed and diffusion combustion. Soot is predicted using the Kinetic soot model, which is a reduced model based on a detailed chemical reaction scheme [32–34]. The soot particle parameters such as mean particle size, particle number density and particle size distribution function are constructed with the so called MACRON code in the soot particle size and distribution model [35,36].

In this study, diesel fuel, used the baseline fuel, has the molecular formula $C_{13}H_{23}$. The complete detailed kinetic scheme of the soot formation process incorporates 1850 gas-phase reactions 186 species and 100 heterogeneous reactions [36]. The effect of fuel type on mean soot size and number density was conducted including three blends of biodiesel/diesel in different proportions B10 (10% biodiesel and 90% pure diesel fuel), B20, B50 and B0 (pure diesel). Some important properties of the fuels are given in Table 2.

The piston bowl diameter (Dr) and depth (T) along with the re-entrant bowl radius (R4) and the bowl depth (T) are the four main parameters (as shown in Fig. 1a) modified for their effect on mean soot size and PN within the cylinder. The compression ratio of the engine is locked at 19:1 for all piston models in order to make sure that results are only affected by the geometry.

To verify correctness of the model, computed in-cylinder pressure histories and heat release rate were compared with experimental results. The operating conditions for validation of computation results are given in Table 3. As shown in Fig. 2, the pressure profiles and the combustion phasing were well-predicted for two cases, and the errors between computed and experimental results were considered acceptable for the purpose of this study. Therefore, the computational models and operating conditions of the numerical simulation are credible.

3. Results and discussion

This section describes evolution of the soot size and number density and factors to them in two subsections. The first subsection is mainly about effects of operation conditions on the soot size and number density. The second focuses on effects of injection and nozzle parameters, fuel types and piston bowl geometry on the soot size and number density.

3.1. Effect of engine load and speed on soot mass fraction

Fig. 3 shows the temporal evolution of the soot mass fraction inside the combustion chamber vs. crank angle under different speeds and loads. The soot mass fraction is relatively unaffected by changes in the light and middle loads. However, more soot yields at heavier and full loads due to higher equivalence ratios which dominates mass of soot formation. Except for the case of full loads, the mass fraction of soot shows unimodal distribution and almost keeps a constant value after 40° CA ATDC due to the balance between the soot formation and oxidation. It is also found that the engine speeds have little effects on the soot mass fraction except for the cases of full loads. As can be seen from Fig. 3, the soot mass fraction for the case of 2000 rpm and full load is less than those for the cases of other three speeds and full loads. This is because lower gas-flow velocity at lower engine speeds affects the mixture of fuel and air while the oxidation time at higher engine speeds is shorter. These factors are dominant in lower and higher speeds, respectively.

3.2. Effect of engine load and speed on mean soot size and number density

The temporal evolution of in-cylinder mean soot size and number