



# Structural evolution of soot particles during diesel combustion in a single-cylinder light-duty engine



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## ARTICLE INFO

### Article history:

Received 8 April 2015

Received in revised form 9 April 2015

Accepted 9 April 2015

Available online 23 April 2015

### Keywords:

Diesel combustion

Soot morphology

TEM

Jet-wall interaction

## ABSTRACT

The structural evolution of soot particles in a single-cylinder, light-duty diesel engine has been investigated by conducting thermophoretic soot sampling and subsequent transmission electron microscope (TEM) imaging. The location of TEM grid with respect to a diesel flame is varied so that soot particles are sampled at three different combustion stages including (1) when the impingement of flame on the wall occurs, (2) after the flame impingement, and (3) during the late-cycle burn-out. For comparison purposes, engine-out soot particles are also collected at the same operating conditions. The results show that diesel soot particles are aggregates of varying numbers of primary particles. It is found that the flame impingement on the wall makes a significant impact on the soot aggregate structures, evidenced by the decreased mean radius of gyration of the aggregates from 38 to 26 nm between the wall-impinging and post-impingement stages. This was due primarily to the fragmentation of large soot aggregates while the mean diameter of primary particles remains the same. From the post-impingement to late-cycle burn-out stages, most of the soot aggregates disappear due to the oxidation leaving only highly agglomerated substructures. As a result, soot aggregates show higher fractal dimension in the late-cycle burn-out stage than that in the previous stages. The intensive soot oxidation also reduces primary particle diameter from 19 to 15 nm through surface oxidation. The engine-out soot samples show similar particle size and structure to the late-cycle samples, suggesting that the late-cycle soot particles experienced little oxidation before exiting through the exhaust. This leads to a conclusion that the highly agglomerated substructures of soot aggregates can survive the late-cycle burn-out and become a major contributor to exhaust soot emissions.

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## 1. Introduction

Soot particles are a major portion of particulate matter (PM) emissions from diesel engines [1,2] that are strictly regulated due to their negative impacts on the environment and human health [3–7]. While modern common-rail diesel engines achieve very low soot emissions by mass, ultra-fine soot particles from these engines are suspected to be more toxic due to the increased defects in particle nanostructures and higher surface reactivity [8,9]. This issue presents the need for an improved understanding of the size and structure of soot particles during diesel combustion. The improved knowledge about the soot fractal structures would also help develop soot models to clarify underlying physics [10,11].

The size distribution of diesel soot particles is widely investigated using a scanning mobility particle sizer (SMPS) [12–15]. Also, there are many fine papers reporting the morphology of

exhaust soot particles from a tail-pipe particle sampling and transmission electron microscopy (TEM) imaging [16–22]. However, the soot particles in the exhaust stream represent only the product of complex soot processes that involve multi-stage formation and oxidation steps occurring inside the engine cylinder. For example, Tree and Svensson [1] summarised that during diesel combustion, soot is formed from the super-saturated gas-phase precursors in fuel-rich reaction zones and then undergoes nucleation, coalescence, agglomeration as well as oxidation inside engine cylinder before exiting through the exhaust. Therefore, the exhaust soot particles provide limited information about the structural evolution of soot particles during formation and oxidation processes.

The in-flame soot is widely investigated using optical/laser-based diagnostics for the measurement of soot area, optical thickness (i.e., KL value), soot volume fraction, and the size of soot particles [23–27]. However, the information about particle structures was very limited until a direct soot particle sampling from a quasi-steady diesel jet flame and subsequent TEM imaging was implemented in a constant-volume combustion vessel [28–31],

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which provided an improved understanding of size and structures of in-flame soot particles. For instance, soot precursor-like structures are found immediate downstream of the flame base while aggregates of soot primary particles with complex fractal structures dominate at the peak soot volume fraction location. In the jet head region, smaller size and simpler structure aggregates are observed, evidencing soot oxidation. Soot morphology was also studied in a working diesel engine using a bulk-gas sampling technique [32–35], which reported the decreased primary particle size and the increased aggregate fractal dimension during diesel combustion. However, this bulk-gas sampling approach raises a question about whether or not the structures of soot particles were affected by the sampling process. Our previous study addressed this issue by placing a TEM grid within the flame for direct sampling of soot particle via thermophoresis (i.e., positive thermal diffusion) [36]. This sampling technique has been used to understand structural changes of in-flame soot particles for various engine operating conditions [37,38].

The present study further utilises this in-flame soot sampling technique to better understand the structural evolution of soot particles occurring inside the cylinder of a diesel engine. Of particular interest is how the flame impingement on the wall impacts the soot particle morphology. The flame–wall interaction is well known to influence local fuel/air mixing and flame temperature significantly which in turn affects combustion and soot processes [39–47]. This question was addressed by sampling the in-flame soot particles at two different combustion stages including (1) when the diesel flame impinges on the wall and (2) after the flame–wall impingement. Moreover, the location of the TEM grid with respect to the flame is varied so that soot particles are sampled in the late-cycle burn-out stage. For comparison purposes, engine-out soot particles are also collected at the same operating conditions.

