A Study of Grid Resolution and SGS Models for LES under Non-reacting Spray Conditions

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Abstract

Large eddy simulation (LES) is widely applied for multiphase reacting flows and can obtain levels of predictability that cannot be achieved by the traditional Reynolds Averaged Navier-Stokes (RANS) technique. In addition to required numerical accuracy of LES solvers, the sub-grid scale models and mesh dependence of LES still need to be addressed. This work examines the effects of grid resolution and Sub-Grid Scale (SGS) model performance for fuel spray simulations under non-reacting conditions in a constant volume chamber. Four different turbulence models namely: (1) LES with Smagorinsky, (2) one-equation dynamic structure SGS model, (3) no SGS model and (4) RANS with RNG k-\(\varepsilon\) are investigated in the commercial code CONVERGE and compared in this study. For each turbulence model, simulations are performed with different minimum grid sizes ranging from 500 microns to 62.5 microns using adaptive mesh refinement. Two Diesel surrogates, \textit{n}-heptane and \textit{n}-dodecane, are studied. Experimental data from Sandia National Laboratory through the Engine Combustion Network (ECN) are used for validation purposes. Predicted global spray characteristics of liquid spray and vapor penetration as well as radial mixture fraction profiles at different axial locations are compared between the different turbulence models against the measurements. The mixture fraction and temperature contours are also compared between the predictions and the measurements. Grid-convergence is studied and the required grid resolution for LES spray simulations is discussed. Additionally, five different injections are simulated for all the models with a minimum grid size of 0.125 mm to capture cycle-to-cycle variations. The predicted global quantities and local values are compared between these injections. With the dramatic increase in computational resources in the past decade, this study indicates that LES is a viable alternative to RANS since it is more predictive in nature and wall-clock times are also reasonable.

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Introduction

Non-uniform fuel and air mixing is mainly due to the transient turbulent nature of the flow inside the combustion chamber. Subsequently, local inhomogeneity in equivalence ratio can result in varied ignition and emission characteristics [1]. Direct Numerical Simulations (DNS) offer potential to completely resolve all the relevant flow scales, however, the computational cost associated is not practical for engine studies [2]. Reynolds Averaged Navier Stokes (RANS) and more recently Large Eddy Simulation (LES) based approaches are typically employed for engine simulations. The RANS approach is based on ensemble averaged governing equations and hence it is less suitable for predicting the local unsteadiness in the flow. The LES approach, which is based on spatially filtered governing equations, can capture the large scale flow structures based on the filter size. However, the unresolved small scale structures are still modeled. Since LES can capture local unsteadiness and is computationally more tractable than a DNS based approach, it has received significant attention in the past decade, especially for simulation of internal combustion engines. A review of different LES modeling approaches can be found in the literature by Pope [3].

Our literature study reveals several groups using a RANS based approach [4-11]. In general, the global flow characteristics such as spray and vapor penetration, liquid length, ignition delay, flame liftoff length, heat release rates, and pressure traces etc., can be fairly well predicted by a RANS approach. This is not surprising since these global experimental parameters are reported in an ensemble averaged fashion [13-15]. More recently different flavors of LES models have been applied, and a review can be found in the literature by Rutland [16]. Broadly they can be classified as viscosity and non-viscosity based. Pope [17] implemented a one equation non-viscosity dynamic structure model since it is known to be less dissipative compared to the viscosity based models. Banerjee et al. [18] applied this model together with a sub-grid mixing model to predict the combustion characteristics under low-temperature conditions.

While different flavors of LES models have been applied for predicting combustion and emission characteristics, the grid resolution associated with these models must be investigated to determine the necessary cell size for practical engine simulations. Senechal et al. [24] showed that spray simulations using the dynamic structure LES model converged with cell sizes of around 0.0625 mm. This study extends that work by investigating grid convergence for additional LES models. Thus, the primary objectives of this work are to (1) study the grid convergence of LES models, and (2) compare the RANS and LES models with measurements under non-reacting spray conditions for their ability to qualitatively and quantitatively predict the spray structures.

