

Analysis of Averaging Methods for Large Eddy Simulations of Diesel Sprays

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ABSTRACT

Large Eddy Simulations (LES) provide instantaneous values indispensable to conduct statistical studies of relevant fluctuating quantities for diesel sprays. However, numerous realizations are generally necessary for LES to derive statistically averaged quantities necessary for validation of the numerical framework by means of measurements and for conducting sensitivity studies, leading to extremely high computational efforts. In this context, the aim of this work is to explore and validate alternatives to the simulation of 20-50 single realizations at considerably lower computational costs, by taking advantage of the axisymmetric geometry and the Quasi-Steady-State (QSS) condition of the near nozzle flow at a certain time after start-of-injection (SOI). Three different approaches are proposed and carefully investigated: the first combines ensemble with spatial averaging techniques based on the estimation of the azimuthal integral length scales to assess the maximal number of independent profiles; the second proposes in addition a time averaging technique that relies on the QSS assumption, whereas a third approach merges all the mentioned techniques together. Results show that for axisymmetric constant volume geometries, converged statistics (mean and standard deviation values) can be obtained from one single LES realization with up to 252 statistically independent samples. These results are very promising and could potentially reduce computational costs up to 50 times, allowing for numerical setup optimizations and sensitivity studies at computational efforts comparable to Reynolds-averaged Navier-Stokes (RANS) simulations.

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INTRODUCTION

In the last decade the role of 3-dimensional numerical simulations in combustion research has steadily grown, and thoroughly validated high fidelity numerical methods increasingly complement experimental findings towards a deeper understanding of complex turbulent combustion processes. The more practical and simpler RANS approach is commonly adopted when predictions of the mean phenomena are the main concern, in which case time (or ensemble) averaged variants of the Navier-Stokes equations are solved and the resulting Reynolds-stress tensor is modeled. Such approaches have found to perform adequately for less complex flows, e.g. [1, 2, 3, 4], however for more complex and highly time dependent flows, Large Eddy Simulations (LES) which resolve the large turbulence scales of motion leaving to the modeling side only the smaller scales are considered state-of-the-art, see e.g. [2, 5, 6]. This is motivated by the fact that most of the energy is contained in the large scale eddies and the small scale structures are considered to be of a more universal character [5, 7]. LES is therefore well suited for highly turbulent complex flows and despite the higher computational costs compared to RANS, LES are often preferred in such cases [4, 5, 7, 8].

Since LES solves filtered Navier-Stokes equations, the results provide instantaneous conditions of the flow field. Thus multiple simulations are generally necessary, followed by significant post-processing efforts to manage the large amount of generated raw data. Averaging statistics - mean and rms values overall - are therefore essential in order to validate the numerical framework with measurements as well as to conduct comparison studies with other simulations, especially with RANS. In this context, different techniques for statistical averaging have been extensively developed in the literature and their suitability heavily depends on the configuration investigated. For non-stationary flows without a direction of homogeneity ensemble averaging is the only solution [9, 10, 11]. In [9, 10], a convergence study with respect to the LES ensemble size has been conducted for a time-evolving plane wake problem and 16 realizations were found to yield accurate converged results. Ensemble phase-dependent averaging is usually adopted also in the context of periodic time-varying configurations, as shown in Hasse et al. [2] for gasoline engines.

As soon as the flow can be assumed to be in a Steady-State (SS) or Quasi-Steady-State (QSS) regime, time averaging can be introduced. Samples separated by a defined time interval are stored and averaged as proposed in [12] for a flow past a cylinder and in [13] for a flow past a manikin. Time averaging can also be applied for more complex

configurations, as shown in Byskov et al. [14], where the averaged velocity fields inside a radial pump were determined over 2000 time steps. Time averaged statistics for a gas turbine combustor (Sandia Flame D) were determined by Pitsch et al. for the axial velocity and mixture fraction distributions [15]. Here the time averages were carried out over two flow-through times.

