

Modeling Split Injections of ECN “Spray A” Using a Conditional Moment Closure Combustion Model with RANS and LES

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ABSTRACT

This study investigates n-dodecane split injections of “Spray A” from the Engine Combustion Network (ECN) using two different turbulence treatments (RANS and LES) in conjunction with a Conditional Moment Closure combustion model (CMC). The two modeling approaches are first assessed in terms of vapor spray penetration evolutions of non-reacting split injections showing a clearly superior performance of the LES compared to RANS: while the former successfully reproduces the experimental results for both first and second injection events, the slipstream effect in the wake of the first injection jet is not accurately captured by RANS leading to an over-predicted spray tip penetration of the second pulse. In a second step, two reactive operating conditions with the same ambient density were investigated, namely one at a diesel-like condition (900K, 60bar) and one at a lower temperature (750K, 50bar). For the diesel-like condition, both modeling approaches captured first injection ignition delay, overall soot mass and soot location well. Due to an under prediction of spray tip expansion during combustion in combination with the slight over-prediction of the vapor tip penetration, RANS-CMC’s reactive spray penetration length nonetheless agreed well with the experiment. However, RANS-CMC did not capture full combustion recession towards the injector location after the end of the first injection. LES-CMC showed accurate predictions of the second injection ignition delay and improvements with respect to combustion recession, and flame structure. For the low temperature condition, RANS-CMC accurately predicted ignition timing. Here LES-CMC slightly under-predicted ignition delay. Ignition location and flame structure are in reasonable agreement with the experiment for both numerical setups. In accordance to the experiment it was seen that for both RANS- and LES-CMC the first injection does not auto-ignite and the second injection was necessary to create the appropriate local conditions for ignition to occur. Furthermore, the simulations did not predict any soot at the lower temperature, in agreement with the experimental observations. The findings suggest that LES may be necessary in the case of split injections towards accurate two-phase flow field predictions and - even more so - to capture full combustion recession for diesel-like conditions. The proposed RANS- and LES-CMC models show considerable promise for the challenging dynamics of auto-igniting fuel sprays with multiple injections.

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INTRODUCTION

Diesel engines have enjoyed immense popularity for more than a century for passenger, freight and maritime transport as well as power generation due to their reliability, cost and efficiency. In view of increasingly tightening emissions legislation, various spray combustion strategies are being introduced to replace the conventional Diesel operation prone to formation of soot and NO_x, due to energy conversion modes occurring over a wide range of equivalence ratios and at high temperatures. Lowering the reactivity of the ambient air, e.g. by reducing the temperature or oxygen content (e.g. by introducing exhaust gas recirculation - EGR) prolongs ignition and consequently increases time for mixing. Both approaches conceptually reduce the soot formation potential; lower oxygen

contents however affect also soot oxidation. For low EGR rates, the latter has been shown to dominate, resulting in higher engine out soot. At very high EGR rates soot formation can be suppressed altogether, leading to a trend reversal, see e.g. [1], [2], [3], [4]. Lowering ambient temperatures (e.g. by Miller valve timing) has shown to reduce NO_x emissions up to a point; for very low temperatures a NO_x trend reversal has been observed in combination with high cyclic variability of the combustion process [5], [6], [7], [8], [9]. The flexibility of modern injection systems allowing for several fuel injection events during one engine cycle has been exploited for both concepts. For soot reduction, post injections have been extensively studied both experimentally and numerically [10], [11], [12], [13] to identify appropriate dwell time and timing with respect to the underlying mechanisms reducing soot. Concerning low

ambient temperature, pilot injections are routinely employed by engine manufacturers to address on the one hand NVH issues as well as to ensure reliable ignition at low temperatures and pressures.

