

LES of Diesel and Gasoline Sprays with Validation against X-Ray Radiography Data

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ABSTRACT

This paper focuses on detailed numerical simulations of direct injection diesel and gasoline sprays from production grade, multi-hole injectors. In a dual-fuel engine the direct injection of both the fuels can facilitate appropriate mixture preparation prior to ignition and combustion. Diesel and gasoline sprays were simulated using high-fidelity Large Eddy Simulations (LES) with the dynamic structure sub-grid scale model. Numerical predictions of liquid penetration, fuel density distribution as well as transverse integrated mass (TIM) at different axial locations versus time were compared against x-ray radiography data obtained from Argonne National Laboratory. A necessary, but often overlooked, criterion of grid-convergence is ensured by using Adaptive Mesh Refinement (AMR) for both diesel and gasoline. Nine different realizations were performed and the effects of random seeds on spray behavior were investigated. Additional parametric studies under different ambient and injection conditions were performed to study their influence on global and local flow structures for gasoline sprays. It is concluded that LES can generally well capture all experimental trends and comes close to matching the x-ray data. Discrepancies between experimental and simulation results can be correlated to uncertainties in boundary and initial conditions such as rate of injection and spray and turbulent dispersion sub-model constants.

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INTRODUCTION

In the last decade, there has been significant interest in the dual-fuel concept for low-temperature combustion (LTC) engine applications [1, 2, 3, 4]. In a dual-fuel engine, gasoline is typically injected early in the intake valve event with low injection pressure, while the diesel fuel provides the source of ignition and is injected at high pressure. High-fidelity simulations of gasoline and diesel spray breakup, interaction, etc. are critical for the accurate characterization of a dual-fuel combustion system.

Traditional Reynolds Averaged Navier-Stokes (RANS) turbulence modeling approach only solves ensemble averaged transport equations. In contrast, LES solves spatially filtered transport equations, allowing us to capture unsteady, large scale flow structures. Due to a relatively small value for the turbulent viscosity term in LES compared to RANS, LES modeling does not damp out small-scale perturbations. Correspondingly, more flow structures are observed with LES. A comprehensive review of LES approaches and sub-grid scale models for internal combustion engine applications can be found in references [5, 6].

With the aid of parallel processing and highly-scalable Computational Fluid Dynamics (CFD) solvers, LES is being increasingly applied to diesel sprays [7, 8], gasoline [9, 10] sprays as well as diesel combustion [11,12,13] simulations. For example, in order to gain confidence that the relevant flow structures were adequately solved, Senecal et al. [7] proposed smallest cell sizes between 0.0625 and 0.125 mm for LES-based spray simulations to achieve reasonable accuracy, acceptable runtimes, and grid-convergent behavior for both vaporizing and non-vaporizing diesel sprays. They also recommended averaging over a minimum of 9 LES realizations for reasonably representing the diesel spray behavior [14, 15]. Shost et al. [9] studied the effect of nozzle-hole length over diameter ratio (l/d) and fuel injection pressure on spray skew angle, spray plume cone angle, and primary breakup length for a Gasoline Direct Injection (GDI) injector using LES and the Volume of Fluid (VOF) approach. Their results showed that nozzle l/d reduction produced a notable increase of plume cone angle, while injection pressure posed little influence. Som et al. [12] studied diesel combustion using both the LES and RANS turbulence models. They found that the Smagorinsky based LES model captured the instantaneous soot contours under reacting conditions and the equivalence ratio contours under non-reacting

conditions, better than the RANS simulations. The LES model also better predicted volumetric auto-ignition and a fairly stabilized lift-off length, which was more realistic in those conditions.

Another important application of LES is for modeling turbulent flows in internal combustion engines to capture the stochastic nature of cycle-to-cycle variations (CCV) in lean-burn Spark Ignition (SI) engines [17, 18]. Enaux et al. [19] studied the cause of CCV in a spark ignition engine using LES. They successfully reproduced experimental findings and correlated CCV to velocity fluctuations in the flow-field at the spark plug, which induced variations in the early flame kernel growth and the overall combustion duration. More recently, Scarcelli et al. [20, 21] demonstrated that RANS can also capture CCV, provided resolutions and numerical schemes typically employed for LES were implemented in RANS calculations.

In contrast to most previous diesel spray studies on research injectors under well-known boundary conditions [7, 8, 12, 14, 15, 16] or on single-hole GDI injectors [9], this study simulated production multi-hole diesel and GDI injectors, which were equipped in a Chrysler dual-fuel prototype engine. The spray characteristics are critical for investigating the detailed fuel/air mixing and combustion processes in this engine. The main uncertainty originated from limited measurements of initial and boundary conditions for simulations. Due to the fact that cyclic variability may be better reproduced by the LES calculations, the main objective of this study was to implement LES for predicting the spray characteristics. It should be noted that engine simulations were not performed with LES since they were beyond the scope of the current project. Future studies may also focus on performing LES calculations of the dual-fuel engine.

