Influence of different subgrid-scale models in low-order LES of supersonic jet flows

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Received: 2 June 2016 / Accepted: 15 April 2018 / Published online: 24 April 2018 © The Brazilian Society of Mechanical Sciences and Engineering 2018

Abstract
The present work is concerned with a study of large eddy simulations (LES) of unsteady turbulent jet flows. In particular, the present analysis is focused on the effects of the subgrid-scale modeling used when a second-order spatial discretization methodology is employed for the numerical simulations. The present effort addresses perfectly expanded supersonic jets, because the authors want to emphasize the effects of the jet mixing phenomena. The LES formulation is discretized using the finite difference approach, after the equations are rewritten in a generalized coordinate system. Both space and time discretizations are second-order accurate and an explicit time march is adopted. Special care is dedicated to the discretization of the energy equation to appropriately model the set of filtered equations appearing in the LES formulation. The classical Smagorinsky, the dynamic Smagorinsky and the Vreman models are the subgrid-scale closures selected for the present work. The computational results are compared to data in the literature to validate the present simulation tool. Results indicate that the characteristics of numerical discretization can be as important as the effects of the subgrid-scale models for such low-order spatial discretization schemes. A detailed analysis is presented for the performance of each subgrid closure in the numerical context here considered.

Keywords Supersonic jet flow · LES · Subgrid-scale models · Low-order methods

1 Introduction
A novel compressible large eddy simulation (LES) tool has recently been developed at Instituto de Aeronáutica e Espaço (IAE) [17]. This numerical tool was developed, to a large extent, to generate unsteady flow data on large launch vehicle propulsion exhaust jets, for which the noise generated on certain flight conditions can be extremely relevant for dimensioning of payload structures being carried by the launcher. The approach intended was to study the aeroacoustics of such jets using a hybrid approach, based on the Ffowcs Williams and Hawkings analogy [34]. As such, and considering previous capabilities available in the research group [2, 3], the decision was to use a low-order spatial discretization approach for such development. The LES tool developed was denoted JAZzY, and further details of its formulation and computational performance can be found in Refs. [16, 17].

It should be emphasized that the use of low-order spatial discretization for LES calculations is not a new idea, and it is actually suggested by several recognized research groups in the world, as indicated, for instance, in Ref. [8]. The main aspect involved in such proposition is computational efficiency, which can typically be achieved with the low-order spatial discretization. However, the critical question that arises in such context is the effectiveness of the subgrid-scale modeling [20, 33]. Therefore, the present paper is precisely directed towards the study of the effects of the subgrid-scale modeling used when a second-order spatial discretization methodology is employed for the numerical
simulations with a LES formulation. The subgrid-scale closures included in the present study are the classical Smagorinsky model [21, 22, 28], the dynamic Smagorinsky model [13, 26] and the Vreman model [31].

In the present effort, the LES formulation is discretized using the finite difference approach, after the governing equations are rewritten in general curvilinear coordinates [16, 17]. Inviscid and viscous numerical fluxes are calculated using a second-order accurate centered scheme with the explicit addition of artificial dissipation terms. Time march uses a five-stage, second-order accurate, explicit Runge–Kutta scheme. The present formulation for the model uses a five-stage, second-order accurate, explicit Runge–Kutta scheme. The present formulation for the energy equation is based on the System I set of equations [30], to appropriately model the filtered terms of the energy equation. The test cases address numerical simulations of perfectly expanded jet flows, and the current results are compared to both numerical [24] and experimental [7] independent data.

2 Large eddy simulation filtering

The large eddy simulation is based on the principle of scale separation, which is addressed as a filtering procedure in a mathematical formalism. A modified version of the System I filtering approach [30] is used in present work, which is given by

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \mathbf{u}_i)}{\partial x_j} = 0,
\]

\[
\frac{\partial}{\partial t} (p \mathbf{u}_i) + \frac{\partial (p \mathbf{u}_i \mathbf{u}_j)}{\partial x_j} + \frac{\partial \rho}{\partial x_j} \left( \delta_{ij} \mathbf{u}_k \mathbf{u}_k \right) + \frac{1}{3} \frac{\partial}{\partial x_j} \left( \delta_{ij} \sigma_{kk} \right) \mathbf{u}_i + \frac{\partial q_j}{\partial x_j} = 0,
\]

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \mathbf{u}_i \mathbf{u}_j)}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = 0,
\]

in which \( t \) and \( x_i \) are independent variables representing time and spatial coordinates of a Cartesian coordinate system, \( x \), respectively. The components of the velocity vector, \( \mathbf{u} \), are written as \( u_i \) and \( i = 1, 2, 3 \). Density, pressure and total energy per unit volume are denoted by \( \rho, p \) and \( e \), respectively. The \( (\cdot) \) and \( \langle \cdot \rangle \) operators are used to represent filtered and Favre averaged properties, respectively. The System I formulation neglects the double correlation term and the total energy per unit volume is written as

\[
\mathbf{\bar{u}} = \frac{\mathbf{u}}{\gamma - 1} + \frac{1}{2} \rho \mathbf{u}_i \mathbf{u}_i.
\]

The heat flux, \( q_j \), is given by

\[
q_j = (\kappa + \kappa_{\text{sgs}}) \frac{\partial T}{\partial x_j},
\]

where \( T \) is the static temperature and \( \kappa \) is the thermal conductivity coefficient, which can be expressed as:

\[
\kappa = \frac{\mu C_p}{Pr}.
\]

The thermal conductivity coefficient is a function of the specific heat at constant pressure, \( C_p \), of the Prandtl number, \( Pr \), which is equal to 0.72 for air, and of the dynamic viscosity coefficient, \( \mu \). The SGS thermal conductivity coefficient, \( \kappa_{\text{sgs}} \), is written as

\[
\kappa_{\text{sgs}} = \frac{\kappa_{\text{sgs}}}{Pr_{\text{sgs}}},
\]

where \( Pr_{\text{sgs}} \) is the SGS Prandtl number, which is equal to 0.9 for static SGS models and \( \mu_{\text{sgs}} \) is the eddy viscosity coefficient which is calculated by the SGS closure. The dynamic viscosity coefficient, \( \mu \), can be calculated using the Sutherland law,

\[
\mu(T) = \mu_\infty \left( \frac{T}{T_\infty} \right)^{\frac{8}{5} + S_1} \left( \frac{T}{T_\infty} - S_1 \right), \quad \text{with} \quad S_1 = 110.4 \, K.
\]

Density, static pressure and static temperature are correlated by the equation of state, given by

\[
\bar{p} = \rho RT,
\]

where \( R \) is the gas constant, written as

\[
R = C_p - C_v,
\]

and \( C_v \) is the specific heat at constant volume. The shear stress tensor, \( \tau_{ij} \), is written according to the Stokes hypothesis and includes the eddy viscosity coefficient, \( \mu_{\text{sgs}} \),

\[
\tau_{ij} = 2(\mu + \mu_{\text{sgs}}) \left( \mathbf{\hat{S}}_{ij} - \frac{1}{3} \delta_{ij} \mathbf{\hat{S}}_{kk} \right),
\]

in which the components of the rate-of-strain tensor, \( \mathbf{\hat{S}}_{ij} \), are given by

\[
\mathbf{\hat{S}}_{ij} = \frac{1}{2} \left( \frac{\partial \mathbf{u}_i}{\partial x_j} + \frac{\partial \mathbf{u}_j}{\partial x_i} \right).
\]

The SGS stress tensor components are written using the eddy viscosity coefficient [27],

\[
\sigma_{ij} = -2\mu_{\text{sgs}} \left( \mathbf{\hat{S}}_{ij} - \frac{1}{3} \delta_{ij} \mathbf{\hat{S}}_{kk} \right) + \frac{1}{3} \delta_{ij} \sigma_{kk}.
\]

The eddy viscosity coefficient, \( \mu_{\text{sgs}} \), and the components of the isotropic part of the SGS stress tensor, \( \sigma_{kk} \), are modeled by the SGS closure.
3 Subgrid-scale modeling

The present section is directed towards the description of the turbulence modeling and the theoretical formulation of subgrid scale closures included in the present work. The closure models presented here are based on the homogeneous turbulence theory, which is usually developed in the spectral space as an attempt to quantify the interaction between the different scales of turbulence.

3.1 Smagorinsky model

The Smagorinsky model [28] is one of the simplest algebraic models for the deviatoric part of the SGS tensor used in large eddy simulations. The isotropic part of the SGS tensor is neglected for the Smagorinsky model in the current work. This SGS closure is a classical model based on the large-scale properties and it is written as

$$\mu_{s_{\text{gs}}} = \overline{\rho} C_s (\Delta)^2 | \vec{S} |,$$

where

$$| \vec{S} | = (2\overline{\vec{S}}_{ij} \vec{S}_{ij})^{\frac{1}{2}},$$

$\Delta$ is the filter size and $C_s$ is the Smagorinsky constant. Several attempts can be found in the literature regarding the evaluation of the Smagorinsky constant. The value of this constant is adjusted to improve the results for different flow configurations. In practical terms, the Smagorinsky subgrid model has a flow dependency on the constant, which takes values ranging from 0.1 to 0.2 depending on the flow. The value suggested by Lilly [22], $C_s = 0.148$, is used in the current work.

This model is generally over dissipative in regions of large mean strain. This is particularly true in the transitional region between laminar and turbulent flows. Moreover, the limiting behavior near the wall is not correct, and the model predictions correlate poorly with the exact subgrid-scale tensor [11]. However, it is a very simple model and, with the use of damping functions and good calibration, it can be successfully applied in large eddy simulations.