In addition to the existing challenging physics present in auto-igniting high-pressure fuel sprays, the turbulent flow field evolution of multiple injection events, as well as the chemico-thermal interactions between the first and second pulse complicate matters considerably. Improved fundamental understanding how multiple injections affect combustion at different engine operating conditions is evidently needed. To this end, experimental efforts in optically accessible rigs in combination with advanced numerical methods are indispensable. This numerical study focusses on the experimental work recently presented in [14] and [15] by Skeen et al., where the well-characterized “Spray A” of the Engine Combustion Network (ECN) was studied for a split injection setup (0.5ms injection - 0.5 ms dwell - 0.5 ms injection) using *n*-dodecane as a fuel. Two turbulence treatments have been assessed, namely the Reynold-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES). For both cases, a Conditional Moment Closure (CMC) combustion model has been used to investigate two of the three operating conditions reported in [14], namely a diesel-like environment at 900 K, 60 bar (referred to as Case 1) and a low ambient temperature condition at 750K, 50bar (referred to as Case 2).

For the short split injections of “Spray A”- to the authors best knowledge - the only other modeling study reported was carried out in the RANS-Transported Probability Density Function (TPDF) context by Chishty et al. [16]. Ignition delay times, lift-off lengths and flame structures compare well to the experimental results, suggesting that the RANS-TPDF approach is promising. Difficulties were however reported concerning the spray vapor penetration of the second injection event which were attributed to the RANS turbulence model. Following successful application of CMC to single injections, the present study seeks to assess the predictive capability of the model for split injections. In addition to RANS-CMC, LES-CMC has been used here specifically to study if turbulence model related processes governing the flow field evolution and mixing processes present for multiple injections can be accurately reproduced.

For single injections at “Spray A” conditions, a number of studies have been reported in the literature both in the RANS context [15] as well as for LES [17], [18], [19], [20], where a variety of combustion models ranging from “well-mixed” to transported PDF approaches were followed. The CMC combustion model used in this study has seen extensive application in conjunction with RANS to spray rigs of different sizes [21], [22], [23], [24], [25], [26], [27], [28], [29], optically accessible engines [2], [11], [12], [30], [31] as well as full metal engines [32], [33], [34], while application to constant pressure and constant volume spray test rigs at Diesel engine conditions in using LES-CMC is reported in [20], [35], [36]. LES-CMC has also been applied with success to turbulent single phase flames by various other groups, e.g. [37], [38], [39], [40]; for a review of auto-igniting flames see [41].

This paper has the following layout: first the non-reactive vapor penetration length and mixing is analyzed for both flow-field solvers. Reactive calculations of Case 1 and Case 2 are subsequently

performed with RANS-CMC and LES-CMC and discussed in terms of ignition delay times of first and second injections, flame structure (e.g. temperature, formaldehyde, acetylene and OH contours) and soot predictions and compared to experiments.

METHODOLOGY

Flow-Field Solvers and Numerical Setups

The commercial CFD program Star-CD [42] was used for both RANS and LES computations. The two-phase flow-field (i.e. fuel injection and ambient gas mixture) was solved according to the Lagrangian/Eulerian formulation [43]. The used spray injection calibration and droplet primary and secondary break-up models (described in detail in [42], [44], [45]) for the RANS and LES simulations were taken from previous works of [46] and [47] where the same *n*-dodecane “Spray A” setup was validated for single injections at the equivalent ambient density as the operating conditions that are investigated in this paper. Therefore the spray calibration was not repeated here.

Thermo-physical properties of *n*-dodecane droplets are calculated internally by Star-CD, which returns specific heat capacity, viscosity, latent heat, vapor pressure, density and surface tension as a function of temperature. The initial flow-field turbulent energy is set to 1.25 J/kg for both numerical solvers. With the flame developing far away from the reactor walls, wall boundaries are assumed as adiabatic [48].

The split injection profile is an approximation of the measured mass flow rate taken from [49] as shown in Figure 1.

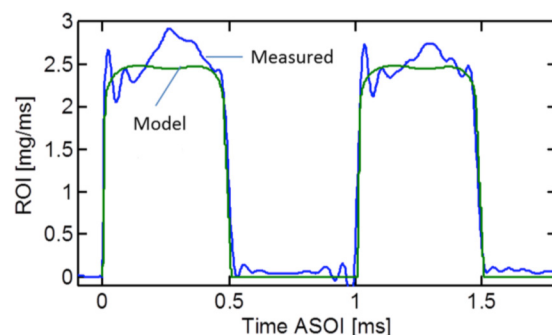


Figure 1. Illustration of the split injection profile as specified by Sandia National Laboratories [49].