In the past decade, several studies were performed by researchers at Sandia National Laboratories and IFP Energies Nouvelles to provide high-fidelity measurements of parameters such as spray penetration, liquid length, vapor penetration, mixture-fraction, axial velocity [19-21], ignition delay, LOL, and soot emissions for a range of ambient and injection conditions, in a constant volume combustion vessel. A variety of fuels and fuel surrogates, such as diesel #2, biodiesel, n-heptane, and n-dodecane, were studied in these experiments, and the resulting dataset can be accessed through the Engine Combustion Network [22]. Only recently, this high-fidelity dataset has been used for spray combustion model development and validation. These data provide realistic information for LES model validation.

The paper is organized in the following way. First a brief introduction is provided for the spray and combustion models and the governing equations for the LES Smagorinsky and dynamic structure models. Details can be found elsewhere [17, 23, 24]. The experimental dataset from Sandia National Laboratory which is extensively used for validation purposes is discussed next. The results and discussion section is mainly divided into Spray A with spray global parameters and local values and Spray H with instantaneous spray structure. The performance of each turbulence model is evaluated against measurements in terms of vapor and liquid penetrations, local axial velocity and mixture fraction profiles on different grid resolutions. The instantaneous spray structure is also plotted for different models on different grid resolution and compared with experimental data. Finally, conclusions are drawn.

Spray and LES Models

Fuel spray simulations were performed using the Eulerian-Lagrangian approach in the computational fluid dynamics software CONVERGE [4, 25, 26]. It incorporates state-of-the-art models for spray injection, atomization and breakup, turbulence, droplet collision, and coalescence. The gas-phase flow field is described by using either the Favre-Averaged Navier-Stokes equations in conjunction with the RNG k-ε or the LES based turbulence model, which includes source terms for the effects of dispersed phase on gas phase turbulence. These equations are solved by using a finite volume solver. The details of these models can be found in previous publications [26], so only a brief description is provided here.
The Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) models are used to predict the subsequent secondary droplet breakup [27, 28]. Droplet collisions are modeled with the No Time Counter algorithm [29]. A droplet evaporation model based on the Frossling correlation is used. Also used is a dynamic drag model based on the postulation that the drag coefficient depends on the shape of the droplet, which can vary between a sphere and a disk. The effects of turbulence on the droplet are accounted for using a turbulent dispersion model. It should be noted that for both RANS and LES, the same set of spray constants was selected for validation purposes, as shown in Table 1.

<table>
<thead>
<tr>
<th>B_0</th>
<th>B_1</th>
<th>C_i</th>
<th>C_s</th>
<th>C_RT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.60</td>
<td>7.0</td>
<td>0.188</td>
<td>1.0</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 1: Spray model constants used in this study.

A brief description of the LES models is provided here. Further details about the RANS and LES models can be obtained from authors’ previous publications [17,24,30,31]. The basic governing equations for the three LES models investigated in this study are outlined.

An LES Favre-averaged compressible momentum equation is given:

\[
\frac{\partial \bar{p} \bar{u}_i}{\partial t} + \frac{\partial \bar{p} \bar{u}_i\bar{u}_j}{\partial x_j} = -\frac{\partial \bar{\rho}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial \bar{T}}{\partial x_i} \tag{1}
\]

where, \(\tau_{ij}\) is the sub-grid stress tensor.

Smagorinsky based LES Model:
The sub-grid stress tensor if modeled by

\[
\tau_{ij} = -2\bar{\rho} \Delta^2 C_s^2 \left[ \overline{S_{ij}} + \frac{1}{3} \delta_{ij} \bar{\rho} \right] \tag{2}
\]

where,

\[
\overline{S_{ij}} = \sqrt{2 \overline{S_{ij}^2}} \Delta^2 \Delta_{cell}
\]

\[
\Delta_{cell} = \frac{1}{2} \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right]
\]

It should be noted that the Smagorinsky based LES model has a model constant, \(C_s\), which is set to 0.2 in the study.