3.2 Vreman model

Vreman [31] proposed a turbulence model that can correctly predict inhomogeneous turbulent flows. For such flows, the eddy viscosity should become small in laminar and transitional regions. This requirement is unfortunately not satisfied by existing simple eddy viscosity closures such as the classic Smagorinsky model [10, 21, 28]. The Vreman SGS model is also very simple and it is given by

$$\mu_{s_{\text{gs}}} = \overline{\rho} c \sqrt{\frac{B_{ij}}{\alpha_{ij} \alpha_{ij}}}$$

with

$$\alpha_{ij} = \frac{\partial \vec{u}_{ij}}{\partial x},$$

$$B_{ij} = \beta_{11} \beta_{22} - \beta_{12}^2 + \beta_{11} \beta_{33} - \beta_{13}^2 + \beta_{22} \beta_{33} - \beta_{23}^2,$$

and

$$\beta_{ij} = \Delta_m^2 \alpha_{mj} \alpha_{mj}.$$  

The $c$ constant is related to the Smagorinsky constant, $C_s$, and it is given by

$$c = 2.5 C_s^2,$$

and $\Delta_m$ is the filter width in each direction. In the present work, the isotropic part of the SGS tensor is neglected for the Vreman model. The $\alpha$ symbol represents the matrix of first-order derivatives of the filtered components of velocity, $\vec{u}$. The SGS eddy viscosity coefficient is defined as zero when $\alpha_{ij} / \alpha_{ij}$ equals zero. Vreman [31] states that the $\beta_{ij}$ tensor is proportional to the Clark model [9, 19] in its general anisotropic form [32].

The Vreman model can be classified as a very simple model because it is expressed in terms of first-order derivatives and it does not involve explicit filtering, averaging and clipping procedures, and it is rotationally invariant for isotropic filter widths. The model was originally created for incompressible flows and it has presented good results for two incompressible flow configurations: the transitional and turbulent mixing layer at high Reynolds number and the turbulent channel flow [32]. In both cases, the Vreman model is found to be more accurate than the classical Smagorinsky model and as good as the dynamic Smagorinsky model.

3.3 Dynamic Smagorinsky model

Germano et al. [12] developed a dynamic SGS model to overcome the issues of the classical Smagorinsky closure. The model uses the strain rate fields at two different scales and, thus, extracts spectral information in the large-scale field to extrapolate the small stresses [26]. The coefficients of the model are computed instantaneously in the dynamic model. They are a function of the positioning in space and time rather than being specified a priori. Moin et al. [26] extended the work of Germano for compressible flows. The dynamic Smagorinsky model for compressible flow configurations is detailed in the present section.

The dynamic model introduces the test filter, $\hat{\vec{S}}$, which has a larger filter width, $\hat{\Delta}$, than the one of the resolved grid.
filter, $\overline{\cdot}$. The use of test filters generates a second field with larger scales than the resolved field. The Yoshizawa model [35] is used for the isotropic portion of the SGS tensor and it is written as

$$\sigma_t = 2C_1\overline{p}\Delta^2|\overline{S}|^2,$$

where $C_1$ is defined by

$$C_1 = \frac{\left(\overline{\mu_t\mu_t} - \overline{\mu_t\mu_t/\overline{p}}\right)}{2\Delta^2\overline{p}\Delta^2|\overline{S}|^2}.$$  

A volume averaging, here indicated by $\langle \cdot \rangle$, is suggested by Moin et al. [26] and by Garnier et al. [11] to avoid numerical issues. The eddy viscosity, $\mu_{sgs}$, is calculated using the same approach used by static Smagorinsky model,

$$\mu_{sgs} = (\rho C_{ds}\Delta^2)|\overline{S}|,$$

where

$$|\overline{S}| = \left(2\overline{S}_{\eta}\overline{S}_{\eta}\right)^{1/2},$$

and $C_{ds}$ is the dynamic constant of the model, which is given by

$$C_{ds} = \frac{\left(\overline{\mu_t}\overline{\mu_t} - \overline{\mu_t}\overline{\mu_t/\overline{p}}\right)}{2\Delta^2\left(\overline{p}\overline{S}_{\eta}\overline{S}_{\eta} - \frac{1}{2}\overline{p}\overline{S}_{\eta}\overline{S}_{\eta}\right)}.$$  

The SGS Prandtl number is computed using the dynamic constant, $C_{ds}$, and written as

$$Pr_{sgs} = C_{ds} = \frac{\left(\Delta^2\left(\overline{p}\overline{S}_{\eta}\overline{S}_{\eta}\right)\overline{\tau}_{\eta}\overline{\tau}_{\eta} - \Delta^2\overline{p}\overline{S}_{\eta}\overline{\tau}_{\eta}\overline{\tau}_{\eta}\right)}{\left(\overline{\mu_t}\overline{T} - \overline{\mu_t}\overline{T}/\overline{p}\right) - \frac{\overline{\tau}_{\eta}\overline{\tau}_{\eta}}{\overline{\tau}_{\eta}\overline{\tau}_{\eta}}}.$$  

4 Transformation of coordinates

In the present work, the filtered Navier–Stokes equations are written in strong conservation law form for a 3-D general curvilinear coordinate system as

$$\frac{\partial \hat{Q}}{\partial t} + \frac{\partial}{\partial \xi}\left(\hat{E}_e - \hat{E}_c\right) + \frac{\partial}{\partial \eta}\left(\hat{F}_e - \hat{F}_c\right) + \frac{\partial}{\partial \zeta}\left(\hat{G}_e - \hat{G}_c\right) = 0.$$  

The general coordinate transformation adopted in the present case can be written as

$$\xi = \xi(x, y, z),$$
$$\eta = \eta(x, y, z),$$
$$\zeta = \zeta(x, y, z).$$  

For the simulations performed in the present paper, $\xi$ is the axial jet flow direction, $\eta$ is the radial direction and $\zeta$ is the azimuthal direction. The new vector of conserved properties in general curvilinear coordinates can be written as

$$\hat{Q} = J^{-1} \begin{bmatrix} p^U \\ \overline{p}\hat{u} + p^z \xi \\ \overline{p}\hat{v} + p^z \eta \\ \overline{p}\hat{w} + p^z \zeta \end{bmatrix}.$$  

Here, $J$ is the Jacobian of the transformation, which could be expressed as

$$J = \left(x_{\eta}Y_{\eta}\xi + x_{\xi}Y_{\xi}\eta + x_{\zeta}Y_{\zeta}\eta - x_{\eta}Y_{\xi}\xi - x_{\xi}Y_{\zeta}\xi - x_{\zeta}Y_{\xi}\zeta\right)^{-1}.$$  

The inverse metric terms of the transformation, which are used to compute the transformation Jacobian, can be directly computed by central finite differences from the mesh information. Such computation is given by

$$x_{\xi} = \frac{\partial x}{\partial \xi}, \quad x_{\eta} = \frac{\partial x}{\partial \eta}, \quad x_{\zeta} = \frac{\partial x}{\partial \zeta},$$
$$y_{\xi} = \frac{\partial y}{\partial \xi}, \quad y_{\eta} = \frac{\partial y}{\partial \eta}, \quad y_{\zeta} = \frac{\partial y}{\partial \zeta},$$
$$z_{\xi} = \frac{\partial z}{\partial \xi}, \quad z_{\eta} = \frac{\partial z}{\partial \eta}, \quad z_{\zeta} = \frac{\partial z}{\partial \zeta}. $$  

The inviscid flux vectors in general curvilinear coordinates, $\hat{E}_e$, $\hat{F}_e$ and $\hat{G}_e$, can be written as

$$\hat{E}_e = J^{-1} \begin{bmatrix} p^U \\ pU + p^z \xi \\ p\hat{v} + p^z \eta \\ \overline{p}\hat{w} + p^z \zeta \end{bmatrix}, \quad \hat{F}_e = J^{-1} \begin{bmatrix} pV \\ p\hat{u} + p^z \eta \\ \overline{p}\hat{v} + p^z \xi \\ \overline{p}\hat{w} + p^z \zeta \end{bmatrix},$$
$$\hat{G}_e = J^{-1} \begin{bmatrix} pW \\ p\hat{u} + p^z \zeta \\ \overline{p}\hat{v} + p^z \eta \\ \overline{p}\hat{w} + p^z \xi \end{bmatrix}.$$  

The contravariant velocity components, $U$, $V$ and $W$, are calculated as

$$U = \xi \hat{u} + \xi \hat{v} + \xi \hat{w},$$
$$V = \eta \hat{u} + \eta \hat{v} + \eta \hat{w},$$
$$W = \zeta \hat{u} + \zeta \hat{v} + \zeta \hat{w}.$$  

The metric terms are given by
\[
\xi_x = J(y_\eta z_\xi - y_\xi z_\eta), \quad \xi_y = J(z_\eta x_\xi - z_\xi x_\eta), \quad \xi_z = J(x_\eta y_\xi - x_\xi y_\eta), \\
\eta_x = J(y_\eta z_\eta - y_\eta z_\xi), \quad \eta_y = J(z_\eta x_\eta - z_\eta x_\xi), \quad \eta_z = J(x_\eta y_\eta - x_\eta y_\xi), \\
\zeta_x = J(y_\xi z_\eta - y_\eta z_\xi), \quad \zeta_y = J(z_\xi x_\eta - z_\eta x_\xi), \quad \zeta_z = J(x_\xi y_\eta - x_\eta y_\xi).
\]

(32)

The viscous flux vectors in general curvilinear coordinates, \( \mathbf{E}_v, \mathbf{F}_v \) and \( \mathbf{G}_v \), are written as

\[
\mathbf{E}_v = J^{-1} \begin{pmatrix}
\xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz} \\
\xi_x \tau_{yx} + \xi_y \tau_{yy} + \xi_z \tau_{yz} \\
\xi_x \tau_{zx} + \xi_y \tau_{zy} + \xi_z \tau_{zz}
\end{pmatrix}, \\
\mathbf{F}_v = J^{-1} \begin{pmatrix}
\eta_x \tau_{xx} + \eta_y \tau_{xy} + \eta_z \tau_{xz} \\
\eta_x \tau_{yx} + \eta_y \tau_{yy} + \eta_z \tau_{yz} \\
\eta_x \tau_{zx} + \eta_y \tau_{zy} + \eta_z \tau_{zz}
\end{pmatrix}, \\
\mathbf{G}_v = J^{-1} \begin{pmatrix}
\zeta_x \tau_{xx} + \zeta_y \tau_{xy} + \zeta_z \tau_{xz} \\
\zeta_x \tau_{yx} + \zeta_y \tau_{yy} + \zeta_z \tau_{yz} \\
\zeta_x \tau_{zx} + \zeta_y \tau_{zy} + \zeta_z \tau_{zz}
\end{pmatrix}.
\]

(33-35)

The \( \beta_x, \beta_y \) and \( \beta_z \) terms, which appear in the energy equation in the viscous flux vectors, can be calculated as

\[
\beta_x = \tau_{xx} \hat{u} + \tau_{xy} \hat{v} + \tau_{xz} \hat{w} - \overline{q}_x, \\
\beta_y = \tau_{xy} \hat{u} + \tau_{yy} \hat{v} + \tau_{yz} \hat{w} - \overline{q}_y, \\
\beta_z = \tau_{xz} \hat{u} + \tau_{zy} \hat{v} + \tau_{zz} \hat{w} - \overline{q}_z.
\]

(36)

5 Dimensionless formulation

In the present effort, the governing equations, given by Eq. (25), are made dimensionless by an appropriate selection of reference variables. From the perspective of the authors, the main advantage of the nondimensionalization process is that all flow properties are scaled to the same order of magnitude, which has important computational advantages [2]. In the present work, the dimensionless time, \( \tau \), is obtained as a function of the speed of sound of the jet at the inlet, \( a_j \), and the jet entrance diameter, \( D \).

