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Modelling of soot formation in a heavy-duty diesel engine with conditional moment closure

Q1 Michele Bolla *, Daniele Farrace, Yuri M. Wright, Konstantinos Boulouchos

Q2 *Swiss Federal Institute of Technology, ETH Zurich, Switzerland*

HIGHLIGHTS

- First application of multidimensional CMC model for soot to diesel engine.
- Comparison of quantitative in-cylinder soot, pressure and AHRR evolutions.
- Methodology for derivation of line-of-sight "numerical soot luminosity".
- Spatial soot predictions validated by optical data for 5 reference cases.
- In-sights into soot inception, formation and oxidation modelling uncertainties.

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ABSTRACT

This study presents the first application of a multidimensional conditional moment closure (CMC) combustion with a two-equation soot model to study the evolution of in-cylinder soot in diesel engines. Five high-fidelity reference cases from an optically accessible heavy-duty diesel engine were used to validate the model predictions; these include two high-temperature cases and two low-temperature cases with two different injection timings and one low-temperature case with a split injection strategy. Simulation results have been compared with experimental data by means of non-reactive fuel vapour distribution, apparent heat release rates (AHRR), temporal evolutions of quantitative in-cylinder soot mass and natural luminosity. The model was capable to reproduce semi-quantitative trends of soot mass for all five cases. In particular for low-temperature conditions the evolution of soot formation and oxidation is very well captured. A line-of-sight transformation of the computed 3D soot is proposed to ensure a consistent comparison with the measured 2D soot natural luminosity images. With this methodology additional effects related to radiation adsorption were observed. Evolutions of line-of-sight soot natural luminosity were qualitatively very well reproduced. Overall the findings suggest that the presented two-equation soot model implemented in the CMC framework is a highly promising candidate for predicting time evolutions of in-cylinder soot for diesel engines operating in different combustion modes.

1. Introduction

Diesel engines are among the highest efficiency energy conversion devices and therefore heavily relied upon for power generation, seaborne and land transport for freight as well as for passenger cars. The success of the quality controlled, non-premixed operation is however aggravated by significant in-cylinder emissions due to rich and lean regions of the combustion zones leading to substantial amounts of soot and nitric oxides. Soot is particularly difficult to model because most of the soot, which is formed during the mixing controlled part of the combustion, is oxidised after end of injection (EOI) [1]. Therefore an improved understanding of the in-cylinder processes is needed to further develop simulation tools towards reliable predictions for wide ranges of operating conditions and hence aiding in the development of future lowest emission diesel engines.

Traditionally soot is measured in the exhaust by means of smoke meters or photo-acoustic methods, both of which return the net soot amount, i.e. the difference between the soot generated and oxidised. As a consequence, no isolation of effects is possible which would allow for an independent validation of the soot formation and oxidation models. Optically accessible test rigs and engines in conjunction with the emergence of cycle-resolved measurement techniques and high-speed imaging in recent years has significantly improved the situation with respect to the availability of large data-sets for validation of models under well-controlled conditions with quantifiable measurement

* Corresponding author. Address: ETH Zurich, Institute of Energy Technology, Aerothermochemistry and Combustion Systems Laboratory, ML L20, Sonneggstrasse 3, CH-8092 Zurich, Switzerland. Tel.: +41 1 632 49 80. Q3
E-mail address: mbolla@lav.mavt.ethz.ch (M. Bolla).

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uncertainties. It should be noted however, that the major advantage of optical accessibility lies not solely in the provision of additional spatial and temporal information relating to soot and hence complementing tail-pipe measurements. Important benefits stem from the fact that all the important pre-processes leading to soot, viz. spray morphology development, ignition location and subsequent flame structure evolution can be recorded as well, processes which greatly affect soot formation and oxidation and hence call for well validated, high fidelity models. Experimental work done at the Sandia optical heavy-duty diesel engine has contributed to an improved understanding of in-cylinder processes resulting in conceptual models for conventional [2] as well as for advanced combustion strategies, e.g. for low-temperature combustion (LTC) with early [3] and with split injection [4] and for which a review can be found in [5,6]. In recent years this engine has received increasing interest for model validation purposes, e.g. [7–14]. Predictions of soot emissions have been attempted with different combustion models and with different fuel chemical mechanisms as well as soot precursor chemistry complexities [7,9,11,12,14].

