

# Predicting In-Cylinder Soot in a Heavy-Duty Diesel Engine for Variations in SOI and TDC Temperature Using the Conditional Moment Closure Model

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## ABSTRACT

Numerical simulations of in-cylinder soot evolution in the optically accessible heavy-duty diesel engine of Sandia National Laboratories have been performed with the multidimensional conditional moment closure (CMC) model using a reduced *n*-heptane chemical mechanism coupled with a two-equation soot model. Simulation results are compared to the high-fidelity experimental data by means of pressure traces, apparent heat release rate (AHRR) and time-resolved in-cylinder soot mass derived from optical soot luminosity and multiple wavelength pyrometry in conjunction with high speed soot cloud imaging. In addition, spatial distributions of soot relevant quantities are given for several operating conditions.

A broad range of operating conditions has been considered: a sweep in start of injection (SOI) at unchanged top dead center (TDC) ambient conditions and a sweep in TDC temperature at an ambient oxygen volume fraction of 12.7 percent, corresponding to a high level of exhaust gas recirculation (EGR). Ignition delays were captured very well, using unaltered model constants and kinetic parameters. The model was found to reproduce pressure and AHRR traces fairly well, although the premixed portion of combustion was in general slightly underpredicted. Concerning emissions, a quantitative comparison of soot mass evolution is presented. Considering the broad range of conditions the model was capable to reproduce the soot trends well; the predicted peak soot mass agreed within a factor of approximately two for almost all operating conditions considered.

Overall, the findings suggest that the presented semi-empirical soot model integrated into the CMC framework is a highly promising approach for the prediction of in-cylinder soot evolution for various diesel engine operating conditions.

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## INTRODUCTION

In the last decades, diesel engines have undergone a wide diffusion in both industrial and private related applications due to their high reliability and operational flexibility, but also due to their high energy conversion efficiency. In conjunction with low production and maintenance costs, these factors allowed their fast spread in stationary energy

production facilities, sea and on-road transportation, as well as for passenger cars. However, the complex characteristics of diesel combustion are further complicated by significant pollutant emissions, which are formed on the fuel rich and lean sides of the flame leading to high amounts of soot and nitrogen oxides. Recent legislations concerning pollutant emissions have inspired research towards a deeper understanding of in-cylinder emissions formation processes,

with the purpose of their minimization. Since soot related processes lie at the end of the chain of combustion events, physical understanding of all affecting phenomena is essential in order to identify the most suitable strategies for pollutants abatement. In this context, an increasing part of engine research is conducted using CFD tools. Supporting experimental investigation, numerical simulations allow for deep analysis of all in-cylinder events, however models validation is a prerequisite to ensure reliable and accurate predictions. In this sense, optically accessible experimental test rigs in conjunction with high-speed imaging permit cycle-resolved measurements and two-dimensional visualizations of many in-cylinder processes, creating a large database available for CFD validation.

In recent years, the engine facilities installed at the Sandia National Laboratories have attracted increasing interest by the combustion community mostly due to their high-fidelity experimental data; the Sandia heavy-duty optical diesel engine in particular has been widely referenced for validation purposes, e.g. [1, 2, 3, 4, 5, 6, 7]. These studies employ a variety of combustion models, which include eddy dissipation concepts as well as more sophisticated approaches allowing for the inclusion of detailed chemistry, namely flamelet models and direct integration (also termed “well-mixed” model, which neglects turbulence-chemistry interaction). Specifically with respect to soot processes, Pang [8] investigated the influence of model constants for a soot model based on Moss-Brookes and reported normalized in-cylinder soot evolutions. Quantitative in-cylinder soot mass evolution predictions have been presented in [5]. The five “reference cases” of this engine have been investigated with respect to soot formation in [9], where a conditional moment closure combustion (CMC) model coupled with the two-equation soot model proposed by Leung [10] was used to model quantitative in-cylinder soot mass. The latter combustion model has seen successful application to various gaseous flame configurations for which a comprehensive review is presented in [11], and has also been used to study different auto-igniting sprays at diesel engine conditions in generic test rigs [12, 13, 14, 15, 16, 17] and in real diesel engines [18, 19]. Motivated by the results shown in [9] showing comparisons of quantitative in-cylinder soot mass evolutions for all five “reference cases” from [20] and demonstrating highly promising capabilities of the mentioned combustion and soot model, the primary motivation of this work is to validate the same numerical platform for a substantially broader range of engine operating conditions. To this end, two different paths are followed: I) a sweep in start of injection (SOI) starting from  $-12^\circ$  crank angle (CA) up to the misfire limit at  $+15.5^\circ$  CA after top dead center for constant TDC temperature. II) an ignition delay sweep which is “actuated” experimentally by modifying the TDC temperature (from 1000 K down to 800 K) while maintaining the same ambient density and injection profile. The first sweep has already been studied by Yoshikawa and Reitz [6] where particular attention was placed on the effect of