This paper is organized as follows: first, experimental setup (from x-ray radiography measurements) and simulation approach will be briefly introduced. Then, non-evaporating diesel and GDI spray simulation results of global and local parameters will be presented and analyzed in detail. Finally, conclusions are drawn.

EXPERIMENTAL SET-UP

The gasoline and diesel sprays were characterized experimentally using x-ray radiography measurements at the 7-BM beamline of the Advanced Photon Source (APS) at Argonne National Laboratory. A focused x-ray beam ($5 \times 6 \mu\text{m}$) with a mean energy of 8 keV was passed through a pressurized chamber which houses the injector nozzle. Polyimide windows were used to both hold pressure and allow transmission of the x-ray beam. A PIN (intrinsic semiconductor region between p-type and n-type semiconductors) diode was used to measure the transmitted signal during “spray on” and “spray off” times, which was digitized by a Yokogawa oscilloscope and stored on a personal computer. The chamber was mounted on vertical and horizontal translations stages to allow a raster scanning of the x-ray beam through the spray. In the experiments, 32 independent measurements were performed at each one of a total of ~ 2000 beam coordinates and then averaged. Data were mapped into a single plot to deliver a 2-D projected density contour (see Figure 1). This contour is a two dimensional representation of an inherently three dimensional flow field. Liquid penetration can be obtained by

measuring the length of the isolated spray plume. The transverse integrated mass (TIM) at certain axial location can be obtained by integrating the projected density along the transverse distance at a single axial location. The operating conditions for the experimental data are listed in Table 1. Uncertainty in liquid length measurements is estimated to be about 5%. Details about the advanced diagnostics carried out at APS can be found in Ref. [22].

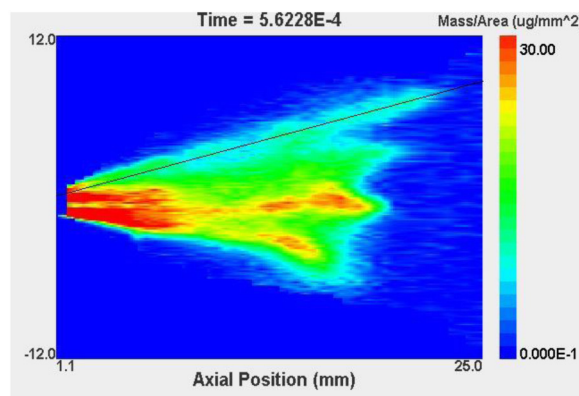


Figure 1. 2-D projected density contour plot from x-ray measurements at APS for the Gasoline Injector of interest.

Table 1. Experimental conditions for non-evaporating gasoline direct injection (GDI) and diesel sprays.

Parameters	GDI	Diesel
Chamber Pressure (bar)	1	20
Chamber Temperature (K)	300	300
Chamber Gas	N ₂	N ₂
Commanded Injection Pressure (bar)	100	1000
Commanded Injection Duration (ms)	1	0.442
Nozzle Diameter (μm)	180	110
Fuel Injection Temperature (K)	300	310
Number of holes	6	3

It should be noted that x-ray radiography measurement cannot provide a complete rate of injection (ROI) profile throughout the injection event. This is due to the fact that the fuel mass is calculated through the integral of density over the visualization domain. Therefore, injected mass versus time curve can only be obtained until the spray tips move out of the measurement window. After the spray tips leave the measurement boundaries, the injected mass used in this study was obtained by extrapolation. The ROI profiles were defined as the derivative of mass over time and shown for both diesel and gasoline injections in Figure 2. It can be seen that the actual diesel and GDI injection start at 0.23 and 0.33 ms after the commanded SOI, respectively. The same duration of delay was added to the corresponding simulation set-up. Thus the timings mentioned in the following text refer to the command SOI ($t = 0$ s), instead of actual SOI. It should also be noted that although the experiments were conducted under non-evaporating condition, the ambient density was comparable to relevant diesel and gasoline engine operating conditions during injection.

In GDI experiments, all the sprays were in the measurement window and hence, all were simulated. However, for the diesel injector, only a single plume (out of the three) of interest was within the measurement window, and was used for validation. Correspondingly, only one diesel spray plume was simulated. Recent internal nozzle flow studies showed that, due to needle off-axis lateral motion, mass flow rate may vary among different holes [23]. In this study, for the diesel injector, it was presumed that injected mass was identical among all the holes with the total injected mass divided by three, since internal nozzle measurements or simulations were unavailable.