Reynold-Averaged Navier-Stokes (RANS) Numerical Setup

Solution of the unsteady RANS equations computes the ensemble average and allows for symmetry to be exploited. For the current setup, an axisymmetric quasi-2D domain is hence employed, leading to a significant reduction of computational cost. The RANS numerical setup was taken from Pandurangi et al. [46], whose work already prepared and validated the CFD setup for *n*-dodecane “Spray A” single injection at the same ambient conditions. Here only the split-injection profile was updated. Based on the grid sensitivity analysis undertaken in [50], an optimal cell size of 0.5x0.5 mm in the injector vicinity and along the center axis was chosen. The cell size was gradually increased to a maximum of 2x2 mm in the far field.

outwards in radial direction from the injector, with the spray always inside the 0.5 mm zone. The total number of cells in the 2D-CFD axisymmetric mesh with a two degree opening angle was 17,820.

Closure of the Reynolds Stress Tensor was completed with the well-known k - ε model using the recommended model constants for diesel spray combustion seen in Table 1 k - ε [15], [51], [52].

Table 1. k - ε model constants for RANS simulation.

C_μ	$C_{\varepsilon,1}$	$C_{\varepsilon,2}$	$C_{\varepsilon,3}$	$C_{\varepsilon,4}$	κ	Pr
0.09	1.52	1.92	1.44	-0.33	0.419	0.9

Large Eddy Simulation (LES) Numerical Setup

LES on the other hand solves filtered variants of the Navier-Stokes equations, using a spatial filter Δ which is correlated to cell volume V as $\Delta = \sqrt[3]{V}$. Turbulent motion that is larger than the filter width is hence resolved. Any turbulent motion below the threshold Δ , i.e. sub-grid scale (SGS), which is responsible for dissipation of turbulent kinetic energy, is modeled. In this study, the k - l model is used to compute the SGS turbulent kinetic energy k_{SGS} and the SGS viscosity μ_{SGS} with model constants set to their default values as detailed in [42]. A full 3D mesh is necessary, making these computations considerably more expensive than RANS. The same LES mesh as used by Farrace et al. [47] - already applied for *n*-dodecane “Spray A” single injections at the same density as studied here - was retained. A rendering of a planar slice of the mesh is depicted in Figure 2 with the injector located at the center of the x-axis, spraying upwards in z-direction. Similar to the RANS mesh, the LES mesh is more refined in the near-nozzle region. After a mesh sensitivity analysis conducted by [47], the densest grid along the center-line has a characteristic length of 0.125 mm, while the largest cells close to the walls are 2 mm. Exact values of the refinements are documented in [47].

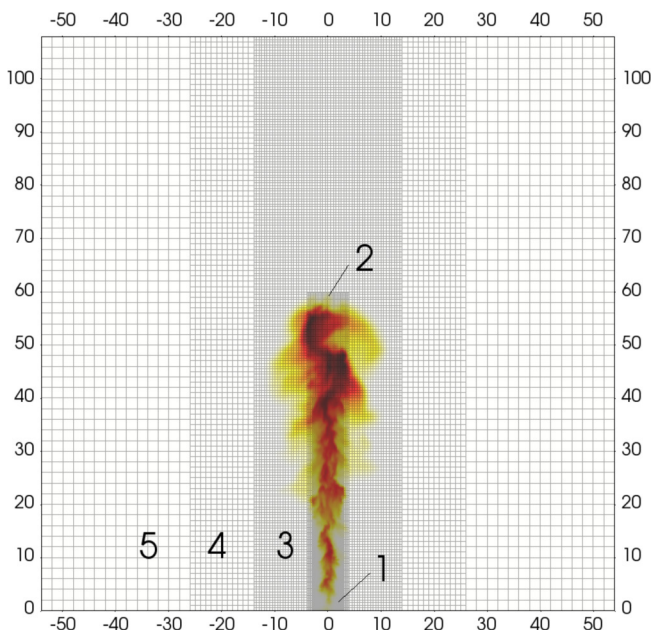


Figure 2. Rendering of the LES mesh (planar slice) of “Spray A” with five different refinement zones as described in [47]. Cell sizes are the smallest in the near-nozzle vicinity. Total mesh size: circa 1.9 million. A representative spray diffusion flame is also shown. All units in mm.

