

Assessment of Large-Eddy Simulations of Turbulent Round Jets Using Low-Order Numerical Schemes

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ABSTRACT

The basic idea behind large-eddy simulation (LES) is to accurately resolve the large energy-containing scales and to use subgrid-scale (SGS) models for the smaller scales. The accuracy of LES can be significantly impacted by the numerical discretization schemes and the choice of the SGS model. This work investigates the accuracy of low-order LES codes in the simulation of a turbulent round jet which is representative of fuel jets in engines. The turbulent jet studied is isothermal with a Reynolds number of 6800. It is simulated using Converge, which is second-order accurate in space and first-order in time, and FLEDS, developed at Purdue University, which is sixth-order accurate in space and fourth-order in time. The high-order code requires the resolution of acoustic time-scales and hence is approximately 10 times more expensive than the low-order code. It is shown that the high-order code is able to accurately capture both the potential core length and the radial spreading rate, whereas the low-order code over-predicts the potential core length by 200% and the spreading rate by 15%. A systematic study of the influence of the SGS model and the amplitude of the inflow perturbation is then performed with the low-order code to determine if its results can be altered to more closely match those of the high-order code. Based on this study, the recommendation is to increase the amplitude of the inflow perturbation by 10 times to predict the correct potential core length and to use the dynamic structure (DS) SGS model instead of the Smagorinsky model to more accurately predict the radial spreading rate. It is also shown that by employing the DS model, the low-order code is able to correctly predict the energy cascade from the resolved scales to the subgrid scales. The low-order code is then employed to simulate a non-isothermal turbulent round jet with a Reynolds number of 250,000 which is relevant for gasoline direct injection (GDI) engine applications. It is shown that using the recommended values for the vortex ring amplitude and the choice of the SGS model, the low-order code is able to predict the correct potential core length and spreading rate for the jet.

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INTRODUCTION

With increasing computational capabilities in recent years, there has been increasing use of large-eddy simulations (LES) for simulating practical flows like internal combustion engines (ICEs) [1] and gas turbines [2]. In LES, the large turbulent scales of the flowfield are fully resolved, whereas the effects of the smaller scales are modeled. Since the larger scales are explicitly represented, LES provides significant advantages over Reynolds-Averaged Navier-Stokes (RANS) simulations in which all the scales are modeled. Several commercially available computational fluid dynamics (CFD) packages now provide capabilities to perform LES for complicated geometries.

In LES, the effect of the unresolved scales on the energy-containing scales of the flow are modeled using subgrid-scale (SGS) stresses, species fluxes and heat fluxes. The smallest resolved scales are

typically used in modeling these SGS terms. For instance, the Smagorinsky model, which is the most commonly used SGS model, uses the local grid size to determine the eddy viscosity, which is then used to calculate the SGS stresses. Hence, it is essential that these small scales be resolved accurately to model the subgrid terms. Ghosal [3] performed a comprehensive mathematical analysis of the effect of numerical errors in LES of turbulent flows. He showed that the finite-differencing error for a second-order scheme remained significantly larger than the subgrid term over a wide range of cases, and an extremely fine grid is required when such schemes are used. Morinishi et al. [4] developed fully conservative fourth order central difference schemes generalized for the case of a non-uniform mesh. They showed that these high-order schemes result in significant improvements over a second-order scheme, when used by the

simulation of a turbulent channel flow. An alternative to the use of high-order schemes to improve the accuracy of LES is to employ explicit filtering [5].

For complex geometries, high-order methods are difficult to implement and are expensive computationally. For these reasons, most commercial codes which are designed to achieve fast turnaround times use low-order numerical schemes which can compromise numerical accuracy. Tsang and Rutland [6] studied the effects of numerical schemes for a planar gas jet and a diesel spray using OpenFOAM, a popular commercial CFD code. They showed that using a cubic central differencing scheme for spatial discretization and the Euler implicit time integration scheme lead to the best predictions. They also showed that use of a first-order upwind scheme for spatial discretization lead to large discrepancies. Converge [7] is another popular commercial CFD code which has been extensively employed for engine simulations [8, 9], due to its unique mesh generation capabilities. The spatial discretization employed in Converge is less than 2nd-order accurate globally while the temporal discretization is only 1st-order accurate. The adequacy of performing LES with this code based on relatively low-order scheme is assessed in this work. This is achieved by comparing LES of canonical flows using Converge and the Flow Large-Eddy and Direct Numerical Simulations (FLEDS) code, which is a high-order academic code developed at Purdue University. FLEDS has been extensively employed in direct numerical simulation (DNS) [10, 11, 12] and LES studies [13, 14]. A simple canonical flow problem - the non-reacting turbulent round jet - is chosen for the comparison of the two codes. Turbulent round jets have been studied in detail, both experimentally and computationally, by several researchers. Ball et al. [15] provides a comprehensive review of experimental and numerical studies of turbulent round jets. Modeling the structure of the turbulent jet accurately is critical in accurate modeling of the fuel injection process in both ICEs and gas turbine engines.

