

Simulations of Diesel Sprays Using the Conditional Moment Closure Model

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ABSTRACT

Numerical simulations of diesel sprays in a constant-volume vessel have been performed with the conditional moment closure (CMC) combustion model for a broad range of conditions. On the oxidizer side these include variations in ambient temperature (800-1100 K), oxygen volume fraction (15-21 %) and density (7.3-58.5 kg/m³) and on the fuel side variation in injector orifice diameter (50-363 µm) and fuel pressure (600-1900 bar); in total 22 conditions. Results are compared to experimental data by means of ignition delay and flame lift-off length (LOL). Good agreement for both quantities is reported for the vast majority of conditions without any changes to model constants: the variations relating to the air side are quantitatively accurately predicted; for the fuel side (viz. orifice diameter and injection pressure) the trends are qualitatively well reproduced. For the reference case, three different *n*-heptane chemical mechanisms (with 22, 29 and 67 species) have further been compared with respect to the ignition process and the subsequent flame stabilization and the flame structure is compared to conceptual models presented in the literature. At those conditions all three mechanisms showed comparable results. Based on the findings reported, CMC is seen as a highly promising approach to model spray combustion for a very broad range of diesel engine relevant conditions.

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INTRODUCTION

Diesel engines are the most used propulsion system for transportation due to the high energy density and thermal efficiency. However, because of increasingly stringent legislations concerning pollutant emissions, as NO_x and soot, there is the need to improve understanding of in-cylinder processes. For example, the flame lift-off length has a strong influence on spray combustion and therefore on exhaust emissions because of the different air entrainment within the spray [1, 2]. A review concerning LOL behavior in diesel jets depending on operating conditions can be found in [3].

In the last decades the computational fluid dynamics (CFD) approach has received increased attention towards the understanding and development of modern diesel engines. Due to well characterized conditions and easier optical access, the validation of simulation models for diesel sprays has often been carried out in constant-volume or -flow configurations. In particular, the constant-volume combustion chamber from Sandia National Laboratories has received much attention by modelers in the last years. For the data reported therefore, numerous reactive fuel spray simulations under diesel engine conditions have been carried out using a

variety of combustion models capable of inclusion of detailed chemistry. Such approaches include e.g. the perfectly stirred reactor (PSR) [4, 5, 6], partially stirred reactor (PaSR) [7, 8], flamelet generated manifold (FGM) methods [9], one-dimensional flamelet models [10] and the transported probability density function (PDF) approach [11]. Even for these high-fidelity combustion systems with well-defined initial and boundary conditions, substantial sensitivity has been found e.g. for different chemical mechanisms or measurement uncertainties [12] and large differences are reported for different spray and combustion modeling approaches in [13]; where results from different groups are compared side-by-side in a joint effort to improve and establish best practices concerning both modeling as well as experiments.

Models used in engineering practice for high pressure spray combustion of diesel, typically resolve only part of the turbulence spectrum and must hence rely on closures for the source terms of the chemical processes occurring at the unresolved scales. Due to overlap between the various time-scales relating to turbulence with the ones pertaining to the oxidation of hydrocarbon fuels and pollutant formation, decoupling is conceptually not feasible. Various models

neglecting turbulence-chemistry interaction (TCI) have nonetheless seen highly successful application to spray combustion. In a recent study, Pei et al. [11] discussed the influence of TCI by comparing results for *n*-heptane sprays from two modeling approaches: the PDF and the PSR method. A significant difference in flame structure was reported, where the PDF method predicted a broader reaction zone and better results for ignition delay and LOL for most cases were achieved.

The CMC model employed in this study belongs to the category of presumed PDF approaches, which allows for inclusion of detailed chemistry and accounts for TCI. CMC has seen highly successful application to a very wide range of flames and non-premixed auto-ignition as reviewed in [14]. For auto-igniting sprays at engine relevant conditions, several studies using CMC have also been reported for constant-volume cells [12, 15, 16], constant-pressure reactors [17] as well as real diesel engines [18, 19]. Diesel engine combustion is characterized by substantially varying conditions not only in terms of pressure and temperature levels on the oxidizer side, but also with respect to the composition (e.g. due to Exhaust Gas Recirculation, EGR). Additionally, highly flexible injection systems lead to considerable variability also with respect to the introduction of the fuel. The main focus of this study is hence to assess the model capability using unchanged model constants, chemical mechanisms and CFD as well as CMC grid resolutions for a very broad range of conditions relevant to diesel engine combustion.

