

Influence of EGR on Post-Injection Effectiveness in a Heavy-Duty Diesel Engine Fuelled with n-Heptane

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ABSTRACT

Numerical simulations of a heavy-duty diesel engine fuelled with n-heptane have been performed with the conditional moment closure (CMC) combustion model and an embedded two-equation soot model. The influence of exhaust gas recirculation on the interaction between post- and main- injection has been investigated. Four different levels of EGR corresponding to intake ambient oxygen volume fractions of 12.6, 15, 18 and 21% have been considered for a constant intake pressure and temperature and unchanged injection configuration. Simulation results have been compared to the experimental data by means of pressure and apparent heat-release rate (AHRR) traces and in-cylinder high-speed imaging of natural soot luminosity and planar laser-induced incandescence (PLII). The simulation was found to reproduce the effect of EGR on AHRR evolutions very well, for both single- and post-injection cases. Further a direct comparison of the computed and measured temporal evolution of soot luminosity is presented for the 18% initial oxygen volume fraction case. The spatial extents of the predicted spray plumes and soot clouds are in qualitative agreement with experimental data. Subsequently, the model has been used to investigate the effect of the post-injection on in-cylinder soot evolution, especially with respect to the role of increased mixing and temperature; a detailed analysis highlighting the relative importance of soot formation and oxidation (both O_2 and OH contributions) is presented at two representative EGR levels.

CITATION: Pandurangi, S., Frapolli, N., Bolla, M., Boulouchos, K. et al., "Influence of EGR on Post-Injection Effectiveness in a Heavy-Duty Diesel Engine Fuelled with n-Heptane," *SAE Int. J. Engines* 7(4):2014, doi:10.4271/2014-01-2633.

INTRODUCTION

The diesel engine has enjoyed immense popularity in the fields of transportation and power generation for decades. While often lauded as the most efficient type of internal combustion engine on account of its high fuel economy and low CO_2 footprint compared to other engines, the diesel engine struggles to keep up with the rapid pace of pollution reduction efforts and legislation. Soot emissions from diesel engines are known to adversely affect the environment and human health. Due to their mode of operation, involving stratification and presence of fuel-rich, soot-prone regions and simultaneously lean NO_x -prone regions in the flame vicinity, a number of challenges are posed, necessitating further research effort into in-cylinder pollutant reduction technologies.

One such approach is exhaust gas recirculation (EGR) which has been studied extensively, especially at low-temperature combustion (LTC) regimes with a focus on NO_x reduction (see e.g. [1]). EGR affects combustion by increasing ignition delay, reducing the peak temperature and reducing reaction rates. By itself however, a high level of EGR can cause an increase in the engine-out soot emissions when used in conventional

diesel engines [2, 3] due to the suppression of soot oxidation. This unwanted increase can be countered by adding a small fuel injection, which follows the main injection and is introduced early enough to undergo combustion. The understanding of the efficacy and mechanisms of such post-injections for soot reduction is reviewed in [4] and a detailed experimental study under different EGR conditions (using n-heptane as fuel) is reported in [5].

The computational modelling of diesel engine combustion processes in general poses a number of challenges: highly turbulent and swirling in-cylinder flow coupled with liquid fuel atomization, droplet secondary breakup and evaporation, fuel-air mixing and auto-ignition of complex hydrocarbon fuels followed by premixed and diffusion combustion fuel conversion modes. The modelling of multiple injections involves additional challenges for the correct and separate treatment of each injection. The phenomena related to pollutant generation usually lie at the end of the chain of the above events; the reliable prediction of flow and combustion phenomena is therefore of primary importance for the goal of soot potential reduction of engine emissions.

