

Numerical Study of the Influence of EGR on In-Cylinder Soot Characteristics in a Heavy-Duty Diesel Engine using CMC

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ABSTRACT

This paper presents numerical simulations of in-cylinder soot evolution in the optically accessible heavy-duty diesel engine of Sandia Laboratories performed with the conditional moment closure (CMC) model employing a reduced n-heptane chemical mechanism coupled with a two-equation soot model. The influence of exhaust gas recirculation (EGR) on in-cylinder processes is studied considering different ambient oxygen volume fractions (8 - 21 percent), while maintaining intake pressure and temperature as well as the injection configuration unchanged. This corresponds to EGR rates between 0 and 65 percent.

Simulation results are first compared with experimental data by means of apparent heat release rate (AHRR) and temporally resolved in-cylinder soot mass, where a quantitative comparison is presented. The model was found to fairly well reproduce ignition delays as well as AHRR traces along the EGR variation with a slight underestimation of the diffusion burn portion. Subsequently, the impact of EGR on the mixture formation, spray characteristics and soot evolution is investigated numerically and governing processes are identified and discussed.

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INTRODUCTION

Stricter emission legislations for diesel engines have motivated engine manufacturers to drastically reduce emissions of NO_x and soot. Exhaust gas recirculation (EGR) is a well proven method for the reduction of NO_x emissions in diesel engines, due to the reduction of the in-cylinder combustion temperature. With oxidizer dilution, a monotonic decrease of NO_x formation rate is obtained since in diesel engines NO_x formation is dominated by the thermal pathway (Zeldovich).

For soot emissions the situation is more complex because exhaust soot emissions are only a small part of the in-cylinder soot formed [1], since net soot emission is the competition between formation and oxidation. At lower temperatures, both soot formation and oxidation are slowed down. At moderate

EGR levels, soot emissions are generally increased due to the more rapid decrease in oxidation rate compared to formation [2]. At high levels of EGR soot is again reduced, probably due to a drastic reduction in soot formation as discussed in [3]. Experimentally, there is a wide range of EGR-related work in the literature employing full metal engines, generic optically accessible test rigs and optical engines evidencing a general understanding of the relevant in-cylinder processes.

Numerical simulations have the potential to provide further insights to these observations, however models need careful validation before useful information can be extracted from the results. In this sense, among others, experimental work conducted in the last decade at the Sandia heavy-duty diesel engine has not only contributed to an improved understanding of in-cylinder processes [3] but has also provided a vast

high-fidelity dataset for model validation purposes. Most of the numerical work carried out so far e.g. [4, 5, 6, 7, 8, 9, 10] was concentrated on the five “reference cases” reported in [11]. Prediction of soot formation have been attempted using a variety of combustion models and with different fuel chemical mechanisms as well as precursor complexities [4, 5, 6, 7, 9, 12]. A CMC combustion model is used in this investigation in conjunction with a semi-empirical two-equation soot model. While CMC has seen successful application to various gaseous flame configurations for which a comprehensive review is presented in [13], studies relating to auto-igniting sprays at diesel engine conditions in generic test rigs [14, 15, 16, 17, 18, 19, 20] and in real diesel engines are documented in [21, 22]. For the diesel engine considered in this study, the prediction of semi-quantitative soot evolutions has been demonstrated for all five “reference cases” [7] as well as separated sweeps in start of injection (SOI) and top dead center ambient temperature (T_{TDC}) [23]. Variations of the former influence have also been studied numerically by others, e.g. in [24], while for the influence of TDC temperature so far investigations have only been presented in [23].

In the present investigation, the goal is to assess the influence of EGR while keeping other parameters unvaried for this engine, for which the experimental data reported in [25] has been used for validation and for which, to the authors' best knowledge, no other numerical study has been presented to date.

Motivated by the promising results recently presented in [7, 23] for variations in SOI and TDC temperature respectively, this study seeks to understanding of the effect of EGR on soot formation and, more specifically, also the distinct influence of dilution on formation and oxidation processes. A total of six EGR levels measured in [25] have been considered to assess the predictions: following the validation of the combustion model by means of AHRR, measured quantitative in-cylinder soot mass evolutions have been used to verify the predictions. In the second part, simulation results have been further analyzed to identify the relative importance of soot formation and oxidation for different EGR levels.

The remainder of this paper is structured accordingly: first the model formulation is presented followed by a short description of the test cases considered. Model predictions are first compared with experimental data for apparent heat release rate and soot mass evolution. Subsequently, simulation results on the impact of EGR on soot formation and oxidation are presented. The paper closes with concluding remarks.