Spatial averaging can be applied to problems with a direction of homogeneity as it is shown for channel flows in [16] and for a backward-facing step in [17], where statistics have been evaluated along the axis orthogonal to the flow direction. For the determination of mean temperature and NO mole fraction distributions of a turbulent jet flame (Sandia Flame D) spatial averaging has been applied along the circumferential direction by Pitsch et al. [18]; a similar procedure has also been adopted for pipe flows in [19, 20]. Nevertheless, spatial averaging in circumferential direction can lead to correlation of the velocity fluctuations close to the centerline due to the reduced distance between the considered samples [19, 21]. Here, spatial averaging in combination with time averaging has been applied in order to increase the number of flow independent samples at lower radii necessary for statistics.

Different approaches are stated in the literature for averaging statistics for three-dimensional spray simulations. In Moin et al. [22], statistics for a gas turbine spray were obtained by averaging LES results along the circumferential direction and then compared in terms of velocity fields (mean and standard deviation values) with experimental data showing adequate accuracy. Habchi et al. [23] showed that 30 ensemble averaged realizations are insufficient for the validation of a diesel spray in terms of axial and radial mixture fraction distributions. However, the accuracy was improved by combining ensemble with spatial averaging techniques using multiple azimuthal planes per realization separated by 45°, resulting in a total of 240 profiles available for statistics. Senecal et al. [24] considered the results of 20 LES realizations for diesel spray (Sandia Spray A) as statistically converged and suggested that averaged mixture fraction and velocity profiles over a reduced number of 9 realizations fall within the desired tolerances for 95% of the time. Despite the reduced number of simulations, the fine mesh that LES requires leads to very high to prohibitive computational costs, especially if sensitivity studies need to be conducted.

In this context, this study seeks to explore and validate alternatives to the simulation of numerous single realizations at considerably lower computational costs, by taking advantage of the axisymmetric geometry and the QSS condition of the near nozzle flow at a certain time after SOI for the Sandia “Spray A” non-reacting reference case.

METHODOLOGY

The turbulent flow field is calculated by means of the widely adopted commercial CFD solver Star-CD [25]. A Large Eddy Simulation (LES) approach is followed where flow variables are decomposed into resolved and subgrid scales by applying an implicit spatial filtering technique. While the resolved scales are directly solved by the flow field solver, the Dynamic Structure Model (DSM) is adopted to model the subgrid scalar flux and dissipation terms [6]. Compared

to the more commonly used Smagorinsky model, DSM was reported to be less dissipative allowing for coarser grid resolutions, as discussed in detail in [26].

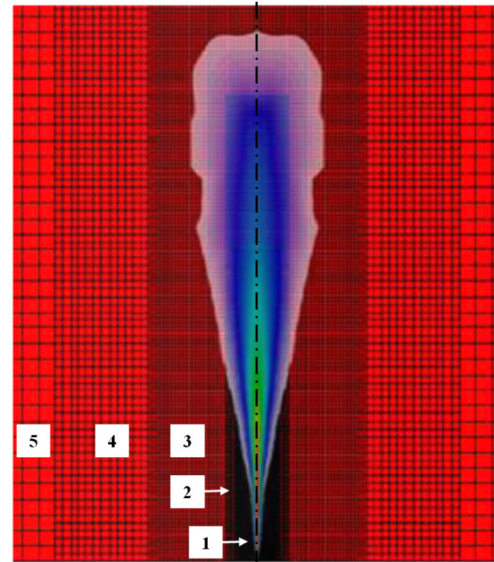


Figure 1. Midplanar section of the computational domain, showing the 5 refinement regions of the cartesian multi-grid mesh. The spray position is superimposed.