radiation on  $\text{NO}_x$  formation. On the contrary, to the authors' best knowledge, no numerical work has been presented to date for the TDC temperature sweep, where the high EGR rate represents an additional challenge in terms of soot prediction.

The remainder of this paper is structured as follows: initially the model formulation is briefly explained, followed by a short description of the considered operating conditions. Then, the results are compared with experimental data in terms of ‘global’ quantities, i.e. evolutions of pressure, AHRR and in-cylinder soot, first for the SOI and then for the TDC temperature sweep. For the former, also the simulated exhaust NO levels trends are presented. Subsequently, the spatial distributions of soot relevant quantities for a selection of six different operating conditions are presented and discussed. The paper closes with concluding remarks.

## NUMERICAL METHODOLOGY

### Flow Field Solver

The commercial CFD solver STAR-CD [21] has been used for the calculation of the turbulent two-phase flow field. Reynolds Averaged Navier Stokes (RANS) equations are solved and turbulence is treated by means of the RNG variant of the  $k$ - $\epsilon$  model with the corresponding ‘standard’ wall functions [21]. Due to the symmetric arrangement of the injector in the cylinder head with eight equally spaced orifices, only one eighth of the combustion chamber is discretized. Simulation of the intake and exhaust strokes has not been attempted, therefore a flat firedeck without valves/pockets is considered, as it is common practice. Figure 1 displays the computational mesh at TDC. Drawn in black is the 3D CFD grid and overlaid in red is the coarser 2D CMC grid (discussed in the “CMC formulation” section below). The CFD characteristic mesh size within the piston bowl is  $1 \times 1 \times 1 \text{ mm}^3$  and in the sweep volume of  $1 \times 1 \times 1.3 \text{ mm}^3$ , resulting in approximately 50,000 cells at TDC and 240,000 cells at bottom dead center (BDC). Note that, for simplicity, the crevice length has been reduced and its width has been increased in order to maintain the same crevice volume and therefore the same geometric compression ratio.

The STAR-CD built-in Lagrangian-Eulerian formulation is employed for the two-phase treatment. For atomization, the widely adopted ‘blob’ model is used and the secondary breakup of droplets is modeled according to Reitz-Diwakar [22]. Possible impingement of droplets with solid walls is treated with the splashing model of Bai. For droplet drag and heat/mass transfer the standard correlations implemented in STAR-CD have been activated. Further details as well as references to the respective models can be found in [21]. Droplet thermo-physical properties have been approximated by  $n$ -dodecane, for which STAR-CD internally calculates the relevant quantities as a function of temperature ( $c_p$ , viscosity, latent heat, vapor pressure, density and surface tension).