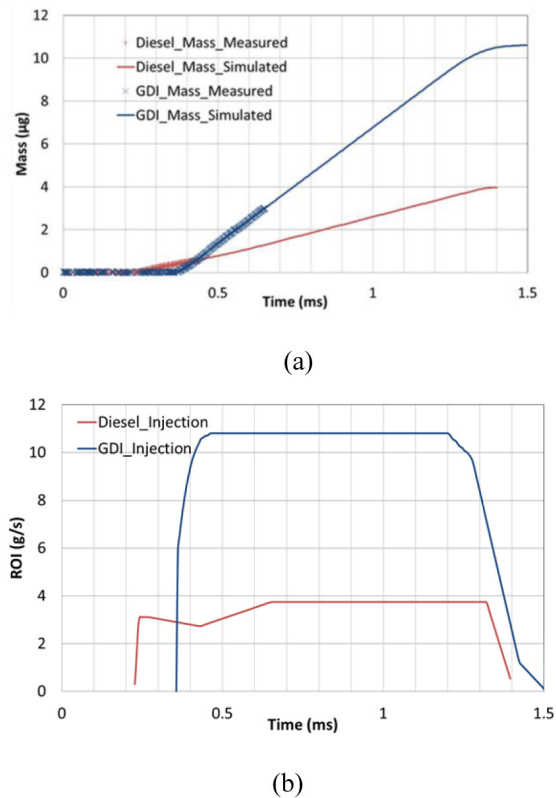


Figure 2. (a) Injected mass vs. time, and (b) ROI for diesel and GDI injections.

SIMULATION SET-UP

The multi-dimensional simulations were performed using CONVERGE, a commercial CFD tool developed by Convergent Science Inc. [24]. It uses an innovative modified cut-cell Cartesian method that eliminates the need for the computational grid to be morphed with the geometry of interest while still precisely representing the true boundary shape. This approach allowed for the use of simple orthogonal grids and completely automates the mesh generation process. Fixed embedding was specified in a small volume close to the nozzle exit and at boundaries. AMR was added to capture important under-resolved flow features (velocity field).

In this study, a second order accurate spatial discretization scheme was used for the governing conservation equations. The transport equations were solved using the Pressure Implicit with Splitting of Operators (PISO) method of Issa [25]. Variable time-stepping was used in the study. The time-step was automatically calculated each

computational cycle based on maximum allowed CFL numbers as well as spray, evaporation, and combustion time-step control methods. All the simulations shown in this paper were run in parallel on distributed memory machines using the Message Passing Interface (MPI). CONVERGE includes an automatic load balancing throughout the calculation as the distribution of cells can change significantly due to AMR [26].

Simulations employed the “blob” injection method of Reitz and Diwakar [27] in which “Lagrangian parcels” of liquid with a characteristic size equal to the effective nozzle diameter were injected into the computational domain. The atomization of the liquid blobs and subsequent droplets was simulated with models based on the Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instability mechanisms without the use of a breakup length model. The standard KH-RT model is implemented for LES calculations. Future studies will also explore different atomization models with LES implementation.

The No Time Counter (NTC) collision method of Schmidt and Rutland [28] was used in the present simulations. When collision occurs, the outcome was predicted to be bouncing, stretching separation, reflexive separation, or coalescence, based on the conditions at impact [29]. In addition to the breakup and collision models described above, models were also included for dynamic drop drag [30]. These models have already been used in the authors' previous publications [1, 2] and details can also be found in [24]. It should be noted that the Lagrangian models for break-up, drag, evaporation, collision etc. are similar between RANS and LES implementations. The authors believe that the existing Lagrangian models are applicable for both RANS and LES implementations since the influence of the LES implementation is transposed to the Lagrangian parcels through source terms in the mass, momentum, and energy equations. Also, a stochastic turbulence dispersion model is used to account for the influence of flow field fluctuations on Lagrangian parcel location. The spray model constants may need to be further calibrated for LES calculations and this will be the focus of future studies.

Unlike the RANS turbulence model, the transport equations for LES models can be decomposed into resolved and sub-grid fields. An LES Favre-averaged compressible momentum equation is given as:

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (1)$$

where the sub-grid stress tensor τ_{ij} is given by:

$$\tau_{ij} = \bar{\rho}(\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) \quad (2)$$

The sub-grid stress tensor needs to be modeled by LES sub-models. In this study, the one-equation Dynamic Structure LES model [24, 31] was used. This non-viscosity based model calculates the sub-grid stress tensor using the sub-grid turbulent kinetic energy and Favre averaged velocities.