## 2. Experiments

### 2.1. Engine specifications and operating conditions

The engine and soot particles sampling system are illustrated in Fig. 1. The specifications and operating conditions are summarised in Table 1. Soot sampling experiments were carried out in an optically accessible, single-cylinder, small-bore diesel engine. Figure 1 shows two soot sampling probes that were used to hold a TEM grid; one probe was installed on the cylinder liner by replacing one of four quartz windows and the other probe was installed in the exhaust manifold. To enable in-flame soot sampling while the engine was running, a portion of the piston bowl-rim (30-mm wide) was removed. This was to avoid the potential crash between the sampling probe and fast-moving engine parts such as the piston and intake/exhaust valves. This piston modification resulted in a reduced compression ratio of 15.2, which is still relevant to the production engines of today. The swirl ratio of the engine was fixed at 1.4. Heated water of 90 °C temperature constantly flowed through the cylinder liner and engine head to simulate a thermally-stable, warmed-up engine condition. The engine was naturally aspirated and the air temperature at the intake port was measured at 30 °C throughout the experiments. All tests were conducted at fixed engine speed of 1200 revolution per minute (rpm) using a 37-kW AC motor.

A second-generation Bosch common-rail injection system was used to deliver ultra-low-sulphur diesel fuel with cetane number of 51. The original injector had a 7-hole nozzle with the same inter-jet spacing and a 150° included angle. Similar to our previous studies [36,37], the nozzle was modified for single-hole injection by blocking six holes using a laser-welding technique. This

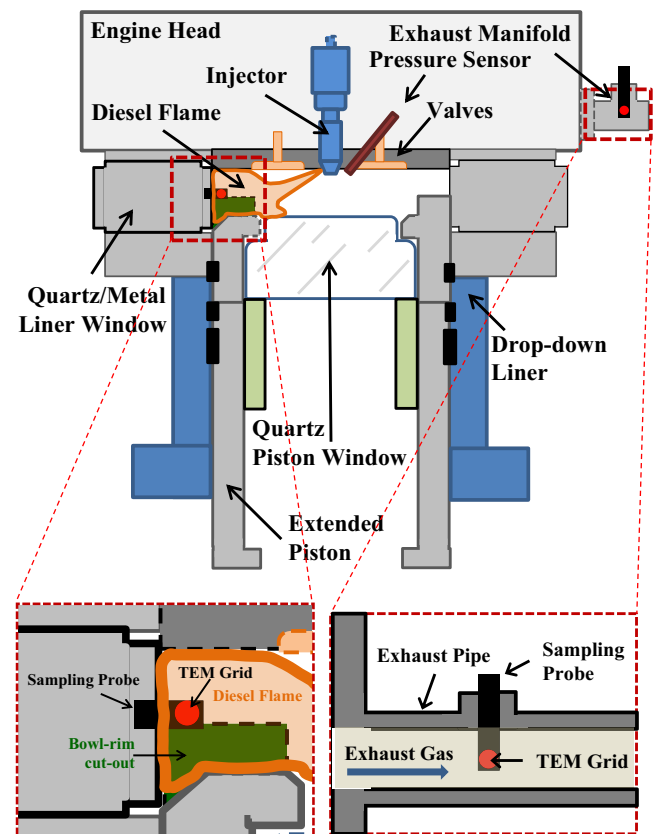


Fig. 1. Cross-sectional sketch of the diesel engine (top) and the close-up views of the soot sampling regions inside the cylinder (bottom left) and exhaust (bottom right).

Table 1

Engine specifications and operating conditions.

Displacement volume	498 cm <sup>3</sup> (single cylinder)
Bore/stroke	83 mm/92 mm
Compression ratio	15.2
Swirl ratio	1.4
Coolant temperature	90 °C
Intake air temperature	30 °C
Engine speed	1200 rpm
Injection system	Bosch second-generation common-rail injector
Fuel	Ultra-low-sulphur diesel
Cetane number	51
Nozzle hole diameter	134 μm (nominal)
Mass per injection	9 mg
Injection pressure	70 MPa
Injection timing	−7°CA aTDC

approach was to isolate a single diesel jet from complex jet–jet interactions and at the same time to allow for long injection duration while keeping the in-cylinder pressure below the burst pressure of the quartz windows. The injection duration of 2.34 ms (actual) was selected for all tested conditions in the present study. At 70-MPa injection pressure, this injection duration corresponds to 9 mg of diesel fuel per injection for a single hole. If all 7 holes were used, the injected mass would be relevant to upper-mid to high-load conditions where soot emissions are most problematic. The injection timing was fixed at −7 crank angles after the top dead centre of the compression stroke (°CA aTDC). Throughout the experiments, the in-cylinder phenomena were monitored by measuring in-cylinder pressure at various crank angle locations using a piezo-electric pressure transducer (Kistler 6056A). The measured in-cylinder pressure traces were used to calculate

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