Dynamic Structure LES model:
The sub-grid stress tensor is modeled by

\[
\tau_{ij} = 2k \frac{L_{ij}}{L_{mk}} \tag{3}
\]

where, \(L_{ij}\) is the Leonard stress and is given by

\[
L_{ij} = u_i u_j - u_j u_i ,
\]

and \(k\) is the sub-grid kinetic energy which is modeled with a transport equation. It should be noted that the dynamic structure model does not have any model constants.

No Sub-grid Scale (SGS) Model:
The sub-grid scale turbulence is not modeled in this approach. Instead, numerical diffusion (upwinding) is used to maintain a stable flow field.

Sub-models
The effect of the sub-grid (or under-resolved) flow field \((u_i)\) on the drop parcels is accounted for via a sub-grid droplet dispersion model. This model is similar to conventional RANS-based turbulent dispersion models. The sub-grid kinetic energy is used in place of the RANS turbulent kinetic energy and the sub-grid dissipation rate is used in place of the RANS turbulent dissipation rate. For the Smagorinsky model and the no sub-grid model approach, a sub-grid kinetic energy is not available and thus a model for the sub-grid kinetic energy is needed. For these models, the sub-grid kinetic energy is modeled by

\[
k \equiv C_s \frac{\Delta^2 \overline{\partial u_i \partial u_j}}{24 \overline{\partial x_i} \overline{\partial x_j}} \tag{4}
\]

where, \(C_s\) is set to 2.0 in this study.

The present CFD software uses a modified cell Cartesian method for grid generation [25,26]. The grid is generated internally at runtime. For all cases, the base grid size is fixed at 1 mm. In order to resolve the flow near the injector, a fixed grid embedding is employed. Apart from this region, it is rather difficult to determine a priori where a refined grid is needed. Hence, different levels of adaptive mesh refinement (AMR) are employed for the velocity field to obtain the various minimum grid sizes of interest which are 0.5 mm, 0.25 mm, 0.125 mm, 0.0625 mm, and 0.003125 mm. For example, a minimum grid size of 0.0625 mm was obtained with fixed and adaptive embedding of 4. Further details about the meshing strategy can be obtained from the
authors’ previous publications [32]. The computational parcels injected to stochastically represent the liquid fuel spray are also chosen based on the methodology highlighted by Senecal et al. [32]. To match the combustion chamber geometry used in the experimental studies, a cubical geometry of 108 mm on each side is generated.

**Numerical Algorithms**

In the present CFD solver, all computed values are collocated at the center of the computational cell. To prevent checker-boarding, the Rhie-Chow [33] algorithm is employed. The conservation equations are solved using the finite volume method.

In the present study a second-order-accurate spatial discretization scheme is used for the governing conservation equations. In order to maintain stability, time accuracy is set to first order by running fully implicit.

The transport equations are solved using the Pressure Implicit with Splitting of Operators (PISO) method of Issa [34]. A geometric multigrid solver is used for the pressure solution.

Variable time-stepping is used in the current study. The time-step is automatically calculated each computational cycle based on maximum allowed Courant-Friedrichs-Lewy (CFL) numbers for convection, diffusion and the speed of sound. Note that these CFL constraints are maintained for accuracy, and not for stability. In addition, spray and evaporation time-step control methods are used in the present simulations.

The calculations in this study are run in parallel on distributed memory machines using the Message Passing Interface (MPI). An automatic domain decomposition technique is employed which allows for efficient load balancing throughout the calculation as the distribution of cells can change significantly due to AMR.