Hence, it can be written as

\[
\tau = \frac{a_j}{D}.
\]

(37)

Dimensionless velocity components are referred to the speed of sound of the jet at the inlet as

\[
\mathbf{u} = \frac{\mathbf{u}}{a_j}.
\]

(38)

Density, pressure and total energy per unit of volume are made dimensionless with regard to the density and speed of the sound of the jet at the inlet. Hence, they can be written as

\[
\rho = \frac{\rho}{\rho_j}, \quad p = \frac{p}{\rho_j a_j^2}, \quad e = \frac{e}{\rho_j a_j^2}.
\]

(39)

Similarly, the viscosity coefficients, both bulk viscosity and subgrid-scale viscosity coefficients, are nondimensionalized by the laminar viscosity coefficient at the jet exit temperature, \( \mu_j \). The governing equations can, then, be rewritten, in terms of dimensionless variables, as

\[
\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{F}_v}{\partial \xi} + \frac{\partial \mathbf{F}_v}{\partial \eta} + \frac{\partial \mathbf{G}_v}{\partial \zeta} = M_j Re \left( \frac{\partial \mathbf{F}_v}{\partial \xi} + \frac{\partial \mathbf{F}_v}{\partial \eta} + \frac{\partial \mathbf{G}_v}{\partial \zeta} \right).
\]

(40)

The jet exit Mach number and jet exit Reynolds number are given, respectively, by

\[
M_j = \frac{U_j}{a_j} \quad \text{and} \quad Re = \frac{\rho_j U_j D}{\mu_j}.
\]

(41)

6 Numerical formulation

The governing equations previously described are discretized in a structured finite difference context for a general curvilinear coordinate system [2]. The numerical flux is calculated through a central difference scheme with the explicit addition of the anisotropic scalar artificial dissipation model of Turkel and Vatsa [29]. The time integration is performed by an explicit, second-order, five-stage Runge–Kutta scheme [14, 15]. Conserved properties and artificial dissipation terms are properly treated near boundaries to assure the physical correctness of the numerical formulation.

6.1 Spatial discretization

For the remainder of the paper, the authors will drop all underbars and tildes in the formulation for the sake of simplicity. Nevertheless, the reader should be advised that all equations are referring to filtered dimensionless quantities. Furthermore, the \( M_j/Re \) factor is assumed to be incorporated into the definition of the viscous flux vectors, again with the objective of simplifying the notation for the forthcoming discussion. The work uses a finite difference framework to discretize the governing equations, Eq. (40).
Hence, the result of the discretization of the spatial derivatives in the governing equations can be written as
\[
\left( \frac{\partial Q}{\partial t} \right)_{i,j,k} = -\text{RHS}_{i,j,k}. \tag{42}
\]

Here, RHS\(_{i,j,k}\) represents the residue for the (i, j, k) grid point. It is very convenient to write RHS\(_{i,j,k}\) as a function of the numerical flux vectors at the interfaces between grid points, following a nomenclature similar to the one used in Ref. [29]. Therefore, the residue can be written as
\[
\text{RHS}_{i,j,k} = \frac{1}{\Delta \xi} \left( E_{v(i, j+\frac{1}{2}, k)} - E_{v(i, j, k)} - E_{v(i, j-\frac{1}{2}, k)} + E_{v(i, j, \frac{1}{2}, k)} \right)
= \frac{1}{\Delta \eta} \left( F_{e(i, j+\frac{1}{2}, k)} - F_{e(i, j, k)} - F_{e(i, j-\frac{1}{2}, k)} + F_{e(i, j, \frac{1}{2}, k)} \right)
= \frac{1}{\Delta \xi} \left( G_{e(i, j, k+\frac{1}{2})} - G_{e(i, j, k, \frac{1}{2})} - G_{e(i, j, k, \frac{1}{2})} + G_{e(i, j, k, \frac{1}{2})} \right). \tag{43}
\]

Since a centered spatial discretization is being considered, the interface numerical flux vectors are defined as the arithmetic average of the corresponding physical flux vectors at the two grid points that share that interface. However, still due to the use of a centered scheme, the inviscid numerical fluxes must be augmented by artificial dissipation terms, to maintain numerical stability. In the present case, the scalar, non-isotropic, artificial dissipation model proposed by Turkel and Vatsa [29] is used. Hence, the numerical inviscid interface fluxes are written as
\[
E_{v(i, j, \frac{1}{2}, k)} = \frac{1}{2} \left( E_{v(i, j, k)} + E_{v(i, j+1, k)} \right) - J^{-1} d_{i,j,\frac{1}{2},k},
F_{e(i, j, \frac{1}{2}, k)} = \frac{1}{2} \left( F_{e(i, j, k)} + F_{e(i, j+1, k)} \right) - J^{-1} d_{i,j,\frac{1}{2},k},
G_{e(i, j, \frac{1}{2}, k)} = \frac{1}{2} \left( G_{e(i, j, k)} + G_{e(i, j+1, k)} \right) - J^{-1} d_{i,j,\frac{1}{2},k}, \tag{44}
\]
where the \(d_{i,j,\frac{1}{2},k}\) terms are the artificial dissipation operators. For instance, the operator in the \(\xi\) direction, at the (i + 1/2) interface, can be expressed as
\[
d_{i+\frac{1}{2},j,k} = \lambda_{\xi(i+\frac{1}{2},j,k)} \left[ \epsilon^{(2)}_{i+\frac{1}{2},j,k}(W_{i+1,j,k} - W_{i,j,k}) \right]
- \epsilon^{(4)}_{i+\frac{1}{2},j,k} (3W_{i+1,j,k} - 3W_{i,j,k} - W_{i-1,j,k})]. \tag{45}
\]

In this equation, the \(\epsilon^{(2)}\) and \(\epsilon^{(4)}\) terms are written as
\[
\epsilon^{(2)}_{i+\frac{1}{2},j,k} = k^{(2)} \max \left( v_{i+1,j,k}^d, v_{i,j,k}^d \right), \tag{46}
\]
\[
\epsilon^{(4)}_{i+\frac{1}{2},j,k} = \max \left[ 0 , k^{(4)} - \epsilon^{(2)}_{i+\frac{1}{2},j,k} \right]. \tag{47}
\]

The pressure gradient sensor operator, \(v_{i,j,k}^d\), for the \(\xi\) direction, as indicated in Ref. [29], is defined as
\[
v_{i,j,k}^d = \frac{|p_{i+1,j,k} - 2p_{i,j,k} + p_{i-1,j,k}|}{p_{i+1,j,k} - 2p_{i,j,k} + p_{i-1,j,k}}. \tag{48}
\]

The \(\mathbf{W}\) vector in Eq. (45) is calculated as a function of the conserved variable vector, \(Q\). The formulation intends to keep the total enthalpy constant in the final converged solution, for steady-state cases, which is the correct result for the Euler equations, and hence reduce the effect of the artificial dissipation terms. This approach is also valid for the viscous formulation because the artificial dissipation terms are added to the inviscid flux terms, in which they are really necessary to avoid nonlinear instabilities of the numerical formulation. The \(\mathbf{W}\) vector is given by
\[
\mathbf{W} = \dot{Q} + [0 \ 0 \ 0 \ 0 \ 0 \ p]^T. \tag{49}
\]

The spectral radius-based scaling factor, \(\lambda\), for the \(\eta\) direction is written as
\[
\lambda_{\eta(i+\frac{1}{2},j,k)} = \frac{1}{2} \left[ \left( \lambda_{\xi(i+\frac{1}{2},j,k)} \right)^{0.5} + \left( \lambda_{\xi(i+\frac{1}{2},j,k)} \right)^{0.5} \right]. \tag{50}
\]

The spectral radii, \(\lambda_{\xi}\), \(\lambda_{\eta}\) and \(\lambda_{\zeta}\) are given by
\[
\lambda_{\xi} = |U| + a\sqrt{\xi_x^2 + \eta_y^2 + \zeta_z^2}, \tag{51}
\]
\[
\lambda_{\xi} = |V| + a\sqrt{\xi_x^2 + \eta_y^2 + \zeta_z^2}, \tag{52}
\]
\[
\lambda_{\xi} = |W| + a\sqrt{\xi_x^2 + \eta_y^2 + \zeta_z^2}, \tag{53}
\]
in which, \(U, V\) and \(W\) are the contravariant velocity components in the \(\xi, \eta\) and \(\zeta\) directions, previously given in Eq. (31), and \(a\) is the local speed of sound, which can be written as
\[
a = \sqrt{\frac{|p|}{\rho}}. \tag{54}
\]

The calculation of artificial dissipation terms for the other coordinate directions is completely similar and, therefore, it is not discussed here.