NUMERICAL METHODOLOGY

Flow Field Solver

The flow field is calculated by means of the widely adopted commercial CFD solver STAR-CD [26]. A Reynolds Averaged Navier Stokes (RANS) approach is followed using the RNG version of the available k - ϵ turbulence models with ‘standard’ wall functions [26]. The fuel injector is centrally located and has eight symmetrically arranged nozzle exits; the numerical solution domain correspondingly encompasses one eighth of the chamber. No valve motion has therefore been considered and the simulation commences at intake valve closure (IVC) with prescribed temperature and pressure levels taken from the experiment. A swirl ratio of 0.5 (solid body rotation) has been prescribed.

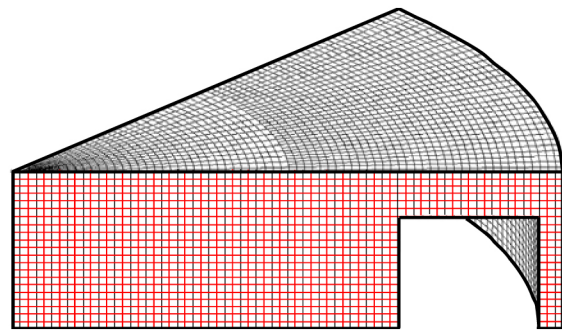


Figure 1. Mesh of engine geometry at TDC. In black is the CFD grid with the CMC grid overlaid in red.

A schematic of the computational domain at TDC is given in Figure 1: in black the fine 3D CFD grid and overlaid in red the coarser 2D CMC resolution are drawn; the latter will be addressed in the “Combustion model” section below. The following resolutions have been chosen for the CFD mesh: in the piston bowl, a uniform spacing of $1 \times 1 \times 1 \text{ mm}^3$ is employed while in the sweep volume the axial ratio has been slightly expanded resulting in a resolution of $1 \times 1 \times 1.3 \text{ mm}^3$. At TDC, cell counts amount to approximately 50,000, while at bottom dead center (BDC) approximately 240,000 cells are present.

Droplets are injected as parcels and tracked in a Lagrangian fashion fully two-way coupled to the gas phase by means of source terms in the conservation equations for momentum, mass, energy and species. For primary break-up, the widely adopted ‘blob’ model has been selected while secondary break-up is treated by the Reitz-Diwakar model [27]. The splashing model of Bai and Gosman has been activated to treat possible impingement of droplets on solid walls [28]. For droplet drag and heat/mass transfer the standard correlations implemented in STAR-CD have been employed for which further details as well as references can be found in [26]. As a surrogate for Diesel, n -dodecane thermo-physical liquid

properties (c_p , viscosity, latent heat, vapor pressure, density and surface tension tabulated as a function of temperature) have been prescribed.

Species mass fractions for the CFD code are obtained by convolution of the respective conditional species mass fractions with a presumed beta Probability Density Function (PDF). The latter is determined by the mean mixture fraction (eq. (1)) and its variance (eq. (2)), for which two transport equations are solved as follows:

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

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

Concerning enthalpy, the 'chemico-thermal' equation is transported by STAR-CD employing polynomial c_p for species.

Evaporating droplets lead to a source term in the mixture fraction eq. (1) while such effects have been neglected in the mixture fraction variance equation following [16], where a negligible impact at conditions similar to the ones in this study was reported. As is evident from eq. (2), the production of variance is due to mixture fraction gradients; the second term on the right hand side (RHS) of eq. (2) denotes the scalar dissipation rate (SDR), which is calculated algebraically using

turbulence quantities as $\tilde{\chi} = c_{\chi} \tilde{\xi}^{\prime\prime 2} / k$ where c_{χ} is a model constant for which a value of 2.0 has been adopted.

Combustion Model

Conditional moment closure has been used to model combustion and, as is common practice in non-premixed combustion, the mixture fraction has been employed as the conditioning quantity. The governing equations for CMC originally put forward in [29] are implemented specifically for engine application as detailed in [21, 22] and therefore not repeated here. In short, in CMC transport equations are solved for conditional species mass fractions and temperature which include convective transport, conditional turbulent fluxes and conditional chemical source terms. Terms due to pressure rate of change (as a consequence of the variable chamber volume) and local effects such as wall heat losses are further accounted for in the conditional temperature. The resulting equations are discretized in space by means of finite differences using a second order scheme for the diffusion

terms and a first order upwind scheme for the convective terms. In time, a full operator splitting technique has been adopted which employs a stiff integrator (DVODE). Further details concerning submodels and implementation can be found in [17, 18, 21]. Mixture fraction space has been discretized into 101 grid points which are clustered around the stoichiometric value, η_{st} , which strongly depends on the level of EGR (cf. Table 5 below).