The transport equation for the sub-grid kinetic energy is given as:

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i k}{\partial x_j} = \frac{\partial}{\partial x_i} \left(\frac{\mu}{Pr_{sgs}} \frac{\partial k}{\partial x_j} \right) + \tau_{ij} \bar{S}_{ij} - \rho \varepsilon \quad (3)$$

where Pr_{sgs} is set to 1.0, and the sub-grid kinetic energy is given by:

$$k = \frac{1}{2} (\tilde{u}_i \tilde{u}_i - \tilde{u}_i \tilde{u}_j) \quad (4)$$

The sub-grid dissipation rate is given by:

$$\varepsilon = C_\varepsilon \frac{k^{1.5}}{\Delta} \quad (5)$$

In the above sub-grid dissipation rate expression, C_ε is a model constant set to 1.0, and Δ is the grid size.

The sub-grid stress tensor was then modeled as follows

$$\tau_{ij} = 2k\bar{\rho} \frac{L_{ij}}{L_{kk}} \quad (6)$$

where the Leonard stress tensor is given by:

$$L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j. \quad (7)$$

The “ $\tilde{\cdot}$ ” indicates the test-level filter which is larger than the grid-level filter. In the present study, the test filter was created from the center cell and the neighbor cells. Each cell was weighted evenly in the test filter operation. Details about other LES sub-grid models can be found in Ref. [6, 24].

RESULTS AND DISCUSSIONS

This section presents the results of the LES spray calculations. First, non-evaporating diesel sprays were simulated. A grid-convergence study was initially carried out. Once the optimum grid resolution was known, nine LES realizations (recommended by Senecal et al. [15]) were simulated by changing the random number seed used in the spray sub-models. This approach has been used in previous studies [6,7,8,14] to introduce perturbations to the calculations to mimic the slightly different conditions during each experimental injection. Except for the spray model random number seed, all other inputs in the nine realizations were identical. Later, GDI spray calculations were performed with an identical approach, and the results are organized in the same pattern.

Diesel Spray Simulations

1. Grid-Convergence

Five different mesh resolutions were tested. The minimum cell sizes (using AMR and nozzle embedding) are listed in Table 2. The number of injected parcels were increased as the mesh was refined based on

the best practices identified by Senecal et al. [7]. It is shown that with the finest resolutions, more than 3 cells were embedded across the nozzle diameter. To the best of our knowledge, these are most resolved diesel spray simulations reported in literature.

Table 2. Minimum cell sizes, number of cells across the nozzle exit, number of injected parcels, peak cell count at 1 ms, and wall clock time for the non-evaporating diesel spray simulations.

Minimum cell size with AMR (mm)	Nozzle diameter/min. cell size	Number of injected parcels (thousand)	Peak cell count at 1 ms (million)	Wall clock time (hours) on 64 CPUs
0.5	0.22	100	0.86	11
0.25	0.44	200	0.95	12
0.125	0.88	800	1.66	17
0.0625	1.76	1,200	6.66	30
0.03125	3.52	1,200	20.0	52 on 128 CPUs

Figure 3 shows the 2-D projected density at 0.4 ms for the five different grid resolutions. In order to be consistent with the experimental procedure to obtaining the predicted fuel density the approach from Som [32] is adopted. The time instant of 0.4 ms was chosen since all the injected mass resides within the visualization window. Very coarse grid (i.e., minimum grid size = 0.5 mm) even shows some axisymmetric behavior, which is expected from RANS simulations. Neither 0.5 mm, nor 0.25 mm grid size can predict a fuel intact core in near-nozzle region (< 3 mm). As the mesh was refined further, the predicted liquid penetration length and the shape of the spray plume became similar to each other at 0.125 mm and finer. All the simulations exhibit an approximately 15 mm long intact core and predict some flow structures.

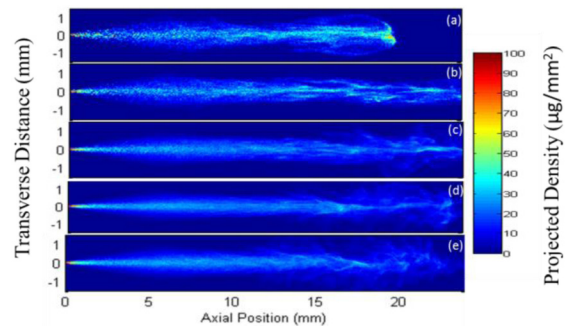


Figure 3. Comparison of predicted 2-D projected density contours ($\mu\text{g}/\text{mm}^2$) at 0.4 ms for different minimum grid resolutions of (a) 0.5, (b) 0.25, (c) 0.125, (d) 0.0625, and (e) 0.03125 mm.

Figure 4 shows liquid penetration as a function of time for measurements and predictions using the five mesh resolutions shown in Table 2. The x-ray data also includes measurement uncertainties of about 5%. Liquid penetration in simulations is defined as the axial distance encompassing 99% of the injected liquid fuel mass. This definition is consistent with previous work