It should be emphasized that the present artificial dissipation model is nonlinear and, hence, it allows for the selection between second and fourth-difference artificial dissipation terms. Therefore, for the problem of interest here, this approach ensures that, throughout most of the computational domain, only the third-order fourth-difference artificial dissipation terms are active, thus reducing the amount of artificial dissipation introduced in the solution. Furthermore, the scaling of the artificial dissipation operator in each coordinate direction, for instance, \(\lambda_{i+\frac{1}{2},j,k}\),
in Eq. (45), is primarily weighted by its own spectral radius of the corresponding flux Jacobian matrix, which gives the non-isotropic characteristics to the model [2, 29]. Further details on the artificial dissipation model here adopted can be seen in the original paper by Turkel and Vatsa [29] or in Ref. [2]. Computational aspects of the present implementation of the model and, in particular, issues associated to the computation of the various terms at partition interfaces, for parallel implementations, are discussed in detail in Refs. [16–18].

6.2 Time marching method

The time marching method used in the present work is a second-order, five-step Runge–Kutta scheme based on the work of Jameson and co-authors [14, 15]. The time integration can be written as

\[ Q_{i,j,k}^{(0)} = Q_{i,j,k}^n, \]

\[ Q_{i,j,k}^{(\ell)} = Q_{i,j,k}^{(0)} - \Delta t \text{RHS}_{i,j,k}^{(\ell-1)}, \quad \ell = 1, 2, \ldots, 5, \quad \] (54)

\[ Q_{i,j,k}^{n+1} = Q_{i,j,k}^{(5)}, \]

The process of validation of the present solver has addressed the issues related to the use of an explicit time integration, and it has indicated that the above time marching scheme is sufficiently adequate for the current purposes. The interested reader can find further details in such studies in Refs. [16–18]. Clearly, in the previous equation, \( \Delta t \) is the time step, and \( n \) and \( n + 1 \) indicate the property values at the current and at the next time step, respectively. The values adopted for the \( \alpha \) parameters are

\[ \alpha_1 = \frac{1}{4}, \quad \alpha_2 = \frac{1}{6}, \quad \alpha_3 = \frac{3}{8}, \quad \alpha_4 = \frac{1}{2}, \quad \alpha_5 = 1, \] (55)

according to the original reference that presents this specific Runge–Kutta method [14]. The time marching scheme is linearly stable for CFL \( \leq 2\sqrt{2} \) [2].

7 Boundary conditions

The geometry used in the present work presents a cylindrical shape which is generated by the rotation of a 2-D plane around a centerline. Figure 1 presents a lateral view and a frontal view of the computational domain used in the present work and the positioning of the entrance, exit, centerline, far-field and periodic boundary conditions. A discussion of all boundary conditions is performed in the following subsections.

7.1 Far-field boundary

Riemann invariants [23] are used to implement far-field boundary conditions. They are derived from the characteristic relations for the Euler equations. At the interface of the outer boundary, the following expressions apply

\[ \mathbf{R}^- = \mathbf{R}^-_\infty = q_{n\infty} - \frac{2}{\gamma - 1} a_{n\infty}, \]

\[ \mathbf{R}^+ = \mathbf{R}^+_e = q_{n_e} - \frac{2}{\gamma - 1} a_e, \]

where \( \infty \) and \( e \) indexes stand for the property in the freestream and in the internal region, respectively. \( q_n \) is the velocity component normal to the outer surface, defined as

\[ q_n = \mathbf{u} \cdot \mathbf{n}, \] (58)

and \( \mathbf{n} \) is the unit outward normal vector

\[ \mathbf{n} = [n_x, n_y, n_z]^T = \frac{1}{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}} [\eta_x, \eta_y, \eta_z]^T. \] (59)

Equation (59) assumes that the \( \eta \) direction is pointing from the jet to the external boundary. Solving for \( q_n \) and \( a \), one can obtain

\[ q_{nf} = \frac{\mathbf{R}^+ + \mathbf{R}^-}{2}, \quad a_f = \frac{\gamma - 1}{4} (\mathbf{R}^+ - \mathbf{R}^-). \] (60)

The \( f \) index is linked to the property at the boundary surface and it is used to update the solution at this boundary. For a subsonic exit boundary, \( 0 < q_{nf} / a_e < 1 \), the velocity components are derived from internal properties as

\[ u_f = u_e + (q_{nf} - q_{ne}) n_x, \]
\[ v_f = v_e + (q_{nf} - q_{ne}) n_y, \]
\[ w_f = w_e + (q_{nf} - q_{ne}) n_z. \] (61)

Density and pressure are obtained by extrapolating the entropy from the adjacent grid node,

\[ \rho_f = \left( \frac{\rho_e^2 a_{e}^2}{\gamma \rho_e} \right)^{\frac{\gamma - 1}{\gamma}}, \quad p_f = \frac{\rho_f a_f^2}{\gamma}. \]

For a subsonic entrance, \( -1 < q_{nf} / a_e < 0 \), properties are obtained similarly from the freestream variables as

\[ u_f = u_{\infty} + (q_{nf} - q_{n\infty}) n_x, \]
\[ v_f = v_{\infty} + (q_{nf} - q_{n\infty}) n_y, \]
\[ w_f = w_{\infty} + (q_{nf} - q_{n\infty}) n_z, \] (62)

\[ \rho_f = \left( \frac{\rho_e^2 a_{e}^2}{\gamma \rho_{\infty}} \right)^{\frac{\gamma - 1}{\gamma}}. \] (63)

For a supersonic exit boundary, \( q_{nf} / a_e > 1 \), the properties are extrapolated from the interior of the domain as
7.2 Entrance boundary

For a jet-like configuration, the entrance boundary is divided into two areas: the jet and the area above it. The jet entrance boundary condition is implemented through the use of the 1-D characteristic relations for the 3-D Euler equations for a flat velocity profile. The set of properties, then, determined is computed from within and from outside the computational domain. For the subsonic entrance, the $v$ and $w$ components of the velocity are extrapolated by a zero-order extrapolation from inside the computational domain and the angle of flow entrance is assumed fixed. The remaining properties are obtained as a function of the jet Mach number, which is a known variable.

$$
(u)_{1,j,k} = u_j, \\
(v)_{1,j,k} = (v)_{2,j,k}, \\
(w)_{1,j,k} = (w)_{2,j,k}.
$$

The dimensionless total temperature and total pressure are defined with the isentropic relations:

$$
T_i = 1 + \frac{1}{2} (\gamma - 1) M_j^2 \quad \text{and} \quad P_i = \frac{1}{\gamma} (T_i)^{\frac{\gamma}{\gamma - 1}}.
$$

The dimensionless static temperature and pressure are deduced from Eq. (67), resulting in

$$
(T)_{1,j,k} = \frac{T_i}{1 + \frac{1}{2} (\gamma - 1)(u^2 + v^2 + w^2)}_{1,j,k} \quad \text{and} \quad (p)_{1,j,k} = \frac{1}{\gamma} (T)_{1,j,k}^{\frac{\gamma}{\gamma - 1}}.
$$

For the supersonic case, all conserved variables receive the jet property values. Such entrance boundary conditions do not include any disturbance to the inlet velocity. The present approach simply generates the so-called “top hat” velocity profile at the jet entrance. The use of a top hat velocity profile is one of the possible procedures for implementing entrance conditions for very high Reynolds number jet flows, as discussed in the literature [4–6]. Actually, one can find in the work of Garnier et al. [11] a very detailed discussion of all possible ways of implementing jet entrance boundary conditions for flows as the one addressed in the present paper. It is clear from the discussion that all approaches have advantages and drawbacks. Therefore, the authors have opted for the simplest form of imposing such boundary conditions. Moreover, the calculations performed in the context of this work have indicated, at least for the cases addressed here, that numerical disturbances already present in the solution process are sufficient to destabilize the flow and induce turbulence transition in the jet.

The far-field boundary conditions are implemented outside of the jet area to correctly propagate information coming from the inner domain of the flow to the outer regions of the simulation. However, in the present case, $\xi$, instead of $\eta$, as presented in the previous subsection, is the normal direction used to define the Riemann invariants.

7.3 Exit boundary conditions

At the exit plane, the same reasoning of the jet entrance boundary is applied. In this case, for a subsonic exit, the pressure is obtained from the outside, i.e., it is assumed

$$
\rho_f = \rho_e, \\
u_f = u_e, \\
v_f = v_e, \\
w_f = w_e, \\
e_f = e_e,
$$

and for a supersonic entrance, $q_n/a_e < -1$, the properties are extrapolated from the freestream variables as

$$
\rho_f = \rho_\infty, \\
u_f = u_\infty, \\
v_f = v_\infty, \\
w_f = w_\infty, \\
e_f = e_\infty.
$$

Fig. 1 Lateral and frontal views of the computational domain indicating boundary conditions

(a) Lateral view of boundary conditions.  
(b) Frontal view of boundary conditions.
given, and all other variables are extrapolated from the interior of the computational domain by a zero-order extrapolation. The conserved variables are obtained as

\[
(p)_{i, j+1/2} = \frac{(p)_{i, j+1} - (p)_{i, j-1}}{2}
\]

(69)

\[
(u)_{i, j+1/2} = \frac{(u)_{i, j+1} - (u)_{i, j-1}}{2}
\]

(70)

\[
(e)_{i, j+1/2} = \frac{(e)_{i, j+1} - (e)_{i, j-1}}{2}
\]

(71)

in which \( I_{\text{MAX}} \) stands for the last point of the mesh in the axial direction. For the supersonic exit, all properties are extrapolated from the interior domain.

7.4 Centerline boundary conditions

The centerline boundary is a singularity of the coordinate transformation and, hence, an adequate treatment of this boundary must be provided. The conserved properties are extrapolated from the adjacent longitudinal plane and they are averaged in the azimuthal direction to define the updated properties at the centerline of the jet.