The outline of the rest of the paper is as follows. In the next section, the numerical features of the two codes employed in this study - Converge and FLEDS - are briefly described. This is followed by a discussion of the computational setup and a description of the subgrid-scale models employed in this study. The results from the two codes for LES of the turbulent round jet are then compared in detail. A systematic study is then performed with the low-order code to determine if boundary and initial conditions can be calibrated to obtain results comparable with the high-order code. Finally, the low-order code with calibrated boundary and initial conditions is employed for a turbulent round jet simulation with a Reynolds number (Re) of 250,000, which is relevant for gasoline direct injection (GDI) engine applications.

NUMERICAL APPROACH

Numerics of the Codes

The high-order code employed in the current study is called FLEDS, which was developed at Purdue University. It solves the 3D compressible equations of motion on a non-staggered Cartesian grid. It employs a 6th-order compact finite difference scheme developed by

Lele [16]. For a generic quantity f at node i along a certain direction, the first derivative of f on a uniform grid with a spacing h is evaluated using the compact scheme as,

$$\frac{1}{3}f'_{i-1} + f'_i + \frac{1}{3}f'_{i+1} = \frac{7}{9h}(f_{i+1} - f_{i-1}) + \frac{1}{36h}(f_{i+2} - f_{i-2}). \quad (1)$$

A compact-storage fourth-order four-stage Runge-Kutta method [17] is implemented in the code for the time integration. A 6th-order accurate spatial filter is employed to remove spurious waves for stability concerns. Navier-Stokes Characteristic Boundary Conditions [18] are employed for inflow and outflow boundaries. The code is written in FORTRAN 90 and has been parallelized using the message passing interface (MPI) libraries. The code has been employed in several LES and DNS studies in the past [10, 13, 19].

The low-order code employed in this study is Converge version 2.3 [7]. The code uses finite volume methods to solve the integral form of the conservation equations on a non-staggered grid. Pressure is solved using a modified Pressure Implicit with Splitting of Operators (PISO) algorithm. A 2nd-order central differencing scheme is used for spatial discretization in which, the first derivative of a generic quantity f is expressed as,

$$f'_i = \frac{1}{2h}(f_{i+1} - f_{i-1}). \quad (2)$$

A 1st-order accurate scheme is used for temporal discretization. This code has been employed in the past for a variety of LES applications [20, 21, 22].

Computational Setup

The non-reacting round jet considered in the current study is an air jet at 300 K injected into a quiescent flow of air at 1 bar and 300 K. The mean jet exit velocity (U_j) is 21 ms⁻¹ while the coflow velocity (U_c) is 0.1 ms⁻¹. The diameter of the jet (d_j) is 5 mm, based on which the Reynolds number is 6800. The computational domain employed for the round jet simulation is shown in Fig. 1. The domain measures 400×125×125 mm (80×25×25 d_j). Fine resolution grids are placed near the jet exit plane and along the centerline by employing either grid stretching (FLEDS) or fixed embedding (Converge). In both codes, the finest resolution is fixed at 0.1 jet diameters. A top-hat profile is used to specify the inflow velocity boundary, i.e.,

$$u(x = 0, r, \theta) = \left(\frac{U_j - U_c}{2} \right) \left[\tanh \left(\frac{r_j - r}{\delta/3} \right) + 1 \right] + U_c, \quad (3)$$

where r and θ are the radius and the azimuthal angle of the cylindrical coordinates; r_j is the radius of the jet and δ represents the momentum boundary thickness of the jet at the exit plane and is selected at 0.1 d_j . Unity Lewis number assumption is employed in both FLEDS and Converge simulations. Bogey et al. [23] suggested introducing small disturbances near the jet exit plane to facilitate laminar-turbulence

transitions. In this work, ten modes of divergence-free vortex ring structures are superimposed onto the shear layers of the jet near the inflow boundary in every iteration. The disturbances are given by:

$$u'_x(x, r, \theta) = \sum_{n=0}^9 \alpha \epsilon_n \cos(n\theta + \psi_n) U_{x_0}(x, r), \quad (4)$$

$$u'_r(x, r, \theta) = \sum_{n=0}^9 \alpha \epsilon_n \cos(n\theta + \psi_n) U_{r_0}(x, r), \quad (5)$$

where

$$\Delta(x, r) = \sqrt{(x - x_0)^2 + (r - r_0)^2}, \quad (6)$$

$$U_{x_0}(x, r) = 2 \frac{r_0}{r} \frac{r - r_0}{\Delta_0} \exp \left[-\ln(2) \left(\frac{\Delta(x, r)}{\Delta_0} \right)^2 \right] U_j, \quad (7)$$

$$U_{r_0}(x, r) = -2 \frac{r_0}{r} \frac{x - x_0}{\Delta_0} \exp \left[-\ln(2) \left(\frac{\Delta(x, r)}{\Delta_0} \right)^2 \right] U_j. \quad (8)$$