The paper is organized as follows: following the presentation of the numerical method, three selected *n*-heptane chemistries are assessed for a reference condition by means of 'standalone' flamelet autoignition calculations and 'full' spray simulations using 2D-CMC. For the selected reduced chemical scheme, results are subsequently presented for a broad range of conditions relevant to Diesel engines, followed by conclusions.

NUMERICAL METHODOLOGY

Flow Field Solver

The STAR-CD CFD solver 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-ε* model with the corresponding 'standard' wall functions [20]. Due to the symmetric arrangement of the spray, a quasi-2D mesh with one degree angle has been employed. The length of the domain is 108 mm and the diameter was chosen to fit the experimental volume of the vessel. The resolution of the mesh was $0.5 \times 0.5 \text{ mm}^2$ in the first 15 mm radially along the entire domain. In the outer part the cell size was set to $1 \times 1 \text{ mm}^2$.

A Lagrangian treatment is adopted for the fuel injection using models offered by STAR-CD: atomization is calculated by means of the Huh/Gosman model [21] which predicts an

initial drop size distribution and the spray cone angle; while secondary break-up is accounted for by the Reitz-Diwakar model [22]. Potential interaction of droplets with walls is treated with the splashing model of Bai. Collisions between droplets are modeled following O'Rourke. For droplet drag and heat/mass transfer the standard correlations implemented in STAR-CD are employed. Further details as well as references to the respective models can be found in [20]. Droplet thermophysical properties have been approximated by *n*-dodecane, for which STAR-CD calculates the relevant quantities internally as a function of temperature (c_p , viscosity, latent heat, vapor pressure, density and surface tension).

The 'chemico-thermal' enthalpy equation is transported by STAR-CD employing polynomial c_p for the species. For the latter, no transport equations are solved, since the respective mass fractions are obtained by convolution of the conditional values calculated by the CMC code (discussed below) with a presumed Probability Density Function (PDF). A beta-PDF is used, constructed by means of the mixture fraction and its variance (eqs. (1) and (2), respectively):

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

In single-phase combustion, the mixture fraction is considered a conserved scalar due to the absence any terms on the right hand side (RHS); while for the spray calculations performed here, evaporating droplets give rise to a source term.

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

The second term on the RHS in eq. (2) denotes the scalar dissipation rate (SDR), which further requires the turbulent kinetic energy, *k*, and its dissipation rate, ϵ , as follows (with the model constant c_χ set to a value of 2.0 as is standard practice):

$$\tilde{\chi} = c_\chi \frac{\tilde{\epsilon}}{k} \tilde{\xi}^{\eta^2} \quad (3)$$

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 [15].

In the experiment, roughly one second elapses between the pre-combustion and the fuel injection events. Based on

the rapid decay of turbulence (as discussed also in [12] relating to the filling process), the flow field is initialized as quiescent. Concerning fuel injection, a top hat mass flow rate profile is used according to experimental data. Walls have been assumed adiabatic.

Combustion Model

The combustion model employed belongs to the group of presumed PDF methods; the methodology and governing equations were originally put forward in [23]. Here, the equations are implemented for the conditional species mass fractions, Q_α , and temperature, Q_T , as follows:

$$\begin{aligned} & \frac{\partial Q_\alpha}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} \\ & + \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[\langle u_i Y_\alpha'' | \eta \rangle \bar{\rho} \tilde{P}(\eta) \right] = \langle w_\alpha | \eta \rangle \\ & + \left[\delta_{\alpha f} - Q_\alpha - (1 - \eta) \frac{\partial Q_\alpha}{\partial \eta} \right] \langle \Pi | \eta \rangle \\ & + \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial \eta} \left[(1 - \eta) \bar{\rho} \tilde{P}(\eta) \langle Y_\alpha'' \Pi'' | \eta \rangle \right] \end{aligned} \quad (4)$$