**Experimental Data and Computational Conditions**

Experimental data to use for comparison are obtained from Sandia National Laboratories and IFP Energies Nouvelles [31], where a constant-volume, quiescent, pre-burn-type combustion vessel is used to generate high-temperature and high-pressure gases to simulate the thermodynamic conditions achieved in a compression ignition engine. A premixed combustible mixture is spark-ignited, which burns to completion. The combustion products cool over a long time due to heat transfer to the vessel walls. Once the desired pressure and temperature are reached, the fuel injector is triggered and injection occurs. The conditions for the ECN data [22] investigated in this work are noted in Table 2. Advanced optical diagnostics are used to obtain liquid and vapor penetration versus time, liquid length, ignition delay, pressure-rise rate, flame lift-off length, and quantitative soot volume fraction. Both the vaporizing “Spray A” and “Spray H” experiments are considered in the current work.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>n-Dodecane</th>
<th>n-Heptane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient composition</td>
<td>0% O₂</td>
<td>0% O₂</td>
</tr>
<tr>
<td>Ambient temperature (K)</td>
<td>900</td>
<td>1000</td>
</tr>
<tr>
<td>Ambient density (kg/m³)</td>
<td>22.8</td>
<td>14.8</td>
</tr>
<tr>
<td>Injection pressure (MPa)</td>
<td>150</td>
<td>150</td>
</tr>
<tr>
<td>Fuel temperature (K)</td>
<td>363</td>
<td>373</td>
</tr>
<tr>
<td>Nozzle diameter (mm)</td>
<td>0.09</td>
<td>0.1</td>
</tr>
<tr>
<td>Injection duration (ms)</td>
<td>1.5</td>
<td>6.8</td>
</tr>
<tr>
<td>Total mass injected (mg)</td>
<td>3.5</td>
<td>17.8</td>
</tr>
</tbody>
</table>

**Table 2:** Nominal conditions for the vaporizing Spray A and Spray H experiments at Sandia National Laboratories.

**Results and Discussion**

This section presents the results of spray simulations under Spray A and Spray H conditions. For Spray A, we compare the spray global parameters, liquid and vapor penetrations, and local mixture fraction and axial velocity between predictions and experimental data. The instantaneous spray structure of temperature and mixture fraction for Spray H is presented. For reference, the calculations of liquid and vapor penetration for simulations are defined in Table 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Penetration</td>
<td>Axial distance encompassing 90% of the injected liquid fuel mass.</td>
</tr>
<tr>
<td>Vapor Penetration</td>
<td>Maximum distance from the injector where the fuel mass fraction is 0.1%.</td>
</tr>
</tbody>
</table>

**Table 3:** Definitions for spray global parameters

**Spray A**

**Grid convergence study**

Figure 1-Figure 4 show the liquid and vapor penetrations as a function of time for measurements and predictions by k ε RNG, LES w/o SGS model, LES Smagorinsky, and LES dynamic structure, respectively. The predictions include results from the four different mesh resolutions. Note that the grid size in the figures refers to the minimum cell size obtained by using AMR. The plots show that 0.5 mm grid is not sufficient for any of the turbulence models to repro-
duce the liquid and vapor penetration characteristics. As the grid is refined, the predicted spray penetration by all the models approaches the experimental data. However, the trend is different between the RANS and LES models. RANS simulations are performed with the RNG k-ε model and predict good spray penetration with 0.25 mm grid. There is not a large variation with further refinement to 0.125 mm and 0.0625 mm grids. We observe that a 0.25 mm grid is not sufficient for LES to resolve the global parameters due to heavy dependence on the SGS models. With the grid resolution increasing, LES models demonstrate convergence of liquid and vapor penetrations. All LES model results show good agreement with experimental data for vapor penetration on 0.0625 mm grid or finer. Liquid penetration shows differences between predictions and measurements. Note that all the spray model constants are tuned based on the RANS model simulations. Our results in the next section show that the liquid penetration prediction can be improved by varying the spray constants. Note that the dynamic structure model predicts a good vapor penetration with 0.125 mm grid, while other LES models do not.

Figure 1: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by k-ε RNG for the Spray A. Four predicted curves are presented for the different cell sizes.

Figure 2: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by LES w/o SGS for the Spray A. Four predicted curves are presented for the different cell sizes.
Figure 3: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by LES Smagorinsky for the Spray A. Four predicted curves are presented for the different cell sizes.

Figure 4: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by LES dynamic structure model for the Spray A. Five predicted curves are presented for the different cell sizes.