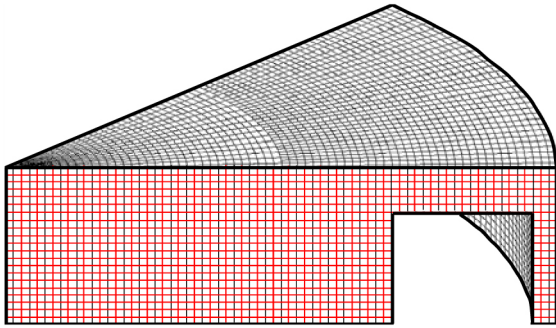


**Figure 1. Mesh of engine geometry at TDC. In black is the CFD grid with the CMC grid overlaid in red.**

The ‘chemico-thermal’ enthalpy equation is transported by STAR-CD employing polynomial  $c_p$  for species. For the latter, no transport equations are solved, since the respective mass fractions are obtained by convolution of the conditional values with the mixture fraction Probability Density Function (PDF). Here, a beta-function is adopted, which is reconstructed by the mean and variance of mixture fraction solved as follows (eqs. (1) and (2), respectively):

$$\frac{\partial \bar{\rho} \tilde{\xi}}{\partial t} + \nabla \left[ \bar{\rho} \tilde{u}_j \tilde{\xi} - \left( \bar{\rho} D_{\tilde{\xi}} + \frac{\mu_t}{Sc_{\tilde{\xi}}} \right) \nabla \tilde{\xi} \right] = \dot{S}_d \quad (1)$$

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{\xi}^{\prime 2}}{\partial t} + \nabla \left[ \bar{\rho} \tilde{u}_j \tilde{\xi}^{\prime 2} - \left( \bar{\rho} D_{\tilde{\xi}^{\prime 2}} + \frac{\mu_t}{Sc_{\tilde{\xi}^{\prime 2}}} \right) \nabla \tilde{\xi}^{\prime 2} \right] \\ = \frac{2\mu_t}{Sc_{\tilde{\xi}^{\prime 2}}} (\nabla \tilde{\xi})^2 - \bar{\rho} \tilde{\chi} \end{aligned} \quad (2)$$

The mixture fraction equation is subjected to a source term due to droplet evaporation (RHS in eq. (1)). On the other hand, no effects of evaporating droplets have been considered in the mixture fraction variance equation since no consensus has been reached hereto and their impact was found to be negligible at similar conditions in [13]. The second term on the RHS in equation (2) denotes the scalar dissipation rate (SDR), which is determined using turbulence quantities, i.e. the turbulent kinetic energy,  $k$ , and its dissipation rate,  $\epsilon$ ,

$$\tilde{\chi} = c_{\chi} \frac{\tilde{\epsilon}}{\tilde{k}} \quad (3)$$

where  $c_{\chi}$  is a model constant set to 2.0 as is common practice.

## CMC Formulation

The combustion model employed belongs to the group of presumed PDF methods. In the case of non-premixed

combustion, the mixture fraction is used as the conditioning parameter. The original governing equations as well as their derivation were originally put forward in [23], while details concerning the implementation and specifics for engine application are well documented in [18, 19] and are hence not repeated here. Transport equations for species and temperature are solved for conditionally averaged species and temperature in each CMC cell. The CMC equations are discretized with finite differences and a second order scheme for the diffusion terms is employed while convective terms are treated with a first order upwind scheme. Time integration is performed by means of a stiff integrator DVODE using a full operator splitting technique. The mixture fraction space is discretized into 101 grid points clustered around the stoichiometric value. Further details concerning sub-models and implementation can be found in [12, 15, 18].

As spatial fluctuations of conditional quantities are much weaker than their corresponding unconditional values [23], a coarser spatial resolution can be employed for the CMC grid compared to the CFD mesh. Results presented in former investigations showed that a two-dimensional CMC formulation is appropriate for simulations of diesel engines [9, 18, 19]. This approach is consequently also followed in this study where the azimuthal direction has been collapsed, allowing for substantial savings in computational costs. In Figure 1 the 2D CMC mesh at TDC is shown in red, where in the piston bowl volume a constant CMC spatial resolution of 1 mm by 2 mm in the cylinder axial and radial directions respectively is employed. This results in 35×20 CMC cells at TDC, whereas during the compression/expansion strokes, CMC cells layers are removed/added as described in [18] in analogy to the CFD cell layer addition.