$$\begin{aligned} & \frac{\partial Q_T}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_T}{\partial x_i} = \langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \\ & \langle N | \eta \rangle \left[\frac{1}{\langle c_p | \eta \rangle} \left(\frac{\partial \langle c_p | \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^N \langle c_{p,\alpha} | \eta \rangle \frac{\partial Q_\alpha}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta} \\ & - \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial x_i} \left[\langle u_i T'' | \eta \rangle \bar{\rho} \tilde{P}(\eta) \right] \\ & + \frac{1}{\langle c_p | \eta \rangle} \left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \right| \eta \right\rangle + \frac{\langle w_T | \eta \rangle}{\langle \rho | \eta \rangle \langle c_p | \eta \rangle} + \frac{\langle w_{WALL} | \eta \rangle}{\langle \rho | \eta \rangle \langle c_p | \eta \rangle} \\ & - \langle \Pi | \eta \rangle \left[\frac{h_{fg}}{\langle c_p | \eta \rangle} + Q_T + (1 - \eta) \frac{\partial Q_T}{\partial \eta} \right] \\ & - \frac{1}{\bar{\rho} \tilde{P}(\eta)} \frac{\partial}{\partial \eta} \left[(1 - \eta) \bar{\rho} \tilde{P}(\eta) \langle T'' \Pi'' | \eta \rangle \right] \end{aligned} \quad (5)$$

where the last two terms in both equations relate to the effect of evaporating droplets which are implemented according to [15].

Conditional turbulent fluxes of species $\langle u_i Y_\alpha'' | \eta \rangle$ and temperature $\langle u_i T'' | \eta \rangle$ are closed with the commonly employed gradient flux hypothesis; $\langle u_i | \eta \rangle$ denotes the conditional velocities for which a linear model is applied.

The conditional chemical source terms $\langle w_\alpha | \eta \rangle$ and $\langle w_T | \eta \rangle$ are closed at first order, i.e. using the conditional species

mass fractions and conditional temperature. Pressure is assumed constant for all values of the mixture fraction; the time derivative is retained in the present formulation to enable calculations for closed combustion chambers and engines with time-varying geometries.

The conditional scalar dissipation $\langle N | \eta \rangle$ rate is modelled based on the unconditional value following the AMC approach [24]:

$$\begin{aligned} \langle N | \eta \rangle &= N_0 G(\eta) \\ G(\eta) &= \exp \left(-2 \left[\text{erf}^{-1}(2\eta - 1) \right]^2 \right) \\ N_0 &= \frac{\tilde{\chi}}{2 \int_0^1 G(\eta) \tilde{P}(\eta) d\eta} \end{aligned} \quad (6)$$

No soot modelling efforts as in [16] have been attempted and any associated radiative heat losses have hence not been accounted for in this study.

Chemical mechanisms

n-Heptane has been used to model the D2 fuel used in the experiment since it has seen successful application to autoigniting diesel sprays, e.g. in [19]. Three chemical mechanisms have been considered: a compact reduced scheme based on a skeletal chemistry documented in [25], a mechanism which has been well demonstrated for engine calculations (using alternative combustion models) [26] and a considerably larger mechanism however still applicable to CMC for comparison [27].

Table 1. Mechanism complexity of the three different chemistries.

	Pitsch [25]	ERCv2 [26]	Hewson [27]
Number of species solved (total no. species)	22 (44)	29	67
Reaction steps	18	52	265

The species and number of reaction steps are summarised in Table 1 above. Since the reduced chemistry employs quasi-steady-state assumptions (QSSA) for some of the intermediates, only a selection of the total of 44 species is solved for.

Numerical method

The CMC equations are discretized with finite differences and employ second order for the diffusion terms while the convective terms are first order. Time integration is performed by means of a stiff integrator using operator splitting. Further details can be found in [12, 17, 18].

A two-dimensional formulation of the CMC equations is employed since the domain is axisymmetric and good results have been previously reported for autoigniting sprays

therewith in [12, 15, 16, 17]. The spatial variations of the conditional quantities is much weaker than their corresponding unconditional values, hence substantially reduced resolutions are possible. Various axial and radial CMC node combinations have been employed to assess the CMC resolution influence as will be discussed later on. In mixture fraction, 101 grid points are used which are clustered around the stoichiometric value.