The fourth-difference terms of the artificial dissipation scheme, used in the present work, are carefully treated to avoid the five-point difference stencils at the centerline singularity. If one considers the flux balance at one grid point near the centerline boundary in a certain coordinate direction, let \( w_j \) denote a component of the \( \nabla \) vector from Eq. (49) and \( d_j \) denote the corresponding artificial dissipation term at the \( j \)-th mesh point. In the present example, \( (\Delta w)_{j+1/2} \) stands for the difference between the solution at the interface for the points \( j + 1 \) and \( j \). The fourth difference of the dissipative fluxes from Eq. (45) can be written as

\[
(d)_{j+1/2} = (\Delta w)_{j+1/2} - 2(\Delta w)_{j+1/2} + (\Delta w)_{j-1/2}.
\]

(72)

Considering the centerline and the point \( j = 1 \), as presented in Fig. 2, the calculation of \( d_{1+1/2} \) demands the \( (\Delta w)_{1+1/2} \) term, which is unknown since it is outside the computational domain. In the present work a extrapolation is performed and given by

\[
(\Delta w)_{1+1/2} = - (\Delta w)_{1-1/2}.
\]

(73)

This extrapolation modifies the calculation of \( d_{1+1/2} \) that can be written as

\[
(d)_{1+1/2} = (\Delta w)_{1+1/2} - 3(\Delta w)_{1+1/2}.
\]

(74)

The approach is plausible since the centerline region is smooth and does not have high gradient of properties.

7.5 Periodic boundary conditions

A periodic condition is implemented between the first \( (K = 1) \) and the last point in the azimuthal direction \( (K = K_{\text{MAX}}) \) to close the 3-D computational domain. There are no boundaries in this direction, since all the points are inside the domain. The first and the last points, in the azimuthal direction, are superposed to facilitate the boundary condition implementation which is given by

\[
(p)_{i,j,K_{\text{MAX}}} = (p)_{i,j,1},
\]

\[
(u)_{i,j,K_{\text{MAX}}} = (u)_{i,j,1},
\]

\[
(v)_{i,j,K_{\text{MAX}}} = (v)_{i,j,1},
\]

\[
(w)_{i,j,K_{\text{MAX}}} = (w)_{i,j,1},
\]

\[
(e)_{i,j,K_{\text{MAX}}} = (e)_{i,j,1}.
\]

(75)

8 Study of supersonic jet flow

Four test cases are addressed in the present work to study the use of second-order spatial discretization on large eddy simulations of a perfectly expanded jet flow configuration. These test cases compare the effects of mesh refinement and SGS models on the results. Two different meshes are created for the grid refinement study. Results for the three SGS models implemented in the code, namely, classic Smagorinsky, dynamic Smagorinsky and Vreman models, are compared in the current section. The present results are compared with analytical, numerical and experimental data from the literature [7, 24, 25].
8.1 Geometry characteristics

Two different computational domain geometries are created for the jet simulations discussed in the current work. One geometry presents a cylindrical shape and the other one presents a divergent conical shape. For the sake of simplicity, the cylindrical geometry is named geometry A and the other one is named geometry B in the present paper. The computational domains are created in two steps. First, a 2-D region is generated. In the sequence, this region is rotated about the jet axis to generate a fully 3-D geometry. An in-house code is used for the generation of the 2-D domain of geometry A. The commercial mesh generator ANSYS® ICEM CFD [1] is used for the 2-D domain of geometry B.

Geometry A is a cylindrical domain with radius of 20D and a length of 50D. Geometry B presents a divergent form whose axis length is 40D. The minimum and maximum heights of geometry B are \( \approx 16D \) and 25D, respectively. Geometry B is created based on results from simulations using geometry A to refine the mesh in the shear layer region of the jet flow. The 2-D coordinates of the zones created for geometry B and further details of the geometry can be found in Ref. [16]. Geometries A and B are illustrated in Fig. 3 which presents a 3-D view of the two computational domains used in the current work. The geometries are colored by an instantaneous visualization of the solution for the axial component of the flow velocity.

8.2 Mesh configurations

One grid is generated for each geometry used in the present study. These computational grids are named mesh A and mesh B. An illustration of the computational grids is presented in Fig. 4.

Mesh A is created using a mesh generator developed by the research group for the cylindrical shape configuration, i.e., geometry A. This computational mesh is composed of 400 points in the axial direction, 200 points in the radial direction and 180 points in the azimuthal direction, which yields a total of 14.4 million grid points. Hyperbolic tangent functions are used for the point distributions in the radial and axial directions. Grid points are clustered near the shear layer of the jet. The mesh is coarsened towards the outer regions of the domain to dissipate properties of the flow far from the jet. Such mesh refinement approach can avoid the reflection of waves back into the domain.

The radial and longitudinal dimensions of the smallest distance between mesh points of grid A are given by \( (\Delta r)_{\text{min}} = 0.002D \) and \( (\Delta x)_{\text{min}} = 0.0126D \), respectively. This minimal spacing occurs at the shear layer of the jet and at the entrance of the computational domain. Mesh A characteristics are chosen based on data provided by the work of Mendez et al. [24, 25], who have also used a second-order accurate spatial discretization scheme for the same jet flow configuration. It should be observed, however, that the cited references have included a nozzle in the simulation. Therefore, it is expected that the present results should be somewhat similar to those in Refs. [24, 25], but not identical, since we are using the top hat inlet velocity profile. Simulations were initially performed using mesh A. This particular calculation has used the static Smagorinsky SGS model, and details of the calculation are discussed in the forthcoming sections. The results indicated that further grid refinement was necessary and they also helped in the decision of which regions of the domain should be refined.

(a) 3-D view of two XZ planes of geometry A. (b) 3-D view of two XZ planes of geometry B.

Fig. 3 3-D view of computational domain geometries used for the LES calculations

\( \odot \) Springer
Therefore, the authors created a second computational grid, mesh B, which also adopted a somewhat different topology for the computational domain, geometry B, as previously discussed.

The more refined computational grid, mesh B, is composed of 343 points in the axial direction, 398 points in the radial direction and 360 points in the azimuthal direction. This yields a mesh with approximately 50 million grid points. The 2-D mesh is generated with ANSYS® ICEM CFD [1]. The points are allocated using different distributions in eight edges of the 2-D domain. The same coarsening approach used for mesh A is also applied for mesh B. The distance between mesh points increases towards the outer region of the domain. This procedure forces the dissipation of properties far from the jet to avoid reflection of waves into the domain. The grid coarsening can be understood as an implicit damping which can smooth out properties far from the jet, in the region where the mesh is no longer refined. Figure 5 illustrates the edges used to generate the point distribution and the direction of the mesh coarsening. Table 1 presents the number of points, the growth factor and the smallest grid spacing for all auxiliary edges used to generate the mesh.

### 8.3 Flow configuration and boundary conditions

An unheated perfectly expanded jet flow is chosen to perform the present studies with the LES tool. The jet entrance Mach number is 1.4. The pressure ratio, \( PR = P_j / P_\infty \), and the temperature ratio, \( TR = T_j / T_\infty \), between the jet entrance and the ambient freestream conditions, are equal to one, i.e., \( PR = 1 \) and \( TR = 1 \). The Reynolds number of the jet is \( Re = 1.57 \times 10^6 \), based on the jet entrance diameter, \( D \). This flow configuration is chosen due to the absence of strong shocks waves. Strong discontinuities clearly create additional numerical difficulties, that the authors did not want to add to the present study. Moreover, numerical and experimental data are

| Edge | Nb. of points | Growth factor | Smallest spacing |
|------|---------------|---------------|-----------------|
| a    | 300           | 1.01912       | \( 1.000 \times 10^{-3}D \) |
| b    | 30            | 1.02739       | \( 2.8231 \times 10^{-1}D \) |
| c    | 15            | 1.30370       | \( 3.4482 \times 10^{-4}D \) |
| d    | 45            | 1.00          | \( 3.40909 \times 10^{-3}D \) |
| e    | 155           | 1.03724       | \( 3.40909 \times 10^{-3}D \) |
| f    | 155           | 1.01034       | \( 1.18655 \times 10^{-2}D \) |
| g    | 40            | 1.07161       | \( 5.73327 \times 10^{-2}D \) |
| h    | 7             | 1.08206       | \( 7.93887 \times 10^{-1}D \) |
available in the literature for this flow configuration, such as the work of Mendez et al. [24, 25] and the work of Bridges and Wernet [7].

The boundary conditions discussed in Sect. 7 are used in the simulations performed in the present paper. Figure 1 presents a lateral view and a frontal view of the computational domain used for the simulations, indicating the positioning of each boundary condition. A top hat velocity profile, with $M = 1.4$, is used at the entrance boundary. Riemann invariants are used at the stagnated ambient regions. A special singularity treatment is performed at the centerline. Periodicity is imposed in the azimuthal direction. Properties of flow at the inlet and at the farfield regions have to be provided to the code to impose the boundary conditions. Density, $\rho$, temperature, $T$, velocity, $U$, Reynolds number, $Re$, and specific heat at constant volume, $C_v$, are provided in the dimensionless form to the simulation. These properties are given by

$$
\begin{align*}
\rho_j &= 1.00, \quad \rho_\infty = 1.00, \\
T_j &= 1.00, \quad T_\infty = 1.00, \\
U_j &= 1.4, \quad U_\infty = 0.00, \\
Re_j &= 1.57 \times 10^6, \quad C_v = 1.786,
\end{align*}
$$

where the $j$ subscript identifies the properties at the jet entrance and the $\infty$ subscript stands for properties at the farfield region.

### 8.4 Large eddy simulations

Four simulations are performed in the present work. The objective is to study the effects of mesh refinement and to evaluate the three different SGS models included into the code. The calculations are performed in two steps. First, a preliminary simulation is performed to achieve a statistically steady-state condition. In the sequence, the simulations are run for another period to collect enough data for the calculation of time-averaged properties of the flow and their fluctuations.

