

Multi-dimensional Conditional Moment Closure Modelling Applied to a Heavy-duty Common-rail Diesel Engine

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ABSTRACT

A multi-dimensional combustion code implementing the Conditional Moment Closure turbulent combustion model interfaced with a well-established RANS two-phase flow field solver has been employed to study a broad range of operating conditions for a heavy duty direct-injection common-rail Diesel engine. These conditions include different loads (25%, 50%, 75% and full load) and engine speeds (1250 and 1830 RPM) and, with respect to the fuel path, different injection timings and rail pressures. A total of nine cases have been simulated.

Excellent agreement with experimental data has been found for the pressure traces and the heat release rates, without adjusting any model constants.

The chemical mechanism used contains a detailed NO_x sub-mechanism. The predicted emissions agree reasonably well with the experimental data considering the range of operating points and given no adjustments of any rate constants have been employed. In an effort to identify CPU cost reduction potential, various dimensionality reduction strategies have been assessed. Furthermore, the sensitivity of the predictions with respect to resolution in particular relating to the CMC grid has been investigated.

Overall, the results suggest that the presented modelling strategy has considerable predictive capability concerning Diesel engine combustion without requiring model constant calibration based on experimental data. This is true particularly for the heat release rates

predictions and, to a lesser extent, for NO_x emissions where further progress is still necessary.

INTRODUCTION

Diesel engines are among the most efficient energy conversion devices in use today for both vehicle propulsion and power generation. In the past, engine development focussed to a large extent on the three 'traditional' engineering goals: optimisation of performance, efficiency and reliability. More recently, the increased awareness of the impact of engine out exhaust gases on health and the environment has lead to progressively stricter legislation standards concerning emissions throughout the world.

The number of degrees of freedom to be optimised for engines has increased by several orders of magnitude in the past decades [1]. For Diesel engines, this is due to developments pertaining in particular to the fuel path, i.e. the availability of highly flexible fuel injection systems. To complement the optimisation by means of engine testing, fast and reliable numerical tools are hence urgently required to help meet future demands and to speed up the development process.

Comparatively simple approaches such as the widely adopted characteristic time scale model [2] which is based on eddy dissipation concepts [3] are nowadays routinely applied to simulate spray combustion processes in Diesel engines. Such calculations usually necessitate careful calibration of model constants based on measured pressure traces, although engine dimension scaling arguments can sometimes be applied

[4]. While 'global' quantities relating to engine performance such as the pressure trace can often be reproduced satisfactorily for conditions close to the ones used for model calibration, quantitative or even qualitative predictions of emissions require more elaborate methodologies. Among the latter category, presumed probability density functions (PDF) approaches such as representative interactive flamelets [5,6,7] have seen highly successful application to different Diesel engine configurations. For HCCI, fully transported PDF models have also been reported [8], exploiting tabulated chemistry to speed up the computations. Both of these approaches enable the inclusion of detailed chemistry and can hence also treat the auto-ignition process avoiding the use of a separate model for this phase (e.g. [2,9]). Generalised flame surface density approaches [10] as well as coherent flame models [11] and extensions thereto proposed in [12] have also seen successful application to combustion in stratified environments.

Conditional Moment Closure (CMC) has been demonstrated to offer a solid and promising framework for modelling a broad range of single-phase turbulent flames [13,14,15,16,17,18] including auto-ignition processes [19] as well as for auto-igniting spray combustion [20,21]. In [22] a fully elliptic CMC formulation capable of accounting for the time-varying geometry inside engine combustion chambers was demonstrated for a heavy duty Diesel engine. In this study, the predictive capability of the model with respect to changes in both the air and fuel paths is further assessed for a total of nine operating conditions. In addition to the comparisons of the pressure traces, predictions of the heat release rates as well as NO_x emissions are presented. Furthermore, the sensitivities with respect to the CFD and the CMC grid resolution for both heat release and NO_x are investigated.

NUMERICAL METHOD

The widely adopted CFD solver STAR-CD [23] has been coupled to an elliptic CMC combustion code. Figure 1 shows a schematic of the coupling; further details as well as information concerning the integration procedure which employs operator splitting techniques can be found in [21,22].