The numerical grid shown in Figure 1 represents the Sandia combustion vessel, which is a cubical constant-volume combustion chamber with a characteristic length of 108 mm [27]. Since the entire combustion vessel is simulated, a multi-grid cartesian mesh is implemented in order to ensure the resolution of the velocity gradients in each part of the domain. Since the velocity difference between the gas and droplets enters the drag force calculation and hence affects spray penetration, the accurate representation of velocity gradients in the jet transversal directions is paramount for Lagrangian-Eulerian spray calculations [28].

As summarized in Table 1, the densest grid with a characteristic length of 0.125 mm is defined for the centerline region and then increases towards the walls where smaller gradients are expected. A total of five grid refinement regions are implemented resulting in approximately 1.9 million cells. This resolution has been adopted following a mesh sensitivity study and the chosen resolutions, in particular in the near-nozzle region, are similar to those employed in other studies [23, 29]. Energy and species equations are discretized using the available second-order monotonic advection and reconstruction scheme (MARS), with no compression applied, whereas for convective terms in the momentum equation a central differencing scheme has been adopted, cf. [25]. A PISO solver is used for time integration with a Courant number limited variable time step; resulting values range between 2.0e-7 s and 2.0e-6 s.

Table 1. Refinement regions of the adopted computational mesh.

Mesh refinement zone	x,y-directions (mm)	z-direction (mm)	cell size, $v^{1/3}$ (mm)
1	0-3	0-40	0.125
2	3-4	0-60	0.25
3	4-14	0-108	0.5
4	14-26	0-108	1
5	26-54	0-108	2

Droplet are injected as parcels and tracked with a Lagrangian method fully two-way coupled to the gas phase by means of source terms in the conservation equations for momentum, mass, energy and species. The spray atomization is mimicked with the widely adopted 'blob' model using a semi-cone angle of 6° . The subsequent secondary break-up is described by the Kelvin-Helmholtz and Rayleigh-Taylor (KHRT) model. A detailed description for these models can be found in [25, 29]. As a surrogate for Diesel fuel, *n*-dodecane thermo-physical liquid properties have been prescribed for heat capacity, viscosity, latent heat, vapor pressure, density and surface tension. The fuel rate-of-injection (ROI) has been implemented according to [27], through an injector for which the main characteristics are given in Table 2.

Table 2. Injector configuration [27].

Injector type	<i>Bosch 210677</i>
Actual nozzle diameter, d	0.0837 mm
Fuel surrogate	<i>n - dodecane</i>
Injection pressure	150 MPa
Discharge coefficient, C_d	0.98
Area-contraction coefficient, C_a	0.89

All simulations have been performed with unchanged parameters for the non-reactive reference case whom initial conditions are summarized in Table 3. The initial random perturbations responsible for the event-to-event variability are introduced through the well established built-in turbulent dispersion model, which assumes each injected parcel to be affected by a stochastically-varying velocity field mimicking the fluctuating velocities within the turbulent eddies, as reported in [25]. The widely adopted O'Rourke model [30] has been selected to consider inter-droplet interactions.

Table 3. Initial conditions for the non-reactive reference case [27].

Oxygen volume fraction	0 %
Ambient temperature	900 K
Ambient density	22.8 kg/m ³
Ambient pressure	6.05 MPa
Fuel temperature	363 K

RESULTS AND DISCUSSION

In this section, the three averaging procedures mentioned above are discussed in detail: spatial and time averaging techniques in particular are further analyzed by means of statistical tools for the estimation of turbulent integral length (ILS) and time scales (ITS), respectively. Further, the results for three different combinations of the general averaging procedures are presented and compared by means of mixture fraction and azimuthal velocity distributions.

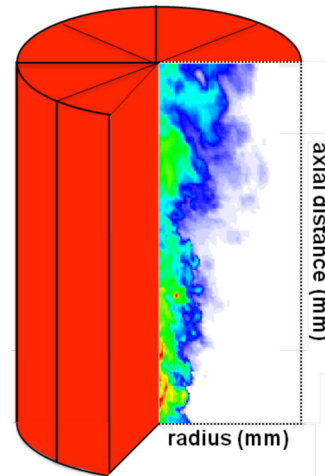


Figure 2. Sketch showing the considered test area for averaging statistics. The test volume is defined in the range 0-10 mm and 20-50 mm in radial and axial direction, respectively. The injector is located on the centerline at 0 mm axial distance (not shown here).