Quantities required at the coarser CMC grid resolution (e.g. scalar dissipation rate, conditional velocities etc.) are obtained by means of PDF weighted volume averaging of the respective quantities from the corresponding finer CFD grid cells. The unconditional species mass fractions (Favre averages) returned to the flow field solver are calculated by means of convoluting the conditional quantities with the beta PDF in each CFD cell. Additional details concerning the derivations can be found in [18], while a schematic concerning the mapping is given in [19].

With these CFD and CMC grid resolutions, the computational cost from IVC up to 50 °CA aTDC amounts to roughly 20 hours on 16 processors.

## Chemical Mechanisms and NO Modeling

Concerning the oxidation chemistry, *n*-heptane has been used to represent the D2 fuel used in the experiment, since it has seen successful application to diesel engine combustion with CMC in [19] using kinetics from [24]. Here, the reduced chemistry documented in [25] has been adopted, mainly due to its computational efficiency and further motivated by the good performance shown in [16] when compared to two larger *n*-heptane mechanisms applied to diesel sprays for a broad range of engine relevant conditions in a constant-

volume optically accessible test rig. In the absence of chemical kinetics for fuel surrogates which are tractable in the framework of 3D-CFD calculations in engines, the use of *n*-heptane to model diesel combustion is common practice, as is evident from other studies for this engine, see e.g. [2, 3, 4, 5, 6].

Concerning NO modelling, in this study a post-processing methodology has been chosen, which calculates NO formation at the CFD resolution based on the Favre averaged temperatures and species mass fractions. It considers only thermal NO and employs the following rate expression from [26]:

$$\frac{d[NO]}{dt} = 2k_1[O][N_2] \quad (4)$$

This approach is in contrast to the methodology utilised in [19] with the same combustion model where a) a detailed NO<sub>x</sub> sub-mechanism (included in the chemical scheme of [24]) was used which accounts also for prompt NO and NO re-burn and b) all NO relevant processes were solved in mixture fraction space. As the main focus of this investigation is the validation of in-cylinder soot evolutions for a broad range of conditions, and since experimental data for NO is only available for the SOI sweep, in a first step a simple NO model has been adopted.

## Soot Model

Soot was modeled according to the semi-empirical two-equation approach first proposed by Leung et al. [10]. Transport equations in mixture fraction space are solved for conditional soot mass fraction and soot number density (eq. (5)).

$$\begin{aligned} \frac{\partial Q_s}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_s}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_s}{\partial \eta^2} \\ + \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[ \langle \rho u_i Y_s'' | \eta \rangle \tilde{P}(\eta) \right] = \langle w_s | \eta \rangle \end{aligned} \quad (5)$$

In analogy to other chemical species, the soot transport equations include terms accounting for spatial convection and diffusion as well as for molecular mixing (the second, third and fourth term in the LHS of equation (5), respectively). This equation is the same as for the other chemical species apart from the chemical source term  $w_s$  describing soot sub-processes. The model accounts for simultaneous soot particle inception, surface growth, coagulation and oxidation by O<sub>2</sub> and OH. This leads to source terms in the soot mass fraction, eq. (6), as follows:

$$\begin{aligned} \langle w_{Y_s} | \eta \rangle = \langle w_{Y_s,inc} | \eta \rangle + \langle w_{Y_s,gro} | \eta \rangle + \\ \langle w_{Y_s,oxidO_2} | \eta \rangle + \langle w_{Y_s,oxidOH} | \eta \rangle \end{aligned} \quad (6)$$

and for the particle number density (eq. (7)) as:

$$\langle w_{N_s} | \eta \rangle = \langle w_{N_s,inc} | \eta \rangle + \langle w_{N_s,coag} | \eta \rangle \quad (7)$$

As soot mass diffusivity is comparatively low due to the high density, soot exhibits a Lewis number higher than unity. Modeling approaches for this soot differential diffusion effect in a mixture fraction based framework have been proposed in the literature (e.g. [27, 28]). However, at diesel engine conditions no validated closures exist hereto which account for differential diffusion. In this study a unity Lewis number has been assumed motivated by the good agreement of soot distributions and quantitative levels demonstrated in a previous study for a constant volume test rig [14] and at the current engine [9].