In combination with computational fluid dynamics, a range of combustion modelling approaches have been applied in recent years ranging from the characteristic time scale (CTC) approach [6], extensions to coherent flame models (ECFM) [7], 2D flamelet models [8], transported probability density function (PDF) methods [9] and presumed PDF methods [10]. The CTC and ECFM models do not require additional modelling for multiple injections and simulation is relatively straightforward. The ECFM-3Z model has been applied [11] to diesel engines for studying the effect of post-injections, and recently the CTC approach [6] has been applied to the same experimental dataset as used in the present study. However, for more elaborate models such as Representative Interactive Flamelets (RIF) or Conditional Moment Closure (CMC) which are based on the mixture fraction, the complexity of the model is considerably increased since two different mixture fractions are needed for describing the two distinct fuel streams. While the first fuel stream exhibits a classical auto-ignition process, the following fuel stream(s) are additionally subject to strong interaction with the preceding stream, which may lead to forced ignition merely due to contact with an established flame [8].

To address these issues, 2D flamelet (RIF) models have been derived [8] and successfully applied to diesel engines [8, 12, 13]. However, difficulties persist in the modelling of terms such as the cross scalar dissipation rate and in obtaining a representative description for the 2D probability distribution needed for convolution. To help reduce such uncertainties, DNS simulations for a three-feed system have been reported in [14] and the processed data supplied as input to separate 2D flamelet calculations. Still, discrepancies were found with respect to heat release rate as well as the evolutions of temperatures conditioned on the respective mixture fractions of the two fuel streams; these were attributed to the use of only one single 2D-flamelet to represent the entire domain. Conceptually, when attempting to incorporate multiple injections into CMC models, difficulties similar to those in the derivation of 2D-RIF can be expected. Additionally, the situation is aggravated by the physical space transport terms in the CMC equations (conditional velocity and conditional turbulent fluxes) [15], for which new closures are likely to be required in the presence of multiple fuel streams. Apart from the modelling challenges, a formal double-conditioning in CMC will also lead to a dramatic increase in computational expense rendering the simulation of diesel engines impractical, since CMC typically discretises the physical domain into thousands of nodes (in contrast to a single 2D flamelet representing the entire domain in the 2D-RIF approach).

The CMC model employed in this study has been successfully and extensively applied to a number of generic test rigs [16,17,18,19,20] and diesel engines [21, 22] using single injections. Extensions to the model have enabled detailed investigations of soot [23,24,25,26] and also the influence of EGR [27] thereupon. Recently the incorporation of arbitrarily spaced multiple injections without requiring formal double-conditioning was reported [28] and successfully applied [29, 30] and the same is used in this work.

The paper is structured as follows. We first discuss the flow field and combustion computation describing the governing equations and the models used. The experimental reference data is then reviewed briefly, followed by results, including validation based on apparent heat-release rates and in-cylinder soot distribution. The results are used to gain an understanding of the effect of EGR on post-injection effectiveness, which forms the subject of discussion, and the main conclusions are then drawn in closing.

NUMERICAL SETUP

The numerical methodology employed in this study follows previous works [23,24,25] except for the model extension to multiple injections. Hence, the latter is described in more detail whereas the rest is only briefly repeated.

Flow Field Computation

The computational domain of the engine is represented as a 45° sector of the entire cylinder, and correspondingly only one of the eight injector holes is considered. The domain is meshed into hexahedral cells with a resolution of 1 mm³ in the piston bowl resulting in approximately 50,000 cells at top-dead-centre position; at bottom-dead-centre the mesh grows to approximately 240,000 cells. The polar configuration of the CFD mesh is the same as used in [25] wherein a grid sensitivity analysis under non-reactive conditions was also shown. The depth of the piston crevice has been reduced to align it with the piston bowl bottom for simplicity, and consequently its thickness is increased to maintain the overall geometric compression ratio. Figure 1 shows the computational domain along with the individual cells. A coarser-resolution but synchronised mesh of the same model is used for the evaluation of quantities related to the CMC combustion model, which is described in the next section.

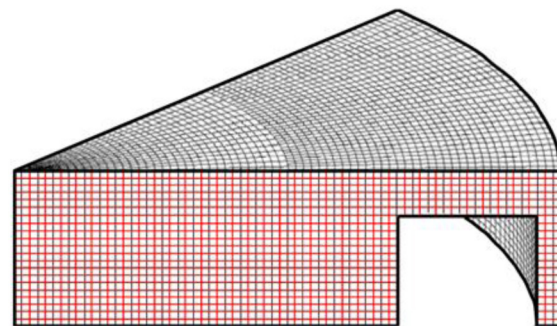


Figure 1. CMC mesh (in red) and CFD mesh (in black) shown overlaid on the same computational domain.