In LES shot-to-shot variability can be accounted for and in this paper a total of 10 realizations (five per Case) were computed motivated by the findings reported by Pei et al. [19], [53] which state that with five LES realizations a 98 to 99% similarity to an equivalent of 16 LES realizations for larger scale fluctuations (e.g. mixture fraction and velocity magnitude) and temperature can be achieved. For variables with shorter scale fluctuations, more LES realizations are necessary. Initial conditions were identical for all realizations and the resulting shot-to-shot variations are due to the turbulent droplet dispersion model employed, which introduces an extra term in the k_{SGS} equation; the same model was also applied in [20], [35], [36]. The fluctuating velocity is derived from the resolved value by means of an approximate deconvolution method, for further details concerning the implementation see [42].

Combustion Model

The Conditional Moment Closure combustion model is a conserved scalar method used to close the chemical source term present in the species and enthalpy transport equations. In non-premixed combustion, it is common practice to use the mixture fraction as the non-reactive scalar, which is a measure of the local state of mixing. CMC solves transport equations for species and temperature conditioned on the mixture fraction and exploits the weaker dependence of the conditional quantities compared to their unconditional counterparts. For more details the reader is referred to the detailed derivation of the method presented by Klimenko and Bilger in [54]. In this paper 2D-CMC meshes were used for both RANS (20 x 54 mesh resolution) and LES (12 x 202 mesh resolution) setups where the azimuthal dimension is collapsed.

The *n*-dodecane chemical reaction mechanism employed in this study was specifically developed by Yao et al. [55] for “Spray A” simulations. It comprises low temperature reactions (of vital importance for Case 2) and is quite compact with only 54 species and 269 reactions.

Conditional Moment Closure in Reynolds-Averaged Navier-Stokes Context

The CMC equations in the RANS context were presented in detail in [21] and are not repeated here for brevity.

Conditional Moment Closure in Large Eddy Simulation Context

For this paper the in-house CMC code, which initially based on the RANS context, needed to be modified for LES computations to solve the conditionally *filtered* variables to ensure consistency with the *filtered* LES equations. The derivation of the LES-CMC equations and considerations concerning the interfacing between LES and CMC are discussed in detail in [56], [57] and not repeated here. The LES-CMC model used in this study was first applied to spray combustion in [39], where validation of the model in terms of ignition delay times, ignition locations and early pressure rise was reported for two high pressure, high temperature constant pressure and constant volume vessels. A

further assessment of the numerical platform was presented by Farrace et al. [20] for *n*-heptane and *n*-dodecane combustion at “Spray A” conditions yielding promising results.

Conditional Moment Closure for Multiple Injections

In literature [58], [59], [60], [61], considerable effort has been put into increasing the dimensionality of flamelet models in order to account for more than one spray, i.e. multiple injections. The Representative Interactive Flamelet (RIF) model was modified to accommodate the two-dimensional flamelet equations with two mixture fractions [58], slightly later it was extended to allow any number of injections [59]. These methods describe a three-feed system in which more than two streams are mixing and the basic equations are depending on mixture fractions ξ_1 and ξ_2 . Extending the dimensionality of the CMC equations would lead to a tremendous increase of complexity and computational costs. Hence, an extended Conditional Moment Closure model was introduced in [62] in a RANS context and was successfully applied in [11], [12]. Since the general structure of RANS-CMC equations and LES-CMC equations are alike, the multiple injection approach developed for RANS can be adapted to the LES case. The main idea of the model is to transform the original temperature and species profiles conditional on the mixture fraction originating from the first injection (MF1) into representative profiles which are conditional on the total mixture fraction (MFT). It has to be pointed out that using one conditional quantity instead of two requires the collapse of one dimension similar to what is seen during initialisation of a 2D-RIF model in case of a subsequent injection [59]. Since the CMC grid is spatially resolved in two dimensions, a detailed determination of time and location of contact between fuel streams as well as their local conditions is possible. The model is based on re-initialisation of the conditional temperature and species profiles in every CMC cell at the time of the first appearance of the of the mixture fraction coming from the second fuel stream (MF2). Further details concerning the re-initialization procedure can be found in [11].