**Table 1. Soot chemistry mechanism.**

|       |                                                              |
|-------|--------------------------------------------------------------|
| (I)   | $C_2H_2 \xrightarrow{R_{inc}} 2C_{(s)} + H_2$                |
| (II)  | $C_2H_2 + nC_{(s)} \xrightarrow{R_{gro}} (n+2)C_{(s)} + H_2$ |
| (III) | $C_{(s)} + 0.5O_2 \xrightarrow{R_{oxidO_2}} CO$              |
| (IV)  | $C_{(s)} + OH \xrightarrow{R_{oxidOH}} CO + H$               |

Acetylene has been considered for both soot inception and surface growth. Chemical reactions involved in the soot mechanism and the corresponding rates are summarized in Table 1 and Table 2 and are identical to the ones employed in [9].

**Table 2. Reaction rate constants in Arrhenius form,  $k_j = A \cdot T^b \cdot \exp(-T_a/T) \cdot S_{Soot}^C$**

|       | $k_j$         | A     | b   | $T_a$  | C   |
|-------|---------------|-------|-----|--------|-----|
| (I)   | $k_{inc}$     | 1.0e4 | 0   | 21,100 | 0   |
| (II)  | $k_{gro}$     | 6.0e3 | 0   | 12,100 | 0.5 |
| (III) | $k_{oxidO_2}$ | 1.0e4 | 0.5 | 19,800 | 1   |
| (IV)  | $k_{oxidOH}$  | 0.36  | 0.5 | 0      | 1   |

Concerning the soot number density transport equation, a primary soot particle is assumed to consist of 100 C-atoms as proposed in [10] resulting in a primary particle diameter of 1.28 nm. Coagulation is the only process that acts as a sink for the particles number and the corresponding rate is computed as:

$$\langle w_{N_s,coagulation} | \eta \rangle = -c_a \left( \frac{24R}{\rho_s N_A} \right)^{\frac{1}{2}} \left( \frac{6}{\pi \rho_s} \right)^{\frac{1}{6}} T^{\frac{1}{2}} (\rho \langle Y_s | \eta \rangle)^{\frac{1}{6}} \langle N_s | \eta \rangle^{\frac{11}{6}} \quad (8)$$

where  $N_A$  is the Avogadro number,  $R$  is the universal gas constant and  $C_a$  is a model constant set to 3 according to [29].

## EXPERIMENTAL SETUP

Experimental high-fidelity data from the optically accessible heavy-duty diesel engine installed at Sandia National Laboratories have been used for comparison with the simulation results. The engine setup consists of a single cylinder, common-rail diesel engine with eight equally spaced injector orifices; further engine and injector specifications are listed in Table 3.

**Table 3. Engine and injector specifications.**

|                              |                   |
|------------------------------|-------------------|
| Engine type base             | Cummins N-14      |
| Swirl ratio                  | 0.5               |
| Bore x Stroke [mm]           | 139.7 x 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                 |