Turbulence model comparison on similar mesh sizes

As shown in Figure 5 and 6, the vapor and liquid penetration predicted by different turbulence models are plotted with experimental data on 0.125 mm and 0.0625 mm grids, respectively. The $k$-$\varepsilon$ RNG model gives good agreement on both grids as expected from the results on the 0.25 mm grid. The LES SGS models show differences on the 0.125 mm grid. The dynamic structure model performs the best of the LES models at the 0.125 mm grid size. On the 0.0625 mm grid shown in Figure 6, more scales are resolved and thus there is less dependence on the sub-grid models. At this level, the three LES models show quite close predictions in terms of liquid and vapor penetrations.
Figure 5: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by RANS and LES models for the Spray A on cell size of 0.125 mm.

Figure 6: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by RANS and LES models for the Spray A on cell size of 0.0625 mm.

The overall conclusion for this section is that the RANS models converge at a coarser resolution (0.25 mm) compared to the LES models. The LES models are observed to grid converge at resolutions of 0.0625 mm and finer. In terms of the global spray characteristics, both RANS and LES models are able to capture the experimental values provided appropriate grid convergent resolutions are chosen. Further study of the spray constants influence on the prediction of global spray parameters will be presented at following subsection.

Cycle-to-cycle variations

The previous spray comparisons were based on a single LES spray injection. Averaging of many injections may be needed when comparing LES simulations to experimental data. To explore the cycle-to-cycle variations, five different injections were simulated for the grid size of 0.125 mm. Various injections were simulated by changing the spray model random number seed for each case.

Figure 7 shows a comparison between measured and predicted vapor and liquid penetrations. The predictions include five injections for each of the four turbulence models. The thinner lines are predictions of each injection, and the thicker line is the averaged value over five injections. The k-ε RNG model shows the same values of liquid and vapor penetration for each injection. We know RANS solves the ensemble-averaged equations hence smaller perturbations are dissipated in the simulation and cycle-to-cycle variations are not captured as well. However, there are noticeable differences between different injections for each of the LES models. Although each case results in a different penetration curve, predictions from the five injections are similar and it is reasonable to look at global parameters such as vapor and liquid penetration using a single injection with LES. Overall conclusion from this section is that RANS is not as suitable for capturing the cycle-to-cycle variations present in this case, however with LES model differences are observed with different realizations.
Figure 7: Comparison of vapor (top) and liquid (bottom) penetration between measurement [22] and prediction by RANS and LES models for the Spray A on cell size of 0.125 mm. The thinner curves and thicker curves represent five injections and averaged values, respectively.

Effect of liquid spray breakup constant
As described in a previous section, the spray model constants used for the current LES simulations are identical to those used for RANS simulations of the same case [32]. As was shown in Figs. 2-4, the predicted average liquid length is longer than the measured value. In order to assess the sensitivity of the results to the spray breakup model, additional LES realizations were simulated with a different value of the Kelvin-Helmholtz (KH) constant $B_1$. This constant is included in the expression for the breakup time of a liquid drop with radius $r_0$:

$$
\tau_{KH} = \frac{3.726 B_1 r_0}{\Lambda_{KH} \Omega_{KH}} \tag{4}
$$

where $\Omega_{KH}$ is the growth rate of the most unstable KH wave and $\Lambda_{KH}$ is the corresponding wavelength.

Figures 8-10 show comparisons of vapor and liquid penetration between the original $B_1=7$ and a new $B_1=5$, as well as measurements. It can be seen that the results with $B_1=5$ is in better agreement with the experimental data for all the three LES models. On the other hand, the vapor penetration does not show much variation with the change of $B_1$. A smaller value of $B_1$ results in earlier breakup and hence the liquid penetration becomes shorter. Hence this section shows that better liquid penetration results can be obtained using LES models with marginal tuning of the spray breakup constants without influencing the vapor penetration characteristics.