#### 8.4.1 Statistically stationary flow condition

The configurations of all simulations are discussed in the current subsection towards the description of the preliminary calculations which are performed to drive the flow to a statistically steady flow condition. In this preliminary stage, the goal is to achieve a starting point to begin the calculation of statistical data. Table 2 presents the operating conditions of all four numerical studies performed in the current research. S1, S2 and S3 simulations were the test cases that admitted stagnated flow conditions as the initial conditions for the preliminary simulations. Differently from the former studies, the S4 simulation used the statistically steady-state condition of the S2 computational study as initial condition for this preliminary stage. S1 is only used in the S1 simulation. The other calculations are performed using the more refined grid, Mesh B. S1, S2, S3 and S4 studies apply, respectively, time increments of $2.5 \times 10^{-5}$, $1.0 \times 10^{-4}$, $5.0 \times 10^{-5}$ and $1.0 \times 10^{-4}$, in dimensionless time units, as indicated in the 4th column of Table 2, respectively. The dimensionless time increment used for all configurations is the largest one which the solver can handle without diverging the solution. The static Smagorinsky model [21, 22, 28] is used in the S1 and S2 simulations. The dynamic Smagorinsky model [13, 26] and the Vreman model [31] are used in simulations S3 and S4, respectively.

The total (physical) time simulated by all numerical studies to achieve the statistically steady-state condition is indicated in the 6th column of Table 2 in flow through time (FTT) units. One flow through time is the necessary amount of time for a particle to cross all the domain considering the inlet velocity of the jet. The S1 simulation is the least expensive test case studied and, therefore, one

---

### Table 2 Overall characteristics of the large eddy simulations performed in the present work

| Simulation | Mesh | SGS               | $\Delta t$       | Initial Condition | FTT   |
|------------|------|-------------------|------------------|-------------------|-------|
| S1         | A    | Static Smagorinsky| $2.5 \times 10^{-5}$ | Stagnated flow   | 52.9  |
| S2         | B    | Static Smagorinsky| $1 \times 10^{-4}$  | Stagnated flow   | 14.2  |
| S3         | B    | Dynamic Smagorinsky| $5 \times 10^{-5}$  | Stagnated flow   | 8.20  |
| S4         | B    | Vreman            | $1 \times 10^{-4}$  | S2                | 19.1  |

### Table 3 Details of the data extraction for mean flow calculations for each test case

| Simulation | Number of extractions | Frequency | Data extraction time |
|------------|-----------------------|-----------|----------------------|
| S1         | 2048                  | 50        | 1.60 FTT             |
| S2         | 3365                  | 50        | 3.30 FTT             |
| S3         | 2841                  | 50        | 2.77 FTT             |
| S4         | 1543                  | 50        | 1.51 FTT             |
could afford to let it run for a longer period of time. It uses a 14 million-point mesh while the other simulations use the 50 million-point grid. On the other hand, simulation S3 is the most expensive numerical test case, because the dynamic Smagorinsky SGS model requires more computational time per time step when compared with the other SGS models implemented in the code. Moreover, the time step restrictions for the dynamic Smagorinsky model are much more stringent, as one can see in Table 2. Hence, the S3 simulation has only been run for 8.20 FTT for this study.

8.4.2 Mean flow property calculations

After the statistically stationary state is achieved, the simulations are restarted and run for another period of time in which data of the flow are extracted and recorded in a fixed frequency. The collected data are time averaged to calculate mean properties of the flow and compare them with the results of the numerical and experimental references. In the present section, time-averaged properties are denoted as $\langle \cdot \rangle$. Table 3 summarizes the information on data collecting and time averaging for the four test cases addressed here. The 2nd column presents the number of extractions performed during the simulations. Data are extracted each 0.02 dimensionless time units in the present work, which is equivalent to a dimensionless frequency of 50. The choice of this frequency is based on the numerical work reported in Refs. [24, 25]. The last column of Table 3 presents the total additional dimensionless time simulated to extract the data to calculate the mean properties.

![Fig. 6 Positioning in the computational domain of surfaces studied in the present work](image)

Table 4 Potential core length and relative error with respect to the experimental data [7]

| Simulation | $d_{95\%}$ | Relative error (%) |
|------------|-------------|-------------------|
| S1         | 5.57        | 40                |
| S2         | 6.84        | 26                |
| Mendez et al. | 8.35      | 8                 |

![Fig. 7 Lateral view of $\langle U \rangle$ for S1 and S2 simulations](image)
8.5 Study of mesh refinement effects

Effects of mesh refinement on compressible LES using the JAZzY solver are discussed in the present section. Time-averaged 2-D distributions and profiles of the axial component of velocity are collected from simulations S1 and S2, and they compared with numerical and experimental results from the literature [7, 24, 25]. Both simulations use the same SGS model, the static Smagorinsky model [21, 22, 28]. Mesh A is used on the S1 simulation while Mesh B is used on the S2 simulation. Figure 6 illustrates the positioning of surfaces and profiles extracted for all simulations performed in the present work.

Cuts (A) through (D) are radial profiles at different positions downstream of the jet entrance. An average in the azimuthal direction is performed, when appropriate, for the calculation of the radial profiles. The last region indicated in Fig. 6, Cut (E), represents the jet axis.

8.5.1 Time-averaged axial component of velocity

One important characteristic of round jet flow configurations is the potential core length, $\delta_j^{95\%}$. The potential core is defined as the region in which the axial velocity component, $U_j^{95\%}$, is at least 95% of the velocity of the jet at the inlet, i.e.,

$$U_j^{95\%} = 0.95 \ U_j.$$  (77)
Therefore, the potential core length can be defined by the point in which the mean axial velocity component reaches $U_j^{95\%}$ along the centerline.

Lateral views of $\langle U \rangle$ for the S1 and S2 simulations are presented in Fig. 7. In these contour plots, $U_j^{95\%}$ is indicated by the black solid line.

Table 4 presents the potential core length for the S1 and S2 simulations. The present calculations are compared to the numerical results from Refs. [24, 25], both in terms of the actual values of $d_j^{95\%}$ as well as in terms of the relative error with respect to the experimental data [7].

There are significant differences between the results for the S1 and S2 test cases, as well as between those and the computational results from Ref. [25]. The results for the S1 simulation present a smaller $d_j^{95\%}$, when compared to the results for the S2 simulation, i.e., 5.57 and 6.84, respectively. The S1 solution is over dissipative when compared to the S2 results and, hence, the jet decays earlier in the S1 simulation. As previously discussed, the mesh used in the

---

**Fig. 9** Evolution of the averaged axial component of velocity, $\langle U \rangle$, along the centerline (Y=0); $0 \leq X \leq 20D$. (Dashed line) S1 simulation; (solid line) S2 simulation; (open squares) numerical data; (filled triangles) experimental data

**Fig. 10** Lateral view of instantaneous pressure contours, in gray scale, superimposed by vorticity magnitude contours, in color, of the jet flow computed in the S1 and S2 simulations

(a) S1 simulation.

(b) S2 simulation.
S1 test case is very coarse when compared to the grid used for the S2 simulation. This lack of spatial resolution can generate very dissipative solutions which yield the under prediction of the potential core length. The mesh refinement reduced in 14% the relative error of the S2 simulation when compared to the experimental data.

Profiles of $hU_i$ along the mainstream direction and the evolution of $hU_i$ along the centerline are compared with numerical and experimental results in Figs. 8 and 9. The centerline is indicated as the (E) cut in Fig. 6. The dash-point and the solid lines stand for the results of the S1 and S2 test cases, respectively, in Figs. 8 and 9. The square symbols are the LES results of Mendez et al. [24, 25], while the triangular symbols indicate the experimental data of Bridges and Wernet [7].

The comparison of profiles indicates that the distributions of $\langle U \rangle$, calculated in the present work, correlate well with the reference data up to $X = 5.0D$. The $\langle U \rangle$ profile, calculated in the S2 case, at $X = 10.0D$ is under predicted when compared with the reference profiles. However, the comparison is still quite a bit better than the one obtained for the S1 results at this axial position. One can observe that the $\langle U \rangle$ distributions along the centerline, for the S1 and S2 cases, correlate well with the reference data in the region in which there is good grid resolution. The averaged axial component of velocity calculated in S1 simulation is always underestimated when compared to the same property calculated with S2 computation. However, as the mesh spacing increases, the time-averaged axial velocity component, computed using S1 and S2 numerical studies, starts to correlate poorly with the references.

Figure 10 presents a lateral view of an instantaneous snapshot of the pressure contours, in gray scale, superimposed by vorticity magnitude contours, in color, for both S1 and S2 numerical studies. It is clear that the finer grid results, that is, the S2 simulation, provide greater details of the pressure and vorticity fields.

A detailed visualization of the jet entrance is shown in Fig. 11, for the two test cases. As before, an instantaneous snapshot of one longitudinal plane of the jet flow is shown. Pressure contours are shown as a background visualization in gray scale, and this is superimposed by vorticity magnitude contours, in color. The better resolution of flow features obtained for the S2 test case is even more evident.
in this detailed plot of the jet entrance. In particular, compression waves generated at the shear layer, and their reflections at the jet axis, are much more clearly visible in the S2 results. At the end, this simulation provides a much richer visualization of flow features.

8.5.2 RMS distributions of time fluctuations of axial velocity component

The time fluctuating part of the flow is also important to be studied. Therefore, the analysis of the effects of mesh refinement is also performed for the fluctuating part of the axial velocity component using the root mean square approach. A lateral view, i.e., a complete longitudinal plane, and a detailed view of the region near the jet entrance of the root mean square (RMS) values of the fluctuating part of the axial velocity component, \( u_{\text{RMS}}^* \), computed in the S1 and S2 simulations, are presented in Fig. 12.

One can observe, for instance, in Fig. 12a, b, that the mesh coarsening in the streamwise direction, towards the farfield, is working as designed. In other words, the mesh stretching destroys structures of the flow towards the exit boundary and, therefore, there are no wave reflections back into the computational domain. As previously discussed, coarse meshes implicitly add dissipation to the solution and, as such, they work as sponge zones in the vicinity of undisturbed flow regions. The detailed views of \( u_{\text{RMS}}^* \), i.e., Fig. 12c, d, indicate that the properties calculated in the S2 study provide a better definition of the potential core and of the near jet entrance region. The results for the S1 test case are more spread and indicating a much reduced potential

![Image](85x315 to 510x732)

Fig. 12 Lateral and detailed views of the RMS values of the time fluctuation of the axial component of velocity, \( u_{\text{RMS}}^* \), for S1 and S2 simulations.
core length. The same effect can be observed on crossflow plane visualizations of $u'_{RMS}$ contours, which, however, are not shown here for the sake of brevity.