For the present study, LES simulations of non-reacting spray injections for the Sandia Spray A reference case have been carried out until 3 ms. As shown in Figure 2, averaging statistics have been applied for a confined test region of 0-10 mm in radial direction and 20-50 mm in axial direction, since high-fidelity experimental data for mixture fraction distribution (both mean and standard deviation) are available from the Engine Combustion Network (ECN) community [27]. The injector is located on the centerline at 0 mm axial distance (not visible here) and the turbulent non-reacting spray develops from the bottom upwards. Analogous to the ECN published data, the results presented in this section are all conducted while the spray can be assumed to be in QSS, as will be further discussed later.

Assessment of Averaging Methods

The most common statistics based on ensemble averaging techniques require a large number of realizations, which - to the literature - generally vary between 20 and 50 for diesel spray or engine related configurations, [24, 31, 32]. In the present work, the ensemble average is obtained by using one plane of the test domain per realization, representing the ideal procedure to conduct statistical studies since the different realizations are certainly not correlating, allowing event-to-event variability studies. However, performing such a bulk of realizations requires an enormous computational effort and is often not practicable, especially for design purposes, since a unique non-reactive simulation with the considered mesh (see Table 1) up to 3 ms requires approximately 18,000 CPU hours due to the small time steps needed to satisfy the specified Courant number.

Compared to ensemble averaging, spatial averaging provides the opportunity to extract more information out of one single realization. For the present setup, the circumferential direction is considered as the direction of homogeneity, since the geometry is axial-symmetric to the injector axis. Thus, the spatial average is determined by evaluating multiple r - z planes separated by a constant azimuthal angle θ as indicated in Figure 2. In order to determine the total amount of independent samples available for statistics, the larger turbulent structures between the sample planes need to be evaluated: If turbulent eddies are larger than the inter-planar distance, the flow field correlates, violating the required condition of independence between statistical samples.

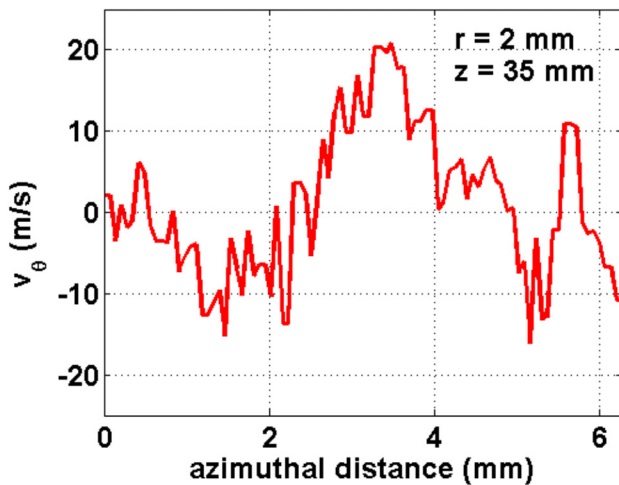


Figure 3. Azimuthal velocity profile along azimuthal axis at 2 mm and 35 mm in radial and axial direction, respectively.