Here, r_0 represents the radius of the vortex ring and is selected as twice the jet radius; x_0 is chosen to be $2.4d_j$ which represents the axial location of the maximum disturbances; ϵ_n and ψ_n are the random amplitudes and phases for each mode of vortex ring, respectively. They are generated every time step from uniform distributions between $[-1, 1]$ and $[0, 2\pi]$, respectively. α is the amplitude of the disturbances and is selected at 0.03 in the FLEDS simulations. It was also shown that, with this formulation, disturbances are not correlated for azimuthal angles greater than 20° apart [23].

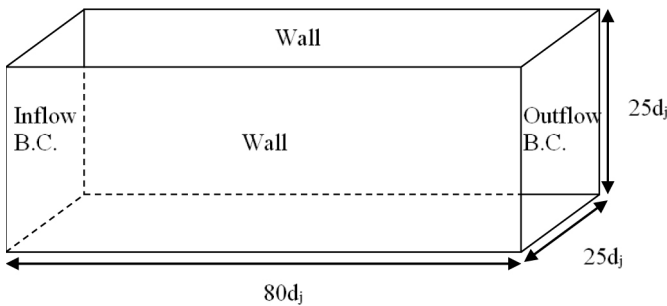


Figure 1. Schematic of the computational domain employed in the simulations with FLEDS and Converge codes.

Sub-Grid Scale Modeling

Large-eddy simulation is based on filtering the full set of conservation equations over a control volume of size Δ . As a result, terms such as the sub-grid scale (SGS) stress $\tau_{ij}^{SGS} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$ arise which require closure. In this work, a constant coefficient Smagorinsky model with compressibility effects is used following a formulation from Moin et al. [24] in FLEDS and Converge

simulations. The Smagorinsky model is an eddy-viscosity based model where the SGS stress is linearly related to the filtered rate of strain $\bar{S}_{ij}$, i.e.,

$$\tau_{ij}^{SGS} = -\nu_T \bar{S}_{ij} = -(C_s \Delta)^2 |\bar{S}| \bar{S}_{ij}. \quad (9)$$

Here, $\bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$, $|\bar{S}| = \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}}$ and $C_s = 0.1095$ is the Smagorinsky coefficient.

In addition, dynamic Smagorinsky [24] and dynamic structure [25] turbulence models are also considered for Converge simulations. In the case of dynamic Smagorinsky model, the Smagorinsky coefficient is dynamically determined from filtering the flow field with a test filter size $\tilde{\Delta}$ that is larger than the grid filter Δ , i.e.,

$$C_s^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}, \quad (10)$$

where $L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j$ is the Leonard stress and $M_{ij} = 2\Delta^2 |\bar{S}| \bar{S}_{ij} - 2\tilde{\Delta}^2 |\tilde{S}| \tilde{S}_{ij}$. The advantage of dynamic Smagorinsky model over the standard Smagorinsky model is that no *a priori* knowledge of the Smagorinsky coefficient is needed. In the case of the dynamic structure model, modeling of the SGS stress does not invoke the eddy-viscosity model, but is related to the Leonard stress through

$$\tau_{ij}^{SGS} = \left(\frac{2k}{L_{kk}} \right) L_{ij}. \quad (11)$$

Here, k is the SGS kinetic energy and is solved from its own transport equation. For the given incompressible flow, the transport equation simplifies to

$$\begin{aligned} \frac{\partial k}{\partial t} + \bar{u}_i \frac{\partial k}{\partial x_i} = & -\frac{1}{\rho} \left[\bar{u}_i \frac{\partial p}{\partial x_i} - \bar{u}_i \frac{\partial p}{\partial x_i} \right] - \frac{\partial}{\partial x_j} \left[\frac{1}{2} \tau_{ij} - \bar{u}_i \tau_{ij} \right] \\ & + \nu \frac{\partial^2 k}{\partial x_j \partial x_j} - \tau_{ij}^{SGS} \bar{S}_{ij} - \epsilon_{sgs}. \end{aligned} \quad (12)$$

Similar to the dynamic Smagorinsky model, there is no need for parameter tuning with the use of dynamic structure model. Furthermore, the dynamic structure model enforces energy balance between the resolved scale and the sub-grid scale flow.

RESULTS AND DISCUSSION

Comparison of Round-Jet LES

Table 1 lists the simulation parameters used in the FLEDS (Case 0) and Converge (Case 1-8) simulations. All simulations are performed until 200 ms and turbulence statistics are collected from 100 to 200 ms. Note that the condition employed in Case 1 of Converge simulation is identical to the FLEDS simulation which is used as the baseline. Simulation using FLEDS is approximately 10 times more