Figure 13 presents the comparison of RMS profiles of $u'$, from the S1 and S2 simulations, with reference results. All profiles of $u'_{RMS}$, calculated using numerical approaches, fit very well with the experimental reference profile at $X = 2.5D$ near the centerline region. However, the numerical calculations overpredict the peaks of $u'_{RMS}$ at the proximity of $Y = 0.5D$ for the $X = 2.5D$ station. The profile obtained with the S2 calculation, at this axial position, presents a good correlation with numerical data, whereas the $u'_{RMS}$ profile calculated in the S1 simulation cannot correctly represent the two peaks of the profile. At $X = 5.0D$, the $u'_{RMS}$ profile calculated using S2 simulation is close to the profiles obtained by the references. The S1 study overestimates the RMS of $u'$ near the centerline region, i.e., $r/D = 0.0$. The same behavior can be observed at $X = 10.0D$, where the profiles of the fluctuating part of the axial velocity component obtained in the S1 and S2 calculations start to diverge from the reference results in the range $-0.5D < Y < 0.5D$. At $X = 15.0D$, the $u'_{RMS}$ profile for the S1 calculation is completely underpredicted when compared to the profiles of $u'_{RMS}$ obtained from the numerical and experimental references. At the same position, the $u'_{RMS}$ profile from the S2 computation seems to somewhat follow the reference profiles, but with fairly large inaccuracies.

Figure 14 presents the distribution of $u'_{RMS}$ along the centerline of the jet. The S2 calculation presents
overpredicted values of $u_{\text{RMS}}$ when compared to the reference data. Nevertheless, the evolution of this property along the centerline presents a similar shape as that presented in the numerical and experimental references. One can notice that the distribution of $u_{\text{RMS}}$ obtained in the S1 calculation presents the same behavior of the distribution obtained from the S2 study for $X \leq 10D$. Both results are overpredicted when compared with the reference data. However, in particular for the S1 simulation, the value of $u_{\text{RMS}}$ decreases quickly in the streamwise direction for $X > 10D$. This behavior of the S1 calculation generates a very underpredicted distribution of $u_{\text{RMS}}$ when compared to the results of the S2 simulation and the reference data. Even the shape of the evolution of the property calculated by the S1 simulation, for $X > 10D$, is completely different from the evolution presented by the reference data.

Therefore, it is clear the significant improvement of the solution with the refinement of the mesh performed for the S2 study.

### 8.6 Subgrid-scale modeling study

The present subsection addresses the comparison of the three SGS models added to the solver. The test cases considered are defined in Table 2. In particular, we discuss here the S2, S3 and S4 simulations, which are performed using the static Smagorinsky [21, 22, 28], the dynamic Smagorinsky [12, 26] and the Vreman [31] models, respectively. The same mesh, with 50 million grid points, is used for all three simulations. The stagnated flow condition is used as initial condition for the S2 and S3 simulations. A restart of the S2 simulation is used as initial condition for the S4 simulation.

#### 8.6.1 Time-averaged axial component of velocity

Effects of the SGS modeling on the time-averaged results of the axial component of velocity are presented in the subsection. A lateral view of $\langle U \rangle$ for S2, S3 and S4 simulations, side by side, are presented in Fig. 15, where $U_f^{95\%}$ is indicated by the solid line.

![Fig. 15 Lateral view of the averaged axial component of velocity, $\langle U \rangle$, for S2, S3 and S4 simulations; solid line: the potential core of the jet, $U_f^{95\%}$](image)

Table 5 Potential core length and relative error of S2, S3 and S4 simulations

| Simulation | $\delta_f^{95\%}$ | Relative error (%) |
|------------|------------------|-------------------|
| S2         | 6.84             | 26                |
| S3         | 6.84             | 26                |
| S4         | 6.28             | 32                |
| Mendez et al. | 8.35         | 8                 |

Fig. 14 Evolution of RMS values of time fluctuation of axial component of velocity, $u_{\text{RMS}}$, along the centerline ($Y=0$); $0 \leq X \leq 20D$. (dashed line) S1 simulation; (solid line) S2 simulation; (open squares) numerical data; (filled triangles) experimental data
Table 5 presents the size of the potential core of S2, S3 and S4 simulations and the numerical reference [24, 25] along with the relative error compared with the experimental data [7].

Comparing the results, one cannot observe significant differences on the potential core length between S2, S3 and S4 simulations. However, the present results are calculating a potential core length which is fairly different from the results obtained by Mendez et al. [24, 25]. Figure 16 presents instantaneous fields of pressure, in gray scale, superimposed by vorticity contours, colored by the vorticity magnitude, for the numerical simulations performed with the more refined grid, Mesh B. Although the comparison is only qualitative, one cannot notice a
significant effect of the SGS model on the pressure and vorticity fields.

Profiles of $h_U i$ from S2, S3 and S4 simulations, along the mainstream direction are compared with numerical and experimental results in Fig. 17. The evolution of $h_U i$ along the centerline is illustrated in Fig. 18. The solid line, the dashed line and the circular symbol stand for the profiles of $h_U i$ computed by the S2, S3 and S4 simulations, respectively. The reference data are represented by the same symbols used in the mesh refinement study.

The comparison of profiles indicates that distributions of $h_U i$ calculated on S2, S3 and S4 simulations correlate well with the references until $X = 5.0D$. For $X > 10.0D$, all simulations performed in the present work underestimate the magnitude of $h_U i$ in the $-0.5D < Y < 0.5D$ region, when compared to the reference data. One can notice that the evolution of $h_U i$ along the centerline, calculated by all three simulations, is in good agreement with the numerical and experimental reference data at the region where the mesh presents a good resolution. Moreover, the three distributions, calculated using different SGS closures, have presented a very similar behavior.

8.6.2 Root mean square distributions of time fluctuations of axial velocity component

Fig. 17 Profiles of averaged axial component of velocity, $\langle U \rangle$, at different positions within the computational domain: (solid line) S2 simulation; (dashed line) S3 simulation; (open circles) S4 simulation; (open squares) numerical reference data; (filled triangles) experimental data
computed by the S2, S3 and S4 simulations, are presented in Fig. 19a–c, respectively.

The corresponding profiles of $u'_{\text{RMS}}$ at the four longitudinal stations previously defined, are shown in Fig. 20. The profiles of $u'_{\text{RMS}}$, obtained in the present study, are in good agreement with the numerical reference data until $X = 5.0D$, as one can observe in Fig. 20. At $X = 10D$, the present results still resemble the reference data, but there are clear differences in the values of $u'_{\text{RMS}}$. At the $X = 15D$, the present calculations clearly have difficulties in representing the distribution of $u'_{\text{RMS}}$, since the grid is already very coarse at this longitudinal location. One should further observe that even the reference numerical data [24, 25] have difficulties in predicting the value of the peaks in the $u'_{\text{RMS}}$ distribution, when compared to the experimental data. Our calculations are not different. Although there is a qualitative agreement with the experimental data for the $u'_{\text{RMS}}$ distributions near the jet entrance, the computed peak values at the lipline locations show some differences with respect to the experimental values.

Moreover, Fig. 20 also shows that, for the stations in which there is very good correlation between the present results and the literature data, there is essentially no difference between the $u'_{\text{RMS}}$ profiles computed with the different SGS models. In other words, for $X = 2.5D$ and $X = 5.0D$, the results for the S2, S3 and S4 cases are essentially identical. Clearly, for $X = 10D$, one can observe some differences among the present results, but, again, at this station one can already observe significant differences between the present calculations and the reference data. As we already discussed, at $X = 15D$, all of the present calculations have difficulties due to the already fairly coarse mesh at that location.

Figure 21 presents the distribution of $v'_{\text{RMS}}$ along the centerline of the domain. All three simulations performed in the current work present overestimated distributions of $u'_{\text{RMS}}$ along the centerline for $X < 10D$. Moreover, one can also observe that, at least for $X < 9D$, there are no large differences between the centerline $u'_{\text{RMS}}$ profiles calculated in the present paper. For $X > 9D$, it seems that the results with the two Smagorinsky models follow trends which are quite different from the behavior of the results with the Vreman model. Unfortunately, for such downstream locations, the mesh is already becoming fairly coarse. This fact together with the results from the crossflow $u'_{\text{RMS}}$ profiles, previously discussed, discourages an attempt to try to interpret such behavior.

### 8.6.3 Root mean square distributions of time fluctuations of radial velocity component

Effects of SGS modeling on the RMS values of time fluctuation of the radial component of velocity are also compared with the reference data. A visualization of the contours of $v'_{\text{RMS}}$, computed for the S2, S3 and S4 test cases, is shown in Fig. 19d–f, respectively. These results seem to indicate that the choice of SGS model does not significantly affect the distribution of $v'_{\text{RMS}}$. However, one can notice that, for $8D < X < 10$, the calculations with the Vreman model seem to be generating somewhat larger values of $v'_{\text{RMS}}$. The contours shown in Fig. 19d, e clearly indicate that there are no relevant differences between the results with the two Smagorinsky models.

Using the same four stations downstream of the jet entrance, profiles of $v'_{\text{RMS}}$ in the radial direction are presented in Fig. 22 at $X = 2.5D$, $X = 5.0D$, $X = 10.0D$ and $X = 15.0D$. One can observe that all profiles calculated in the present work show very good agreement with the experimental data at $X = 2.5D$. Actually, at this station, the peaks in $v'_{\text{RMS}}$ at the lipline locations, calculated in the present case, are in better agreement with the experimental data than the results in Refs. [24, 25]. However, as one analyzes the profiles at $X = 5.0D$, there is already a significant decay in the values of $v'_{\text{RMS}}$ for the present calculations. At this station, the present results still capture the correct trends, compared to the experimental data, but, for instance, the peaks at the lipline locations are considerably lower than the experimental results. The values of $v'_{\text{RMS}}$ at the centerline location, computed in the present case, are slightly higher than the experimental value, but there is good agreement with the numerical reference value for this position, at $X = 5.0D$. As previously discussed with regard to other comparisons in the present paper, at these two
longitudinal stations closer to the jet entrance, there are no significant differences among the results computed in the present paper for the three different SGS models.

