Subgrid modeling approaches for scalar transport and mixing in LES of turbulent shear flows

Olivia S. Sun,* Lester K. Su†

Applied Fluid Imaging Laboratory, Department of Mechanical Engineering
Johns Hopkins University

and

Tristan M. Burton‡

Mechanical Engineering Department
United States Naval Academy

LES models for subgrid scalar transport are assessed through large eddy simulation of passive scalar mixing in a turbulent round jet. The simulation is performed on a spherical coordinate grid using semi-implicit time advancement. The models used to close the subgrid scalar flux term are varied while the same modeling approach is used for the momentum model in order to isolate the effects of the scalar modeling. The subgrid scalar flux models tested include the dynamic eddy diffusivity model and the dynamic one-parameter mixed model. Model performance is analyzed by examining mean, resolved-scale quantities and fluctuations of the resolved scalar concentration field. Also addressed in this paper are particular challenges associated with dynamic modeling in spherical-coordinate, round jet simulations. These include explicit test filtering of resolved-scale quantities and spatial averaging of dynamic coefficients.

I. Introduction

In large eddy simulation (LES), only the large scales of turbulent motion are computed explicitly, while the smallest scales are represented by subgrid scale (SGS) models. The advantage of LES is since most of the turbulent kinetic energy is resolved, accurate representation of complex flows can be obtained at a lower computational cost compared to direct numerical simulation (DNS). Consequently, LES has become a very attractive and powerful tool for many engineering applications, including simulations of reacting flows and combustion systems. Since molecular mixing, the precursor to chemical reaction, occurs exclusively at the subgrid level, it is vital that large eddy simulations accurately represent the mixing process at all scales. Given their importance to the mixing problem, thorough analysis of the performance and behavior of subgrid scale mixing models is essential.

For flows that involve scalar mixing, large eddy simulations require models for the SGS scalar flux to close the scalar transport equation. The main approaches to modeling these variables include gradient-based, or eddy diffusivity, models, where the modeled quantity is assumed to align with the resolved-scale scalar gradient tensor [1], structural models in which the modeled quantity is structurally represented by scale-similarity approximations [2, 3], and combinations of the two (so called ‘mixed’ models).

Analyses of SGS scalar models have been fairly limited. Some previous studies have examined methods for predicting SGS model behavior [4–6]. However, there are currently no universal metrics for assessing the performance of SGS models and, particularly, SGS scalar mixing models. The sparsity of fully resolved direct numerical simulations (at reasonable Reynolds numbers) and suitable experimental measurements preclude many SGS model validation studies. The objective of the present work is to examine the behavior of SGS
mixing models in LES of passive scalar mixing in a round, turbulent jet. For this study, we select two scalar flux models based on the more prevalent, ‘mainstream’ modeling approaches: the gradient-based, dynamic eddy diffusivity model, and the one-parameter, dynamic mixed model. Model assessment is conducted by comparing the evolution of mean, resolved-scale quantities with expected solutions, and examining the fluctuations of the resolved scalar concentration field.

For the spherical-coordinate geometry used in the present simulation, there are several challenges associated with the dynamic modeling of both the subgrid stress and subgrid scalar flux. The inherent spatial anisotropy of the spherical coordinate grid creates difficulties in defining a consistent test filter, necessary for computing terms in the dynamic procedure [7]. Additionally, the round jet lacks an appropriate homogeneous direction to perform spatial averaging required to stabilize the dynamic coefficient [7]. Here, we develop and implement a novel, explicit test filtering method we call ‘Cartesian-fitted test filtering’. The method is based on locally fitting Cartesian grids to the spherical-coordinate LES grid. Dynamic model coefficients, as computed using Cartesian-fitted test filtering in the standard dynamic procedure [7], are presented.

II. Numerical simulations

For large eddy simulation (LES) of passive scalar mixing in a spatially developing, free, round turbulent jet, the flow is governed by the LES-filtered Navier-Stokes equations:

\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \tag{1} \]

\[ \frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{2} \]

where

\[ \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \tag{3} \]

and the filtered transport equation for a conserved scalar, \( C \):

\[ \frac{\partial C}{\partial t} + \bar{u}_i \frac{\partial C}{\partial x_i} = \frac{1}{ReSc} \frac{\partial^2 C}{\partial x_i \partial x_i} - \frac{\partial \tau_{i,C}}{\partial x_i}, \tag{4} \]

where \( Sc \) is the Schmidt number, and the SGS flux term \( \tau_{i,C} \) is defined

\[ \tau_{i,C} = \bar{u}_i \bar{C} - \bar{u}_i \bar{C}. \tag{5} \]

The LES code is based on a direct numerical simulation (DNS) code developed by Burton [8] and originally applied to multiphase turbulence. The equations, (1), (2) and (4) are discretized in spherical coordinates and solved on a spherical grid with geometric stretching in the radial direction similar to that of Boersma et al. [9]. Spatial discretization of the momentum equation (1) is performed using second-order central differencing. The passive scalar transport equation (4) is discretized using the second-order, upwind-biased bounded QUICK scheme [10] to minimize unphysical spatial oscillations in the scalar solution. The equations are integrated in time using a semi-implicit, three-step time advancement algorithm [11], with all viscous terms treated implicitly.