Figure 8: Comparison of measured [22] and predicted vapor (top) and liquid (bottom) penetration. The predictions are single realizations by LES w/o SGs model on 0.0625 mm grid with $B_1=7$ and $B_1=5$.

Local velocity and mixture fraction
In addition to the global spray liquid and vapor penetration comparison, local mixture fraction and axial velocity are compared with the available experimental data [4]. The transverse mixture fraction and axial velocity data is available at 25 mm, 35 mm and 45 mm downstream from injection location, respectively. The axial data is available from 20 mm to 80 mm. The simulation results here are obtained on 0.0625 mm grids. It is necessary to average multiple LES realizations when comparing LES simulations to local quantities [5]. Herein, we present the predictions for both the five individual injections and the average over the five injections for local quantities.
Figures 11-13 show the measured and predicted gas-phase axial velocity in the spray centerline at 1.0 ms and 1.5 ms by three LES models, respectively. We can observe the variations from each LES realization. The predicted averages of the five LES realizations capture the trends fairly well for the different times by all the LES models, although there is difference between the models. In general there are some discrepancies between the simulation results and experiments also which could be caused by several reasons: (1) it should be noted that Meijer et al. [31] note that the uncertainty in measurement of velocity to be ± 5m/s, (2) experiments are averaged over 20 realizations while simulations are averaged over 5, (3) the simulations were performed with the minimum resolution of 0.125 mm in order to speed up the simulations. The authors plan to extend this study by simulating 20 different realizations with all the models at 0.0625 mm minimum grid resolution.

Figure 9: Comparison of measured [22] and predicted vapor (top) and liquid (bottom) penetration. The predictions are single realizations by Smagorinsky model on 0.0625 mm grid with B1=7 and B1=5.

Figure 10: Comparison of measured [22] and predicted vapor (top) and liquid (bottom) penetration. The predictions are single realizations by the dynamic structure model on 0.0625 mm grid with B1=7 and B1=5.

Figure 11: Comparison between measured [31] and predicted by LES w/o SGS gas-phase axial velocity along the spray centerline at 1.0ms (top) and 1.5ms (bottom). The figure includes all 5 LES injections and the averaged value over 5 injections.
Figure 12: Comparison between measured [31] and predicted by LES Smagorinsky model gas-phase axial velocity along the spray center line at 1.0 ms (top) 1.5 ms (bottom). The figure includes all 5 LES injections and the averaged value over 5 injections.

Figure 13: Comparison between measured [31] and predicted by LES dynamic structure model gas-phase axial velocity along the spray center line at 1.0 ms (top) and 1.5 ms (bottom). The figure includes all 5 LES injections and the averaged value over 5 injections.

Figures 14-16 plot the measured and predicted transverse gas-phase velocity at 25 mm, 35 mm, and 45 mm downstream of nozzle exit by three LES models. Again, the plots include all the individual LES realizations and the averaged value. We see the expected variations from individual realizations and fairly good agreement between the predicted averages and experimental data at all three downstream locations for all LES models.
Figure 14: Comparison between measured [31] and predicted by LES w/o SGS gas-phase axial velocity at 25 mm (top), 35 mm (middle), and 45 mm (bottom) from nozzle exit. The figure includes all 5 LES injections and the averaged value over 5 injections.

Figure 15: Comparison between measured [31] and predicted by LES Smagorinsky model gas-phase axial velocity at 25 mm (top), 35 mm (middle), and 45 mm (bottom) from nozzle exit. The figure includes all 5 LES injections and the averaged value over 5 injections.
Figure 16: Comparison between measured [31] and predicted by LES dynamic structure model gas-phase axial velocity at 25 mm (top), 35 mm (middle), and 45 mm (bottom) from nozzle exit. The figure includes all 5 LES injections and the averaged value over 5 injections.

In addition to local axial velocity data, local mixture fraction data is also available through ECN. The measured and predicted centerline mixture fraction is plotted as a function of axial distance from the nozzle exit in Figs. 17-19 for the three LES models. The trends in mixture fraction in the axial distance are predicted by all the LES models. However, the mixture fraction is under-predicted by all the LES models. The dynamic structure model shows better comparison with experimental data than other two LES models.