Figure 3 shows the azimuthal velocity profile along the circumferential direction at a fixed radial and axial position of 2 mm and 35 mm, respectively. The strongly fluctuating velocity distribution is the result of the predicted flow field and provides essential statistical information for the estimation of the larger turbulent structures at this location. The correlation between the flow fields of the different planes can be evaluated by means of the azimuthal ILS ($L_{I,\theta}$) which is calculated based on the autocorrelation function given by

$$a_k = \frac{\sum_{i=1}^{N-k} (x_i - \bar{x})(x_{i+k} - \bar{x})}{\sum_{i=1}^{N-k} (x_i - \bar{x})^2}$$

where a_k denotes the correlation level and x_i the variable of interest such as the azimuthal velocity (v_θ). Figure 4 shows the sample spatial autocorrelation results for the azimuthal velocity profile presented in Figure 3. Auto-correlation values close to 1 indicate a full match of the flow field whereas values approaching zero suggest completely uncorrelated flow patterns. According to Feiereisen, the ILS is derived by numerically integrating the auto-correlation function until the first intersection with the confidence interval, set at 10 % [33, 34]. This procedure was performed for the entire test domain and the resulting azimuthal ILSs distribution is presented in Figure 5 in mm (left). In general, within the superimposed dashed black iso-line denoting the mean spray area, the ILS ranges between 0.1 and 1 mm and tends to increase in radial and axial direction mainly due to lower velocities and accordingly lower Reynolds numbers. Since the

number of points of the computational grid is not enough for a quantitative determination of the ILS using the velocity distribution, the values are not shown in the regions very close to the injector axis. From 40 mm downstream of the nozzle exit the cells size increases and accordingly the region where no quantitative determination of the ILS can be conducted.

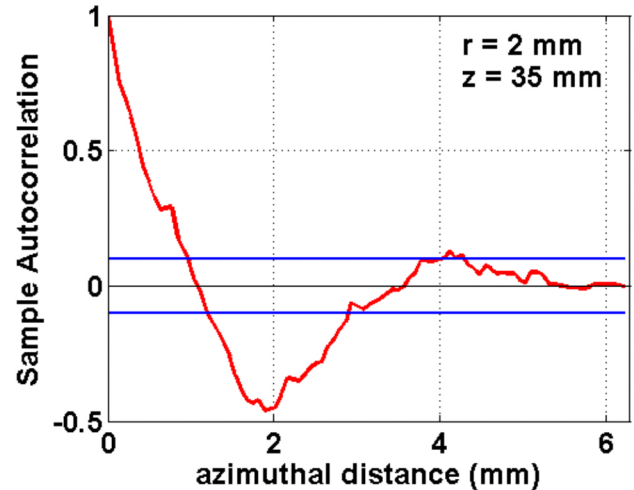


Figure 4. Sample spatial autocorrelation for the azimuthal velocity at 2 mm and 35 mm in radial and axial direction, respectively (red); confidence interval (blue).

The estimation of the available independent planes is obtained dividing the turbulent eddy size represented by the azimuthal ILS from the circumferential distance, as

$$N_{planes,i} = \frac{2\pi r_i}{L_{I,\theta,i}}$$

As is evident from Figure 5 (right), the maximal available number of independent planes increases towards the spray boundary since the physical space between the planes increases proportional to the radius. Accordingly, the region close to the centerline can be considered as the limiting factor for the spatial averaging approach. Spatial averaging analysis performed based on this outcome would be very effective since for each position the maximum number of samples can be considered, increasing the accuracy of the results especially at larger radii. Averaging over a dynamic number of samples requires complex post-processing algorithms and large storage space, therefore a fixed number of planes separated by a constant azimuthal angle is defined a priori by means of a sensitivity study. The evaluation is performed for the azimuthal angles $\theta = 36^\circ$, 30° and 24° which are the equivalent of 10, 12 and 15 equidistant planes per simulation, as illustrated in Figure 6. The green regions indicate where the ILS is smaller than the distance between two consecutive planes suggesting independent samples, while the red regions represent a correlated flow field and occur mostly towards the central axis. Considering 15 planes per realization leads to a relatively large area where significant correlation is present up to a radius of 2 mm. On the other hand, the adoption of 12 planes per realizations displays considerably less correlation that is concentrated up to a radius of about 1 mm, exhibiting results comparable to the method with 10 planes per realization. Nonetheless, areas with correlation cannot be completely avoided since the physical space