EXPERIMENTAL SETUP

The experimental results originate from the ECN “Spray A” split injection campaign presented by Skeen et al. [14], [15]. In the present study, two of the three operating experimental conditions were investigated; cf. Table 2. The available optical experimental data for model validation consisted of planar laser-induced fluorescence (PLIF) and schlieren high-speed imaging. The former was recorded at a wavelength equal to 355nm, ideally allowing for the visualization of formaldehyde (CH_2O). However, as highlighted in [14], CH_2O suffers from fluorescence interference of polycyclic aromatic hydrocarbons (PAH) and laser-induced incandescence (LII) of soot. Therefore all three (i.e. CH_2O , PAH and soot) are all seen in Case 1. For Case 2, at low ambient temperatures, no PAH or soot was recorded by [14]. The schlieren imaging allowed to compute vapor penetration length, first-injection and second-injection ignition.

Table 2. “Spray A” split injection experimental conditions [14].

	Case 1	Case 2
Ambient gas temperature	900 K	750 K
Ambient gas pressure	59.8 bar	49.3 bar
Ambient gas density	22.8 kg/m ³	
Ambient O ₂ content	15 % _{volume}	
Nominal nozzle diameter	90 μm	
Fuel injection pressure	1500 bar	
Fuel	<i>n</i> -dodecane	
Fuel temperature	363 K	
Injection pattern	0.5 ms / 0.5 ms dwell / 0.5 ms	
Injected fuel mass	1 st injection: 1.18 mg 2 nd injection: 1.16 mg	

RESULTS AND DISCUSSION

Non-Reactive Simulations of Vapor Penetration Length

As mentioned above, the spray calibration in RANS and LES was already done in previous works by [46] and [47], respectively, where the *n*-dodecane “Spray A” setup was tuned for a single injection (0-6 ms) setup yielding very good predictions in spray vapor penetration lengths. Therefore these models were adopted for the “Spray A” split injection simulations. In this case one would expect the first injection not to differ from the “Spray A” single injection, since both setups inject *n*-dodecane fuel at an identical injection rate into the same ambient conditions. The capability of these numerical setups to correctly predict the slipstream effect, caused by the momentum of the first spray which creates a low pressure zone at its tail that is seen by the second injection when first injected into the combustion chamber, was of particular interest. This was a key finding by Skeen et al. [14] and completely changed the spray dynamics of the second injection, causing the second pulse to penetrate faster than the first.

Non-reactive spray vapor penetrations of the simulations are illustrated in Figure 3 (RANS) and Figure 4 (LES). Ensemble averages from five realizations are shown for the LES results. For the simulations, the spray vapor penetration was computed by finding the furthest cell from the injector nozzle with $\xi \leq 0.001$. The solid lines starting from time zero indicate the first injection while the dashed lines the second. Experimental data is shown in black with yellow indicating the standard deviations of first and second injection, respectively. Looking at the first injection, RANS under predicts the duration and penetration of primary break-up and slightly under predicts the rest of the vapor penetration. At the time of ignition (roughly 0.35 ms) the computed RANS curve deviates by 7-8% from the experimental penetration length. Similar slight underpredictions were also reported in [50] using RANS in conjunction with comparable spray models and mesh resolutions. The second injection’s penetration is initially very accurately predicted by RANS, however after circa 1.2 ms it shifts to an over prediction, indicating