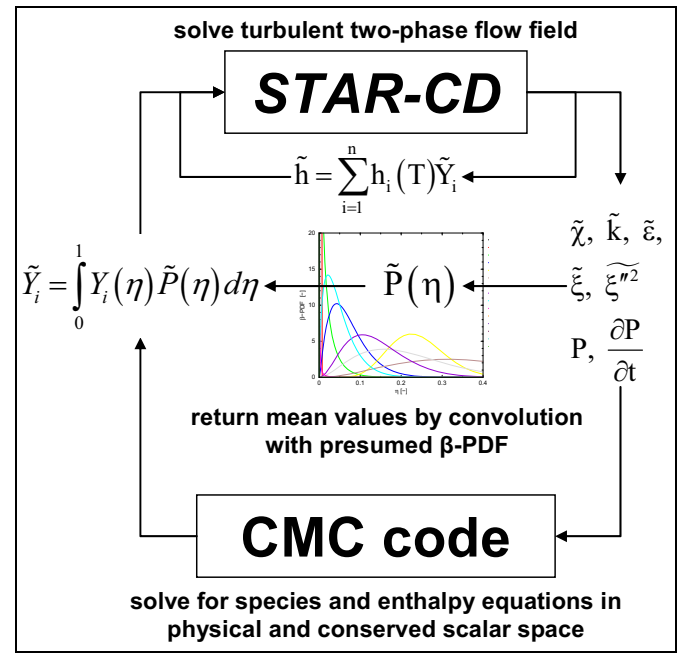


Figure 1 – Schematic of the CFD-CMC coupling

GOVERNING EQUATIONS

The governing equations for CMC have been derived and discussed in detail in [24,25,26]. In brief, CMC solves equations for the conditional expectations of species and temperature denoted by

$$Q_\alpha(\eta, \mathbf{x}, t) = \langle Y_\alpha(\mathbf{x}, t) | \xi(\mathbf{x}, t) = \eta \rangle \quad (1)$$

$$Q_T(\eta, \mathbf{x}, t) = \langle T(\mathbf{x}, t) | \xi(\mathbf{x}, t) = \eta \rangle \quad (2)$$

Where $\langle \bullet | \xi(\mathbf{x}, t) = \eta \rangle$ specifies ensemble averaging with respect to ξ fulfilling the condition on the right side of the vertical bar.

Q_α , the species conditional mass fractions, and Q_T , the conditional temperature, are functions of space, time and conserved scalar space; the latter representing the sample space for all states of mixing. They obey the following equations, respectively:

$$\frac{\partial Q_\alpha}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[\langle u_i Y_\alpha'' | \eta \rangle \bar{\rho} \tilde{P}(\eta) \right] = \langle w_\alpha | \eta \rangle \quad (3)$$

$$\begin{aligned} \frac{\partial Q_T}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_T}{\partial x_i} = & \langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \langle N | \eta \rangle \left[\frac{1}{\langle c_P | \eta \rangle} \left(\frac{\partial \langle c_P | \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^N \langle c_{P,\alpha} | \eta \rangle \frac{\partial Q_\alpha}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta} \\ & - \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[\langle u_i T'' | \eta \rangle \bar{\rho} \tilde{P}(\eta) \right] + \frac{1}{\langle c_P | \eta \rangle} \left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \middle| \eta \right\rangle + \frac{\langle w_T | \eta \rangle}{\langle \rho | \eta \rangle \langle c_P | \eta \rangle} + \frac{\langle w_{WALL} | \eta \rangle}{\langle \rho | \eta \rangle \langle c_P | \eta \rangle} \end{aligned} \quad (4)$$

Hence the dimensionality of the problem to be tackled numerically is increased. As shown e.g. in [25], in many cases the spatial variation of the conditional quantities is much weaker than for their unconditional counterparts allowing for substantial reduction in spatial resolution.

The unclosed terms in equations (3) and (4) are modelled using standard practice, i.e. a gradient transport assumption is followed for the conditional turbulent fluxes $\langle u_i'' Y_\alpha'' | \eta \rangle$ and $\langle u_i'' T'' | \eta \rangle$, the linear model is used for the conditional velocities $\langle u_i | \eta \rangle$ and the conditional scalar dissipation rate $\langle N | \eta \rangle$ is modelled by the Amplitude Mapping Closure (AMC) [26].