**Table 4. Engine operating conditions considered. "S" refers to SOI sweep and "T" to TDC temperature sweep.**

| Case | Speed<br>[rpm] | O <sub>2</sub><br>[%-vol] | T <sub>TDC</sub><br>[K] | SOI<br>[°CA] | DOI<br>[°CA] |
|------|----------------|---------------------------|-------------------------|--------------|--------------|
| S1   | 1200           | 21                        | 900                     | -12          | 10           |
| S2   | 1200           | 21                        | 900                     | -7           | 10           |
| S3   | 1200           | 21                        | 900                     | -2           | 10           |
| S4   | 1200           | 21                        | 900                     | 3            | 10           |
| S5   | 1200           | 21                        | 900                     | 8            | 10           |
| S6   | 1200           | 21                        | 900                     | 13           | 10           |
| S7   | 1200           | 21                        | 900                     | 15           | 10           |
| S8   | 1200           | 21                        | 900                     | 15.5         | 10           |
| T1   | 1200           | 12.7                      | 1000                    | -5           | 10           |
| T2   | 1200           | 12.7                      | 950                     | -5           | 10           |
| T3   | 1200           | 12.7                      | 850                     | -5           | 10           |
| T4   | 1200           | 12.7                      | 800                     | -5           | 10           |

In order to minimize thermal loading, the engine was operated in a skip-fired mode, i.e. combustion occurred every ten cycles. For this reason, a conventional EGR system was technically not possible. EGR is thus mimicked by diluting the intake air with N<sub>2</sub> in order to obtain the desired O<sub>2</sub> concentration. Optical access was gained through the flat piston surface window as well as through windows located on the cylinder head. Different measurement techniques have been employed to evaluate most of the combustion relevant quantities; a detailed description can be found in e.g. [30] and references therein and are not repeated here.

In this study, twelve different cases have been considered: a SOI sweep at a constant nominal TDC temperature of 900 K without EGR [31] and a nominal TDC temperature sweep with unaltered TDC ambient density and injection strategy for an oxygen volume fraction of 12.7 % [30]. The main operating conditions and parameters are listed in Table 4. The engine was run at a speed of 1200 RPM with a TDC nominal motored density of approximately 23 kg/m<sup>3</sup> for all cases, ensuring similar spray penetrations. The nominal gross indicated mean effective pressures (GIMEP) were around 4 bar and 6 bar while the injected fuel masses were 58.1 mg and 74.5 mg for the SOI sweep and the TDC temperature sweep, respectively. The rail pressure was kept constant at 1200 bar for all cases.

## RESULTS AND DISCUSSION

This chapter is divided into two main sections: the SOI sweep and the TDC temperature sweep are first presented and then computed soot relevant scalars distributions are discussed. Simulation results are compared by means of pressure, AHRR and in-cylinder quantitative soot evolutions. For the SOI sweep the exhaust NO trend is also given.

As discussed above, this work employs a well-proven CMC combustion model with an integrated soot model which has seen highly successful application to steady sprays in test-rigs [14] and a first validation by means of five 'reference' conditions of the current heavy-duty engine in [9]. In the latter study, the spray model predictions have been carefully validated by means of non-reactive spray liquid/vapor penetration length and mixture equivalence ratio in three different horizontal planes. Since the chosen mesh represented a good trade-off between accuracy and computational cost, the same grid resolution has been employed here as well.

### Start Of Injection Sweep

Figure 2 shows the comparison between the computed (solid lines) and the measured (dashed lines) pressure traces for different SOI timings while keeping intake conditions unchanged. Nominal motored in-cylinder temperature and pressure at TDC are 900 K and 65 bar. As is evident from Figure 2, the predicted in-cylinder pressure evolutions agree well with the experimental data over the whole SOI sweep range, with the exception of the latest SOI point. For the most extreme case, at SOI 15.5 °CA, the simulation is not able to predict auto-ignition and only a very small part of fuel is converted as can be seen from the small pressure increase from 35 °CA onwards. It is important to note however, that even the experiment is very sensitive to small advances/delays of the SOI close to the misfire limit.

Figure 3 presents the ignition delay (ID) trend by varying the SOI. The ID is defined by the first positive AHRR in the experiment; the simulation considers the time instant of maximal rate of increase of AHRR. The experiments revealed a minimum in ID at -7 and -2 °CA and a considerable