Despite the large amount of soot related studies, most of them reported normalised soot evolutions for comparison with the engine in-cylinder data. To the authors' best knowledge only in [12] soot results have been compared quantitatively for 4 of the 5 reference cases from [15]. Motivated by the results achieved in a previous study [16] reporting semi-quantitative soot distributions for an optically accessible spray combustion chamber at diesel like conditions, in this study all five 'reference' cases from [15] are investigated. The methodology follows the one from [16] and employs a two-equation soot model implemented in the context of conditional moment closure (CMC). The latter combustion model has seen successful application to various gaseous flame configurations for which a comprehensive review is presented in [17], and has also been used to study spray autoignition at diesel engine conditions in generic test rigs [18–22] and in real diesel engines [23–25]. Due to the proven predictive capability of CMC concerning many of the pre-processes such as ignition delay and location, flame lift-off length and flame structure, the approach has demonstrated much promise also for the prediction of soot [16] in a generic spray test rig. This study represents the first assessment of soot formation with a two-phase multidimensional CMC formulation in a diesel engine. In addition, a methodology is presented which enables comparisons between the predicted soot distributions with the measured spatial evolution of soot natural luminosity.

The remainder of this paper is structured as follows: first a short description of the experimental setup and test cases considered is presented, followed by the model formulation. The results start from a spray validation study for non-reactive conditions; followed by an analysis of the 'integral' engine quantities, i.e. pressure traces and AHRR for the 5 operating conditions. Subsequently, a comparison of both integrated as well as spatial distributions of the soot evolutions is presented and discussed also in the context of conceptual models presented in the literature. The paper closes with concluding remarks.

2. Experimental setup

Experimental data available from the optically accessible heavy-duty diesel engine installed at Sandia National Laboratories [15] has been used for model validation. The measurements were obtained on a single-cylinder, common-rail, direct-injection heavy-duty diesel engine based on a Cummins N-series with 139.7 mm bore and 2.34 l displacement. The main specifications of the engine and injector are summarised in Table 1. To minimise thermal loading the engine was operated skip fired where every tenth cycle was fired. The injector has eight equally spaced orifices with a nominal diameter of 0.196 mm. An ultra-low sulphur diesel fuel was employed for which the specification is given in [3]. Optical access is provided by an extended piston and a flat piston-crown window for signal collection as well as windows located around the top of the cylinder-wall for laser-based imaging diagnostics. For a detailed description of the engine specifications and diagnostics employed the reader is referred to [3] and references therein.

Table 1
Engine and injector specifications.

Engine type base	Cummins N-14, Diesel
Swirl ratio	0.5
Bore × stroke (mm)	139.7 × 152.4
Bowl width, depth (mm)	97.8, 15.5
Displacement (L)	2.34
Geometric compression ratio	11.2
Fuel injector type	Common rail
Fuel	Diesel #2
Number of holes	8, equally spaced
Spray included angle	152°
Nozzle orifice diameter [mm]	0.196
Nozzle orifice L/D	5

In this study, all five 'reference' cases reported in [15] have been considered (cf. Table 2). These consist of two high temperature combustion (HTC) cases with different ignition delays, two low temperature (LTC) cases with different start of injection and a LTC case with split injection. HTC and LTC refer to the different adiabatic temperatures as a consequence of the oxygen concentration in the oxidizer caused by dilution. The latter is normally achieved by exhaust gas recirculation; for this engine, pure N_2 is employed due to the skip-fired operation.

The two HTC conditions correspond to 'classical' diesel combustion, which is characterised by a premixed combustion phase followed by mixing controlled energy conversion; the respective modal split for these two cases is 32%/68% and 85%/15%. The LTC cases have been chosen to represent three alternative combustion concepts proposed in the literature, all of which attempt to simultaneously reduce soot and NOx, namely the so-called "Premixed lean diesel combustion", the "Modulated Kinetics" approach as well as the "UNIBUS" concept. For references and further discussion to these combustion strategies the reader is referred to [15].

All cases have been run at a constant engine speed of 1200 RPM. Due to the profound differences in both oxidizer reactivity as well as ignition delays, the operating conditions span between almost fully premixed type combustion to a combination of premixed/diffusion combustion modes. As a consequence, this dataset sets very high requirements for the numerical model.

3. Numerical methodology

The numerical methodology consists of the widely adopted CFD solver STAR-CD coupled with an elliptic first order CMC combustion model augmented by a two-equation soot model. The latter is also solved in the CMC context – as will be discussed next – and hence is not among the "post-processing type" emission models commonly used on the CFD side.

3.1. CMC formulation

The conditional moment closure belongs to the class of presumed PDF methods. In the cases of non-premixed combustion the gas-phase mixture fraction is used as conditional quantity. Transport equations are solved for conditionally averaged reactive scalars. The reader is referred to [26] for a detailed derivation of the CMC governing equations; here only a brief presentation of the

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