Test cases

Data from the constant-volume combustion chamber installed at Sandia National Laboratories [13] and presented in [28, 29] have been used for model validation. All cases were operated with D2 fuel, for which properties specification can be found in [28]. The test cases considered are listed in Table 2, where the reference case is marked in bold. All variations have been considered independently, i.e. not all combinations have been calculated. Operating parameters have been changed only one at a time starting from the reference case.

Table 2. List of test cases considered. Experimental data from [13]. Reference case in bold.

Parameter varied	Quantities computed
Nozzle diameter d_0	50/71/100/ 180 /246/363 μm
Temperature T	800/850/900/950/ 1000 /1100 K
Oxygen concentration $[\text{O}_2]$	15/17/19/ 21 %
Density ρ	7.3/ 14.8 /30/58.5 kg/m^3
Injection pressure Δp	600/900/1100/ 1400 /1700/1900 bar

RESULTS AND DISCUSSION

In the following, comparison of the three different chemical mechanisms for the reference case (cf. Table 1) are first considered by means of “*flamelet*” calculations and then with 2D-CMC. For the latter, the ignition behavior and flame stabilization as well as the structure of the developed flame are analyzed. Subsequently, ignition delay and flame LOL for the Pitsch chemical mechanism were compared with measurements for variations in ambient temperature, oxygen and density and variations in fuel pressure and orifice diameter.

Flamelet Calculations

In a first step “*flamelet*” calculations according to [30] starting from the mixing solution are employed in order to be able to compare the chemistry behavior in a reactive-diffusive system.

The SDR is computed according to equation (6) where N_0 denotes the peak of the bell shaped curve, i.e. $N_0 = \langle N \rangle \eta = 0.5 \zeta$. In [17] the influence of the SDR on ignition delay for

autoigniting flamelets was studied starting from the mixing solution; at the conditions studied it was found that for a peak SDR below 25 s^{-1} the ignition delay was almost independent on SDR. In this study a constant value of $N_0 = 10 \text{ s}^{-1}$ for all test cases has hence been considered. In this way only the chemical component of the ignition delay is considered and the injection and fuel evaporation was not accounted for and therefore the computed delays are expected to be underpredicted. The comparison of the calculated ignition delay is considered in a qualitative way and it should give an impression of the evolution and distribution in mixture fraction of some key quantities in a simplified configuration.

The temperature evolution during ignition is compared as shown in Figure 1: the three mechanisms considered showed a similar evolution of the temperature with an increase of 1000 K within 0.1 ms during the thermal runaway between 0.4 and 0.5 ms. At the very early stages, the Pitsch and Hewson chemistries exhibit the highest activity close to the oxidizer boundary. Radicals produced there however diffuse towards richer mixture fraction values and auto-ignition occurred on the fuel rich side, i.e. at the most reactive mixture fraction, ζ_{MR} , [31] which was at around 0.12. This behavior was also observed in [17] and is in line with results reported in [18] under diesel engine conditions. For the ERCv2 mechanism, the temperature increased by about 100 K almost immediately on the rich side; however ignition proceeds very similarly, with a shorter ignition delay and at a slightly leaner value of ζ_{MR} .

Figure 2 compares the developed flame structures at 5 ms: the peak temperature is the same for all cases. On the lean side the temperature is almost identical for all mechanisms, while on the rich side the ERCv2 shows considerably higher values. E.g. at a mixture fraction of 0.2 the differences amount to approximately 150 K. This is attributed to differences in the conditional CO_2 and CO mass fractions: while the agreement for these species on the lean side is excellent for all chemistries, for mixture fractions between 0.07 and 0.2 the CO_2 values calculated by ERCv2 are up to 50% higher than the other two kinetic schemes (not shown). The OH mass fraction profiles peak at the stoichiometric mixture fraction for all cases as expected. Peak values are of the order of 0.003 with differences amounting to 16 percent at most. The ERCv2 OH profile drops rapidly on the fuel rich side further evidencing an increased high temperature oxidation of CO to CO_2 via OH compared to the other two mechanisms. These discrepancies on the fuel rich side can possibly be attributed to the reduction procedure during the mechanism development: since ERCv2 was targeted at HCCI combustion the optimization was carried out for equivalence ratios between 0.2 and 1.0 for a range of temperatures and EGR rates [26]. As it has been applied to study classical diesel combustion, i.e. mixing controlled modes also in other studies e.g. [5, 32], it has nonetheless been included in this comparison.