The commercial CFD code STAR-CD [31] has been used to compute the turbulent flow field in the domain. The Reynolds-averaged Navier-Stokes equations are solved with the high Reynolds number $k-\epsilon$ model for turbulence. To incorporate the liquid-phase fuel spray in the computation, a Lagrangian approach is used with the 'blob' model for atomization and the model of Reitz & Diwakar [32] for droplet secondary breakup.

The droplets are subject to turbulent dispersion based on a stochastic model. Thermo-physical properties for n-heptane are calculated based on the droplet temperature.

CMC Combustion Model for Single Injection

The conditional moment closure (CMC) model solves transport equations for the conditional mean of temperature and all chemical species, which are weighted with a (presumed shape) beta-PDF function to yield the physical temperature and species fields. The conditioning is performed upon the mixture fraction ξ , for which η denotes the sample space variable, which is resolved with 101 points between the oxidiser and fuel sides ($\xi=0$ and $\xi=1$ respectively) and clustered around the stoichiometric mixture fraction. The conditional expectations of the α -th species mass fraction, Q_α , and temperature, Q_T , are obtained from the following transport equations:

$$\frac{\partial Q_\alpha}{\partial t} + \langle u_j | \eta \rangle \frac{\partial Q_\alpha}{\partial x_j} = \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \frac{1}{\rho_\eta \tilde{P}(\eta)} \frac{\partial}{\partial x_j} [\langle u_j'' Y_\alpha'' | \eta \rangle \rho_\eta \tilde{P}(\eta)] + \langle \dot{\omega}_\alpha | \eta \rangle \quad (1)$$

$$\frac{\partial Q_T}{\partial t} + \langle u_j | \eta \rangle \frac{\partial Q_T}{\partial x_j} = \langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \langle N | \eta \rangle \left[\frac{1}{\langle c_P | \eta \rangle} \left(\frac{\partial \langle c_P | \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^N c_{P,\alpha} \frac{\partial Q_\alpha}{\partial \eta} \right) \frac{\partial Q_T}{\partial \eta} + \frac{\langle \dot{Q}_H | \eta \rangle}{\rho_\eta \langle c_P | \eta \rangle} + \frac{1}{\langle c_P | \eta \rangle} \left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \right| \eta \right] - \frac{1}{\rho_\eta \tilde{P}(\eta)} \frac{\partial}{\partial x_j} [\langle u_j'' T'' | \eta \rangle \rho_\eta \tilde{P}(\eta)] \quad (2)$$

Detailed derivations of the equations are found in [33, 34]. The broad methodology of implementation and CFD-CMC coupling is discussed at length in [21] and is repeated only briefly here. The above equations still contain unclosed terms and a number of sub-models are required for closure. The conditional scalar dissipation rate is treated by the AMC model [35] while a linear relationship is used for the conditional velocity terms. Turbulent fluxes are closed with a gradient flux assumption. The governing equations are discretised with a second-order central differencing scheme for the diffusion terms and an upwind scheme for convective terms. A full operator splitting between the transport in physical and mixture fraction space and chemistry is employed, following conclusions reached in [17]. A stiff integrator is used allowing for substantial performance gains [17].

A simplified reaction mechanism for n-heptane consisting of 22 chemical species in 18 reaction steps is applied [36] based on much success with this compact description in studies of constant-volume combustion [18, 19, 23] as well as diesel engines [24, 25]. Conditional chemical sources are closed at first order; this approach has shown very good results in diesel spray simulations for engines [21, 22] and constant-volume chambers [16, 17, 18, 19, 20]. The computational mesh for solving the conditional transport equations is kept coarser than the flow-field mesh; this is made possible due to the much

weaker spatial dependence of conditional quantities compared to their unconditioned counterparts, as shown in [18, 21]. Data mapping between the two meshes is performed at each time step using PDF-weighted averages. Further, as described in detail in [21], the mesh for CMC computations is two-dimensional where the cells have been collapsed azimuthally into a single vertical plane. This provides for a computationally efficient solution in view of the long process duration and computer-intensive chemical reaction integration, where parallelization alone does not offer a satisfactory reduction in computational time.