A different behavior is observed at the two stations further away from the jet entrance, namely, at $X = 10.0D$ and $X = 15.0D$. Clearly, at $X = 15.0D$, the present results for $v_{RMS}^*$ do not reproduce anything minimally resembling the reference data, either experimental or numerical. However, at $X = 10.0D$, although the present profiles for $v_{RMS}^*$ are quite far from the reference data, one can still observe that there is a tendency of following the same trends. At this station, one can also observe some differences between the results with the Vreman model and those obtained with the two Smagorinsky models for the behavior of $v_{RMS}^*$ around the jet centerline. As we discussed previously, the profiles at this station are already sufficiently far from the reference data that an attempt to further interpret such differences are probably futile.

8.6.4 Shear component of the Reynolds stress tensor

Contours of the $\langle u^*v^* \rangle$ component of the Reynolds stress tensor, computed using the three different SGS models, are presented in Fig. 19g–i for a longitudinal plane of the computational domain. As with other properties, one does not see any dramatic differences in the $\langle u^*v^* \rangle$ contours computed with the different SGS models, at least close to the jet entrance. As one approaches the downstream
portions of the region shown in the figures, it seems that the results with the Vreman model tend to slightly widen the area, in the radial direction, in which there are significant values of $\langle u'v' \rangle$. Moreover, as before, even in such regions in which the computational grid is becoming fairly coarse, there are no significant differences in the $\langle u'v' \rangle$ contours computed with the two Smagorinsky models.

Profiles of the shear component of the Reynolds stress tensor, for the same four stations downstream of the jet entrance, are shown in Fig. 23. It is clear from this figure that the correlation of the present numerical results with the reference data has a few difficulties. For instance, even at the $X = 2.5D$ station, although the trend of the distribution is approximately followed by the present results, the peak values of $\langle u'v' \rangle$ are not correctly captured by the present calculations. A similar behavior is seen at the other three stations. On the other hand, as observed previously, the computations with the three SGS models here addressed yield very similar results with each other for the two stations closer to the jet entrance. In other words, one cannot see any significant differences in the values of $\langle u'v' \rangle$ computed by the three different models at $X = 2.5D$ and at $X = 5.0D$. However, for the two stations which are further away from the jet entrance, there are differences among the present results.

8.6.5 Time-averaged eddy viscosity

The contours of the time-averaged subgrid-scale eddy viscosity coefficients, $\mu_i$, are shown in Fig. 24 for the flow

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**Fig. 20** Profiles of $u'\delta_{\text{rms}}$ for the S2, S3 and S4 simulations at four stations downstream of the jet entrance: (solid line) S2 case; (dashed line) S3 case; (open circles) S4 case; (open squares) numerical reference data; (filled triangles) experimental data
region closer to the jet entrance, for the three SGS closures addressed here. Values of \( \mu_i \) shown in Fig. 24 are already normalized by the reference dynamic viscosity coefficient at the jet entrance conditions. Although the \( \langle \mu_i \rangle \) contours might seem a bit erratic, at a first glance at Fig. 24, one should observe that the maximum values of \( \langle \mu_i \rangle \), in magnitude, are of the order of \( 10^{-9} \) for the static Smagorinsky model, \( 10^{-7} \) for the dynamic Smagorinsky model and \( 10^{-8} \) for the Vreman model. Therefore, these are all residual values of \( \langle \mu_i \rangle \), which means that the SGS models are not really providing any relevant effect in the results of the computations, as we have seen in the several discussions throughout the paper. Moreover, all subgrid-scale closures used in the present work, namely, the static Smagorinsky [21, 22, 28], the dynamic Smagorinsky [13, 26] and the Vreman [31] models, are dependent on the local mesh size by design. This characteristic is exposed in the contours shown in Fig. 24, since the larger magnitudes of \( \langle \mu_i \rangle \) occur in the regions where mesh already presents a lower resolution. Near the domain entrance, where the computational grid is very refined, the eddy viscosity can be essentially neglected.

This last observation goes in the same direction of the conclusions in the work of Li and Wang [20], which indicate that SGS closures introduce numerical dissipation that can be used as a stabilizing mechanism. However, such numerical dissipation does not necessarily add more physics to the LES simulation of the turbulent flow [20]. Therefore, in the present work, the numerical truncation error due to the spatial discretization, which generates the dissipative characteristic of the JAZzY solutions, has been shown to overcome the effects of the SGS modeling. Hence, the mesh needs to be very fine to achieve good results with second-order spatial discretizations. The grid refinement generates very small grid spacing. Consequently, the SGS models, which are strongly dependent on the filter width, cannot have a very decisive effect on the solution. Of course, LES of compressible flow configurations without the use of SGS closures, i.e., implicit LES calculations, would be welcome to complete such discussion. This is, however, beyond the scope of what the authors have set out to do in the present work.

9 Concluding remarks

The current work is concerned with a study of the effects of different subgrid-scale models on perfectly expanded supersonic jet flow configurations using centered second-order spatial discretizations. A formulation based on the System I set of equations is used in the present work. The time integration is performed using a five-stage, second-order, explicit Runge–Kutta scheme. Four large eddy simulations of compressible jet flows are performed in the present research using two different mesh configurations and three different subgrid-scale models. Their effects on the large eddy simulation solution are compared and discussed.

Large eddy simulations of high Reynolds supersonic jet flows using a second-order spatial discretization require high mesh resolution. Special care is necessary at the shear layer region of the jet flow. The mesh refinement study performed in the current effort has indicated that, at least in the region where the grid presents high resolution, the results of the present simulations are in good agreement with experimental and numerical references. For the mesh with 14 million points, the simulation has produced good results for \( X < 2.5D \) and \( -1.5D < Y < 0.5D \). For the finer mesh, with 50 million points, the simulations provided good agreement with the literature up to \( X = 5.0D \) and for \( -1.5D < Y < 0.5D \). The time-averaged eddy viscosity coefficients, calculated by all SGS models here addressed, present very low levels in the region where the current results have good correlation with the data from the literature.

The refined grid used on the mesh refinement study, Mesh B, is selected for the comparison of SGS model effects on the results of the large eddy simulations. Three compressible jet flow simulations are performed using the classic Smagorinsky model, the dynamic Smagorinsky model and the Vreman model. All three simulations present quite similar behavior, at least in the region where the mesh is finer, that is, close to the jet entrance. The present results yield a good agreement with the references up to \( X = 5.0D \). Typically, property profiles in the radial
direction at $X = 10.0D$ still reproduce the trends of the reference data, but the values of such properties are not as close to the reference data as desired. At the most downstream station analyzed, i.e., at $X = 15.0D$, the present computations typically have difficulties, most certainly due to the fact that the computational grid is already very coarse. As discussed, in the region where the grid is very fine and the results correlate well with the literature, the SGS eddy viscosity coefficients, provided by all the SGS models, have very low values. This behavior is understandable considering that the SGS closures used in the present work are strongly dependent on the filter width, which is proportional to the local mesh size. Moreover, it should be emphasized that there are differences among the results with the three SGS models here addressed. However, these differences typically occur in regions of the flow in which the mesh is already fairly coarse.

The present numerical calculations indicate that it is possible to achieve good results using second-order spatial discretizations for LES computations. However, the mesh ought to be well resolved to overcome the truncation errors from the low-order numerical scheme. Moreover, as expected, the numerical discretization can add significant artificial dissipation to the solution in the region where the mesh refinement is not well resolved. One can see this effect as a reduction of the local Reynolds number in such regions, which can, hence, be interpreted as a local overestimation of viscous effects in the flow.

It is also very important to highlight here that very fine meshes yield very small filter widths. Consequently, the

![Fig. 22 Profiles of $v_{rms}$ for the S2, S3 and S4 simulations at four stations downstream of the jet entrance: (solid line) S2 case; (dashed line) S3 case; (open circles) S4 case; (open squares) numerical reference data; (filled triangles) experimental data](https://example.com/fig22.png)
Fig. 23 Profiles of the Reynolds shear-stress tensor component, $\langle u'v' \rangle$, for S2, S3 and S4 simulations at four stations downstream of the jet entrance: (solid line) S2 case; (dashed line) S3 case; (open circles) S4 case; (open squares) numerical reference data; (filled triangles) experimental data.

(a) $X=2.5D; -1.5D \leq Y \leq 1.5D$

(b) $X=5.0D; -1.5D \leq Y \leq 1.5D$

(c) $X=10D; -1.5D \leq Y \leq 1.5D$

(d) $X=15D; -1.5D \leq Y \leq 1.5D$

Fig. 24 Contours of normalized time-averaged eddy viscosity coefficient, $\langle \mu_\text{t} \rangle$, for the S2, S3 and S4 simulations.

(a) S2 case.

(b) S3 case.

(c) S4 case.
effects of the eddy viscosity coefficients, calculated by the SGS models, on the solution become unimportant for the numerical approach used in the present work. There is work reported in the literature, as indicated in the previous section, that arrives at similar conclusions while addressing a simplified problem, namely, the one-dimensional Burgers’ equation. Such work further emphasizes that SGS closures introduce numerical dissipation that can be used as a numerical stabilizing mechanism. However, this numerical dissipation does not necessarily add more physics of the turbulent flow behavior obtained by the LES solution. Therefore, an interesting extension of the present effort would be to revisit the jet flow problem using implicit LES techniques.

Acknowledgements The authors gratefully acknowledge the partial support for this research provided by Conselho Nacional de Desenvolvimento Científico e Tecnológico, CNPq, under the Research Grant nos. 309985/2013-7, 400844/2014-1 and 443839/2014-0. The authors are also indebted to the partial financial support received from Fundação de Amparo à Pesquisa do Estado de São Paulo, FAPESP, under the Research Grant nos. 2013/0735-0 and 2013/21535-0. The authors further acknowledge the National Laboratory for Scientific Computing, LNCC/MCTIC, for providing high-performance computing resources through the Santos Dumont supercomputer, which have contributed to the research results reported within this paper.

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