Figures 20-22 plot the measured and predicted transverse mixture fraction at downstream locations of 25 mm and 45 mm from the nozzle exit by LES w/o SGS, Smagorinsky, and dynamic structure models. Again, we see the variations between the individual LES realizations. The predicted averages show fairly good agreement with experimental data qualitatively and quantitatively for all the models.

Figure 17: Comparison between measured [22] and predicted by LES w/o SGS mixture fraction along the spray center line at 1.5 ms. The figure includes all 5 LES injections and the averaged value over 5 injections.

Figure 18: Comparison between measured [22] and predicted by LES Smagorinsky model mixture fraction along the spray center line at 1.5 ms. The figure includes all 5 LES injections and the averaged value over 5 injections.
Figure 19: Comparison between measured [22] and predicted by LES dynamic structure model mixture fraction along the spray center line at 1.5 ms. The figure includes all 5 LES injections and the averaged value over 5 injections.

Figure 20: Comparison between measured [22] and predicted by LES w/o SGS transverse mixture fraction at 25 mm (top) and 45 mm (bottom) from nozzle exit, respectively. The figure includes all 5 LES injections and the averaged value over 5 injections.

Figure 21: Comparison between measured [22] and predicted by LES Smagorinsky model transverse mixture fraction at 25 mm (top) and 45 mm (bottom) from nozzle exit, respectively. The figure includes all 5 LES injections and the averaged value over 5 injections.
Figure 22: Comparison between measured [22] and predicted by LES dynamic structure model transverse mixture fraction at 25 mm (top) and 45 mm (bottom) from nozzle exit, respectively. The figure includes all 5 LES injections and the averaged value over 5 injections.

Spray H

In addition to the Spray A condition, a further turbulence model performance study is conducted under Spray H conditions, which has instantaneous contours of fuel distribution and gas-phase temperature distribution data for n-heptane fuel at an ambient temperature of 1000 K [20,21]. The instantaneous experimental images obtained using Rayleigh scattering imaging are shown on the left along with the time ASI and the axial length scale (shown in Figure 23 and Figure 24). The field of view is 40 mm x 20 mm in the axial and transverse directions respectively. Note that the experimental contours pertain to a ratio between fuel-air number densities (Nf/Na) and fuel ambient air mixture temperature. Simulations plot the fuel mass-fractions and ambient gas temperatures with single LES realization. Fuel vapor penetration and dispersion can be clearly seen from the experimental and simulation plots. Overall, as shown for Spray A conditions, both RANS and LES simulations predict the vapor penetration fairly well given sufficient grid resolutions are employed. However, remarkable differences in the spray structure are clearly observed between RANS and LES cases. While RANS predicts smooth, averaged profiles, the LES simulations capture the instantaneous structures well.

Grid convergence study

Figures 23 and 24 show the measured gas phase temperature, the predicted gas-phase temperature, and mixture fraction with different grid resolutions at four different times. Spray global parameters, liquid and vapor penetration, can be well predicted by RANS with a 0.25 mm grid. However, the spray structure is smeared out by the RANS simulations compared with measurements. Finer grid resolution is not able to improve the spray structure prediction using RANS k-ε model.

LES solves the filtered NS equations. With the finer grid, the LES models predict the structure as shown in Figs. 25-30. First, we turn off the SGS model and have the fine grid resolve the flow structure. It can be seen in Figs. 25 and 26 that the simulation captures the spray structure of temperature and mixture fraction well on 0.125 mm and 0.0625 mm grids at all the four times. Figures 27-30 shows the predictions of temperature and mixture fraction by Smagorinsky and dynamic structure models with different grid resolutions. They capture well the instantaneous structure for 0.125 mm and 0.0625 mm grids. Note that the LES plots are from single LES realizations. It is interesting to note that at coarse resolutions like 0.5 mm the LES models do not predict any structure. As the grid size is refined more structures are predicted by the LES models, which is expected. This is due to the fact that at the finer resolutions more structures are actually captured by the simulations. In fact, with both 0.125 mm and 0.0625 mm resolutions, the LES model results qualitatively look similar to the experimental images.