As discussed in [29], spatial resolution requirements for *conditional* quantities tend to be much lower than their corresponding unconditional values. As a consequence, a coarser grid resolution can be used for the CMC compared to its CFD counterpart. Former studies using CMC for diesel engines [7, 21, 22] successfully demonstrated, that a two-dimensional formulation of CMC is often sufficient, even for quantities such as NOx emissions, for which a CMC grid sensitivity study is given in [22]. As dimensionality reduction allows for substantial savings in computational cost, a two-dimensional formulation is followed in this study as well which is illustrated in Figure 1: The 2D CMC mesh at TDC is shown in red which employs a constant resolution of 1 by 2 mm in the cylinder axial and radial directions respectively in the piston bowl resulting in 35×20 CMC cells at TDC. During compression and expansion, CMC cells layers are removed/added following the methodology implemented in [21] in analogy to the cell layer addition/removal on the CFD side.

Chemical Mechanisms

Concerning the oxidation chemistry, an *n*-heptane chemistry has been adopted as a surrogate for the D2 fuel used in the experiment. This is motivated by the successful application to diesel engine combustion with CMC in [7, 23] using kinetics from [30], due their computational efficiency and the good performance demonstrated in [14] for auto-igniting D2 sprays in a constant volume chamber at a wide range of engine relevant operating conditions. Although very detailed oxidation schemes including also longer-chain, branched, cyclic hydrocarbons as well as aromatics are emerging (see e.g. reviews in [31, 32], the use of more tractable kinetics for *n*-heptane as a surrogate for diesel is still common practice (due to the very similar cetane number) and this approach has also been followed in similar investigations for this engine, see e.g. [5, 6, 8, 9, 24].

Soot Model

A semi-empirical two-equation approach first proposed by Leung et al. [33] has been adopted to model soot formation. To this end, interacting directly with the *n*-heptane kinetic, two transport equations in mixture fraction space are solved for the conditional soot mass fraction and soot number density (eq. (3)).

$$\begin{aligned} \frac{\partial Q_s}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_s}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_s}{\partial \eta^2} \\ + \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[\langle \rho u_i Y_s'' | \eta \rangle \tilde{P}(\eta) \right] = \langle w_s | \eta \rangle \end{aligned} \quad (3)$$

Similar to the transport equations for the conditional species mass fractions, the soot transport equations include terms accounting for spatial convection, molecular mixing and conditional turbulent fluxes (the second, third and fourth term in the LHS of [equation \(3\)](#), respectively). The conditional chemical source term w_s on the RHS describes all soot related processes, namely soot particle inception, surface growth, coagulation and oxidation by O_2 and OH as follows:

$$\begin{aligned} \langle w_{Y_s} | \eta \rangle = \langle w_{Y_s, inc} | \eta \rangle + \langle w_{Y_s, gro} | \eta \rangle + \\ \langle w_{Y_s, oxidO_2} | \eta \rangle + \langle w_{Y_s, oxidOH} | \eta \rangle \end{aligned} \quad (4)$$

While for the particle number density ([eq. \(5\)](#)) the corresponding conditional chemical source terms read:

$$\langle w_{N_s} | \eta \rangle = \langle w_{N_s, inc} | \eta \rangle + \langle w_{N_s, coag} | \eta \rangle \quad (5)$$

Due to the high density, soot mass diffusivity is comparatively low and soot therefore has a Lewis number higher than unity. Different modeling approaches to account for soot differential diffusion effects in a mixture fraction based framework have been proposed in the literature (e.g. [34, 35]), however, at diesel engine conditions presently no validated closures exist. Motivated by the good agreement of soot distributions and quantitative levels demonstrated in a previous study for a constant volume test rig [19] and at the current engine [7], a unity Lewis number has been assumed here.

Soot inception and surface growth are governed by acetylene only, all soot related reactions are summarized in [Table 1](#) and [Table 2](#) shows the corresponding rate coefficients which are identical to the ones employed in [7].

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)	$C_{(s)} + OH \xrightarrow{R_{oxidOH}} CO + H$

Table 2. Reaction rate constants in Arrhenius form, $k_j = A \cdot T^b \cdot \exp(-T_a/T) \cdot S_{soot}^c$. Units are kg, kmol, m, s, K.

	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

A primary soot particle is assumed to consist of 100 carbon atoms as proposed in [33] which results in a primary particle diameter of 1.28 nm. Coagulation of particles is the only process which acts as a sink in the particle number transport [equation \(5\)](#), for which the corresponding rate is calculated as follows:

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

N_A denote the Avogadro number, R the universal gas constant and C_a is a model constant for which a value of 3 has been chosen following [36].

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](#). 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.

Table 3. Engine and injector specifications [25].

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