The conditional wall heat transfer is modelled as proposed in [7] as

$$\langle w_{WALL} | \eta \rangle = \alpha (Q_T - \tilde{T}_{WALL});$$

$$\text{with } \alpha = \frac{\dot{q}_{wall}^{CFD}}{\int_0^1 (Q_T - \tilde{T}_{WALL}) \tilde{P}(\eta) d\eta} \quad (5)$$

where $\dot{q}_{wall}^{CFD}$ denotes the wall heat flux from the flow field solver.

The conditional source terms from chemical reactions in the specie's $\langle w_\alpha | \eta \rangle$ and temperature equation $\langle w_T | \eta \rangle$ are closed at first order. Investigations employing second order closure have been proposed in [27]; due to the strong increase in computational cost conditional fluctuations have been neglected in the present investigation. As these may be important for ignition/extinction phenomena in certain flow conditions, future, more detailed investigations should assess the importance for the present set-up.

The present formulation of the CMC code does not account for the influence of the liquid phase in the conditional equations, as a clear consensus in this still active field of research is not well established yet. A new, rigorous derivation of the conditional equations and an overview of the existing literature can be found in [28].

Chemical mechanism

The chemical mechanism employed taken from [29] has a total of 59 species, of which 28 are set to steady state based on computational singular perturbation concepts. It was developed for n-heptane, the use of which is motivated by the fact that it shows very similar ignition behaviour as Diesel fuel.

The mechanism has shown good agreement in previous studies of auto-igniting turbulent n-heptane fuel sprays [21] and in Diesel engine simulations [22]. A validation for the mechanism by means of ignition delays for homogeneous mixtures at different equivalence ratios was presented in [21] for the experimental data from [30].

The NO_x submechanism contained in the mechanism developed by [31] accounts for thermal, prompt and nitrous oxide formation and for NO_x reburn by hydrocarbon radicals and amines. For combustion models of the eddy break-up type, NO_x emission computations are often performed in a post-processing fashion by employing an (extended) Zeld'ovich mechanism and evaluating the chemical sources/rates by means of the Favre averaged species concentrations and temperature. The calculation of the NO_x emissions in the CMC code by means of the available comprehensive sub-mechanism conceptually offers two advantages: On the one hand it allows for turbulence-chemistry interactions to be accounted for, i.e. non-linear effects in the rates in particular due to the strongly fluctuating temperature and on the other hand NO_x reburn reactions can be treated due to the availability of radicals and amines in the detailed chemistry.

No soot modelling has been attempted in the framework of this study, although CMC based models have been proposed for turbulent non-premixed methane-air [32] flames and ethylene-air [33] flames. Empirical soot models of the 'production-oxidation'-type could in principle also be applied in a 'post-processing' step using Favre averages of potential soot precursor species and enabling to account also for the soot oxidation by OH – in addition to O₂.

CFD SOLVER

A RANS formulation with the RNG variant of the two-equation k-ε model is used to describe turbulence without adjustment of the model constants. For the two-phase treatment standard modelling practice has been followed by means of the built-in Langrangian-Eulerian formulation. Both droplet atomisation as well as secondary break-up is modelled with the Reitz-Diwakar approach [34] using default model constants; the required cone angle is prescribed at 10 degrees. Droplets impinging on solid walls are treated by means of the available splashing model [35]. Thermo-physical properties of the droplets (viscosity, density, latent heat, c_p, surface tension and saturation pressure) are approximated by the values of n-Dodecane which are computed internally as a function of temperature. Possible inter-droplet collisions are modelled based on the work of [36], which distinguishes three principal behaviours, namely coalescence, separation and bouncing.

All measured points are without exhaust gas recirculation (EGR) and the remaining trapped residual gases have not been accounted for in the simulation. The flow is initialised as technical air with a prescribed swirl profile (based on the measured Tippelmann number) and estimated turbulence parameters at the time of intake valve closure, i.e. no valve motion and intake flow has been simulated.

The piston face, cylinder liner and cylinder head boundaries are set to a constant temperature of 420 K



but allowing for heat losses, hence representing walls with infinite heat capacities. Due to the piston kinematics a velocity boundary condition is additionally imposed on the piston face by means of user coding.

Two computational grids have been used, which both exploit symmetry and hence only model one eighth of the chamber. The standard grid has a cell count of 26,945 at bottom dead centre (BDC), of which 3,680 cells remain active at top dead centre (TDC). In the bowl region, this leads to an average cell volume of approximately 4.6 mm³. To assess the influence of the spatial resolution, a high resolution grid with 181,056 cells has also been tested, which almost halves the cell dimensions in all three spatial directions. The bowl cell count for this refined mesh amounts to 15,936, which leads to an average cell volume in this region of only 0.628 mm³.