CMC Combustion Model with Multiple Injections

An extended CMC model is employed in this study, which is able to account for multiple injections using a single total mixture fraction (MFT) as the conditioning scalar [28]. This approach is supported by findings from [8, 12, 13] reporting a rapid transition in 2D flamelet space along the overall stoichiometric mixture, leading to a quasi-1D structure in the MFT coordinate. The reader is referred to [28] for a detailed discussion of the model; only main points are repeated here.

The original temperature and composition, conditional upon the mixture fraction of the first injection (MF1), are transformed into representative profiles that are conditional upon MFT. The spatial resolution of CMC allows for a detailed determination of the time and location of contact between fuel streams, as well as their local conditions. The model is based on re-initialization of the conditional temperature and composition in every CMC cell, at the time of the first appearance of mixture fraction from the second fuel stream (MF2), using localised spatial information. At the time of first MF2 appearance, it is proposed to start from the doubly conditional temperature distribution, as well as the probability distribution of MF1, in the same way as an initialization of doubly conditioned CMC or 2D-RIF [8] as illustrated in Figure 2. MF1 consists of the original burning temperature profile (MF2=0) and adiabatic mixing is assumed along the MF2 coordinate (MF1=const.). Note that the domain consists of a unity triangle, implying that MFT cannot exceed a value of one.

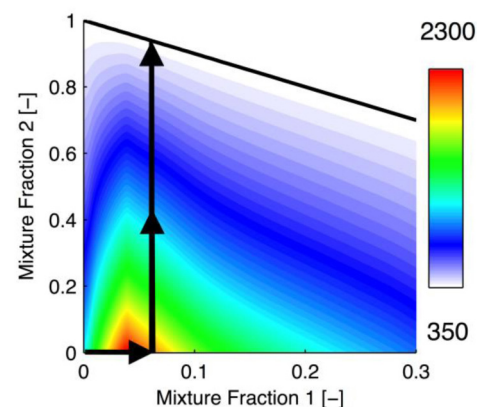


Figure 2. Example of a doubly conditioned temperature distribution at the time of re-initialization.

In order to reconstruct a representative temperature conditioned upon MFT, two fundamental assumptions are introduced: (i) at the time of first appearance of MF2 into a CMC cell, MF1 and its variance both tend to decrease due to convection-diffusion effects and due to the further absence of an MF1 source, implying a temporal separation of MF1 and MF2 sources at a given position; and (ii) when the second fuel stream enters a CMC cell, the increase in MFT is attributed to MF2 only. For the reconstruction of the re-initialised conditional temperature at a given MF1, the left domain of the local MF1 is retained and a vertical line along MF2 is drawn corresponding to adiabatic mixing of the local MF1 with the new incoming MF2, assumed to be the sole MFT source. The new temperature profile, $\langle T_{Double} | \eta_1, \eta_{Tot} \rangle$ for a pre-existing η_1 can be described by:

$$\begin{aligned} \langle T_{Double} | \eta_1, \eta_{Tot} \rangle &= \langle T_{\eta_1} | \eta_{Tot} \rangle [H(\eta_{Tot}) - H(\eta_{Tot} - \eta_1)] \\ &+ \langle T_{mix} | \eta_{Tot} \rangle H(\eta_{Tot} - \eta_1) \end{aligned} \quad (3)$$