Figure 23: Temperature contour plots comparison between the measurement [20,21] and calculations by RNG model with different cell sizes
Figure 24: Mixture fraction Contour plots comparison between the measurement [20,21] and calculations by RNG model with different cell sizes.

Figure 25: Temperature contour plots comparison between the measurement [20,21] and calculations by LES w/o SGS model with different cell sizes.

Figure 26: Mixture fraction Contour plots comparison between the measurement [20,21] and calculations by LES w/o SGS model with different cell sizes.

Figure 27: Temperature contour plots comparison between the measurement [20,21] and calculations by Smagorinsky model with different cell sizes.

Figure 28: Mixture fraction Contour plots comparison between the measurement [20,21] and calculations by Smagorinsky model with different cell sizes.

Figure 29: Temperature contour plots comparison between the measurement [20,21] and calculations by dynamic structure model with different cell sizes.

Figure 30: Mixture fraction Contour plots comparison between the measurement [20,21] and calculations by dynamic structure model with different cell sizes.

Turbulence model comparison
In Figs. 31 and 32 we recompile the temperature and mixture fraction contour plots for all turbulence models on a 0.0625 mm grid. As expected, LES models have the advantage of better prediction of instantaneous structure.
Conclusions

In this work LES and RANS models are employed to simulate Spray A and Spray H conditions and compared with available experimental data from Sandia National Laboratory and IFP Energies Nouvelles. We looked at the grid resolution convergence for RANS k-\(\varepsilon\) and LES models including w/o SGS, Smagorinsky, and dynamic structure.

Using Spray A, we studied four different grid resolutions and evaluated the grid convergence in terms of spray global parameter, liquid and vapor penetrations, and local velocity and mixture fraction profiles. RANS k-\(\varepsilon\) model performs well with a 0.25 mm grid for the liquid and vapor penetrations. With the same spray constants as RANS, LES models show vapor and liquid penetration convergence with increasing grid resolution. However, we see predictions do not converge to the experimental data for liquid penetration. With the change of a break-up constant, LES models improve the liquid penetration and agree well with measurement. With five different injections, we looked at the cycle-to-cycle variation. The vapor and liquid penetration show variation; however, individual realizations are quite close to the predicted averages with LES. It is reasonable to use a single simulation to study the spray global parameters. For local velocity and mixture fraction distributions, individual LES realizations vary from each other. We simulated five LES realizations for each model and plotted the individual and averages with the measurements. The averages agree well with measurements in general. The number of realizations required for averaging needs to be further studied.

With vapor-phase contour data available for Spray H, we compared the temperature and mixture fraction contours with measurements for all the models on different grid resolutions. RANS k-\(\varepsilon\) model gives a smooth instantaneous structure on all the grids. LES models can capture the structures with 0.125mm or finer grids.

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Nomenclature

- \(B_0\) KH model constant for breakup droplet size
- \(B_1\) KH model constant for breakup time
- \(C_1\) KH model constant for breakup droplet normal velocity
- \(C_t\) RT model constant for breakup time
- \(C_{RT}\) RT model constant for breakup size
- \(C_s\) Smagorinsky model constant
- \(C_{les}\) LES Model constant
- \(P\) Pressure of gas mixture [Pa]
- \(S_{ij}\) Symmetric stress tensor [m2/s2]
- \(\tau_{ij}\) LES sub-grid scale tensor [m2/s2]
- \(V_{cell}\) Cell volume [m3]
- \(u\) Gas velocity [m/s]
- \(\Delta\) Filter size [m]
- \(\delta\) Kronecker delta
- \(k\) Sub-grid turbulent kinetic energy [m2/s2]
- \(\mu\) Dynamic Viscosity [Pa.s]
- \(\rho\) Density of the gas mixture

Subscripts

- \(g\) gas
- \(l\) liquid
References

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