Enthalpy in STAR-CD is solved in the form of the total enthalpy with polynomial representation of the specie's c_p . No transport equations for the species mass fractions are required in STAR-CD as the species mean mass fractions are returned from the CMC by convolution of the conditional mass fractions with the PDF, $\tilde{P}(\eta) = P(\tilde{\xi}, \tilde{\xi}^{\eta^2}, \eta)$. A β -function has been presumed, which is governed by two moments; namely the Favre averaged mixture fraction and its variance, obeying the following transport equations:

$$\frac{\partial \bar{\rho} \tilde{\xi}}{\partial t} + \nabla \left[\bar{\rho} \tilde{u}_j \tilde{\xi} - \left(\bar{\rho} D_{\tilde{\xi}} + \frac{\mu_t}{Sc_{\tilde{\xi}}} \right) \nabla \tilde{\xi} \right] = \dot{S}_d \quad (6)$$

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{\xi}^{\eta^2}}{\partial t} + \nabla \left[\bar{\rho} \tilde{u}_j \tilde{\xi}^{\eta^2} - \left(\bar{\rho} D_{\tilde{\xi}^{\eta^2}} + \frac{\mu_t}{Sc_{\tilde{\xi}^{\eta^2}}} \right) \nabla \tilde{\xi}^{\eta^2} \right] \\ = \frac{2\mu_t}{Sc_{\tilde{\xi}^{\eta^2}}} (\nabla \tilde{\xi})^2 - \bar{\rho} \tilde{\chi} \end{aligned} \quad (7)$$

The source term, $\dot{S}_d$, in the right hand side (RHS) of the mixture fraction equation (6) accounts for the evaporating droplets. Standard industrial practice has been followed here neglecting such influences in the equation for the mixture fraction variance; this is an area where improvements are necessary.

The unconditional scalar dissipation rate is computed from the turbulence quantities as:

$$\tilde{\chi} = c_\chi \frac{\tilde{\varepsilon}}{k} \tilde{\xi}^{\eta^2} \quad (8)$$

where a prescribed value of 2.0 has been used for the model constant c_χ following standard practice; despite reported sensitivity with respect to this quantity, e.g. [37,38].

VALIDATION DATA

ENGINE CONFIGURATION

The validation data from [39] has been collected on a four-stroke turbocharged and inter-cooled heavy-duty engine installed in both off-road building machinery as well as on-road vehicles. It has a displacement of roughly 1.6 litres per cylinder; the in-line four-cylinder variant for which the data is reported produces a peak power output of 183 kW at an engine speed of 2,100 RPM. The cylinder head configuration is of a two valves per cylinder type with push-rod actuation. The main engine data is summarised in Table 1 below.

Heavy duty 4-stroke, direct injection, turbocharged, intercooled Diesel engine	
Cylinders	4
Bore x stroke	122 x 142 mm
Displacement	6.64 litres
Compression ratio	17.2
Crank radius / connecting rod length ratio	0.3114
Maximum boost pressure ratio	2.6
Maximum power output	183 kW
Engine top speed	2100 RPM
Maximum BMEP	20 bar
Maximum cylinder pressure	160 bar
Swirl (Tippelmann number)	0.65

Table 1 – Liebherr D924 main engine data

Fuel is injected by means of a common-rail system with a suction throttled pump and an eight-hole solenoid injector for which details are given in Table 2 below; further details can be found in [39]. Needle lifts as well as time-resolved fuel injection rates are available for all setups, the latter were measured on an injection rate analyser.

Injector	Common Rail Technologies AG P2/ETH-LMB prototype
Max. injection pressure	1600 bar
Nozzle diameter	8 x 200 µm
Nozzle L/D ratio	5.16
Fuel pump	ETH development, suction throttled. Max. pressure 2000 bar

Table 2 – Liebherr D924 fuel injection system

To comply with increasingly stringent emission legislation, on-road heavy duty engines need to fulfil the requirements as set out in the European Stationary Cycle (ESC) test [40]. In this test, measurements are taken at 13 different loads and engine speeds and suitable weighting of these points is carried out as depicted in the engine map in Figure 2 to create a representative average engine loading.