Where η_{tot} is MFT, η_1 is the local MF1, H is the Heaviside step function, $\langle T_{\eta_1} | \eta_{Tot} \rangle$ is the original temperature profile before re-initialisation and $\langle T_{mix} | \eta_{Tot} \rangle$ is the mixing temperature obtained following the η_2 coordinate for a constant η_1 on the doubly-conditioned temperature distribution. The probability of encountering a given MF1 inside a CMC cell is assumed to be the current MF1 PDF. The new temperature profile conditional upon MFT, $\langle T_{New} | \eta_{Tot} \rangle$, is computed by considering the marginal PDF for MF1, $P_{\xi|\zeta}(\eta_1|\eta)$, as $P_{\xi}(\eta_1)$ owing to the instantaneous initialisation and the subsequent absence of MF2. It follows that:

$$\langle T_{New} | \eta_{Tot} \rangle = \int_0^1 \langle T_{Double} | \eta_1, \eta_{Tot} \rangle P_{\xi}(\eta_1) d\eta_1 \quad (4)$$

The result of the re-initialization described by equations (3) and (4) is illustrated graphically in Figure 3.

The thick black line is the original profile before re-initialization and the array of thin black curves represents the re-initialised temperatures for different MF1 values. The influence of MF1 PDF is illustrated for three different cases: a low mean MF value with low and high variance (MFV) (blue and green respectively) and a high mean MF value with low MFV (red). For cases with low MFV (blue and red), the new temperature is practically a single “cut” at the local mean MF, and for a larger MFV the profile becomes more rounded. Note that the profiles are continuous and differentiable.

The final solution at the CFD resolution relies on conditional expectations of quantities as is typical in the CMC framework, obtained by the convolution (with the MFT PDF) of the new

profile resulting after re-initialization or its time evolution. The effect of localised initialisation is then transported in physical as well as conserved scalar space, as is also the case for single injections. Note that the number of subsequent injections is not limited: it is sufficient to simply re-initialise the profiles whenever fuel from a new injection enters a CMC cell.

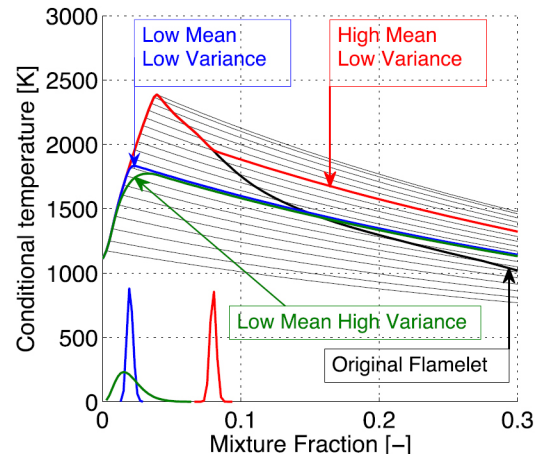


Figure 3. Re-initialised temperature profiles for three different distributions of main mixture fraction.

Soot Modelling

The semi-empirical two-equation model by Leung et al. [37] is used for soot modelling based on prior success in simulations for constant volume test rigs [23] and engines [25]. Transport equations are solved for the conditional mean of soot mass fraction and number. The model considers simultaneous soot inception, surface growth, oxidation by O_2 and OH , and coagulation. Particles are assumed to be spherical and mono-dispersed and a unity Lewis number approach has been considered, neglecting differential diffusion. Acetylene (C_2H_2) is considered as the only soot precursor in this model. The first soot particle consists of 100 carbon atoms [37], corresponding to a primary particle size of 1.28 nm. Chemical reaction rates and constants are described in [24, 25].

EXPERIMENTAL SETUP

High-fidelity experimental data [5] from the optically accessible heavy-duty diesel engine forms the basis of the validation of this study. The engine setup is installed at the Sandia National Laboratories, consisting of the single-cylinder, common-rail direct injection, four-stroke optically accessible engine with eight equally spaced injectors. Windows in the piston and cylinder head enable the imaging of soot by natural luminosity and planar laser-induced incandescence (PLII); details of the setup can be found in [5]. Engine and injector specifications are summarised in Table 1.

From the experimental dataset reported in [5], eight cases have been considered for this study: four levels of EGR resulting in initial ambient oxygen concentrations of 21, 18, 15