The boundary condition at the inflow is a uniform top-hat profile for both the velocity and scalar, imposed across the orifice of diameter \( D \). At the outflow boundary, we use a convective boundary condition. So called ‘traction-free’ or ‘stress-free’ boundary conditions are used on the lateral boundaries of the jet. Simulations are performed at Reynolds number \( ReD = 14,400 \) based on the jet exit diameter, \( D \), and jet exit velocity, \( U_o \), and Schmidt number \( Sc = 1 \), using \( N_r = 112, N_\theta = 32 \) and \( N_\phi = 16 \) grid points in the radial, tangential, and azimuthal directions, respectively. A two-dimensional sketch of the computational domain is shown in Figure 1.

III. Subgrid models

In order to isolate the effects of the scalar modeling, we use the same model for the subgrid scale stress while varying the models used for the subgrid scalar flux. To close the subgrid scale stress term, \( \tau_{ij} \), in
Equation 1, we use the dynamic Smagorinsky model, defined by
\[ \tau_{ij} = -2(C_s \Delta^2 |S| S_{ij}). \] (6)

Two different modeling approaches are used to close the subgrid scalar flux term, \( \tau_{i,C} \), in Equation 4. These include: a gradient-based, dynamic eddy diffusivity model, defined by
\[ \tau_{i,C} = -(C_r \Delta^2 |S| \frac{\partial C}{\partial x_i}), \] (7)

and a one-parameter, dynamic mixed model, given by
\[ \tau_{i,C} = \bar{u}_i \bar{C} - \bar{u}_j \bar{\bar{C}} - (C_m \Delta^2 |S| \frac{\partial C}{\partial x_i}). \] (8)

The eddy diffusivity model (Eq. 7) assumes that the subgrid scalar flux is aligned with the resolved-scale scalar gradient. This model is purely dissipative and only allows forward energy transfer from the resolved to the subgrid scales. The mixed model (Eq. 8) aims to represent the structure of \( \tau_{i,C} \) with the Leonard-type term, \( \bar{u}_i \bar{C} - \bar{u}_j \bar{\bar{C}} \), while additionally tuning the magnitude of \( \tau_{i,C} \) with the eddy diffusivity term, \( (C_m \Delta^2 |S| \frac{\partial C}{\partial x_i}). \) Unlike the eddy diffusivity model, the mixed model also allows energy transfer from the subgrid to the resolved scales, or ‘backscattering’. For both the eddy diffusivity and mixed models, the model coefficients, \( C_r \) and \( C_m \), respectively, affect the magnitude of energy transferred between scales and, consequently, the evolution of the resolved-scale concentration field. The computation of \( C_r \) and \( C_m \), as well as \( C_s \) in Equation 6, is discussed in the following section.

IV. Dynamic modeling

In the dynamic procedure [7], the model coefficient, \( C_s \) in Equation 6 is computed according to:
\[ C_s^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}, \] (9)

where \( \langle \rangle \) denotes averaging,
\[ L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{\bar{u}}_j, \] (10)

and
\[ M_{ij} = 2 \left( \Delta^2 |S| S_{ij} - \Delta^2 |S| S_{ij} \right). \] (11)

An important step in the dynamic procedure is the test filtering, denoted here by \( \langle \rangle \), of resolved-scale quantities, necessary for evaluating \( L_{ij} \) and \( M_{ij} \) according to Equations 10 and 11. On a regular,
Cartesian grid, the test filter is usually defined as a local average of quantities over neighboring grid points in computational space. For example, in 2D, a test-filtered quantity, \( \hat{f} \), at location \((i, j)\) in the domain could be defined as:

\[
\hat{f}_{i,j} = \frac{1}{4}(f_{i-1,j-1} + f_{i+1,j-1} + f_{i-1,j+1} + f_{i+1,j+1})
\]

However, in spherical coordinates, such a test filter is less intuitively defined. Due to the inherent spatial non-uniformity of the spherical-coordinate grid, local averaging performed in computational space results in anisotropic test filters of varying test-to-grid filter ratio, \( \frac{\Delta}{\Delta} \). These are undesirable features in a test filter and can adversely affect the results of the simulation.

### A. Approximate test filter

One possible solution is to approximate the test filter with a derivative-based method, thus eliminating the need for explicit test filtering. This approach, developed by Chester et al. [12], approximates test filtering with Taylor series expansions of resolved-scale quantities. Retaining terms up to second order in the expansion, a test-filtered quantity, \( \hat{f} \), is expressed in terms of the resolved-scale (grid-scale) quantity, \( f \), as:

\[
\hat{f}(x) = f(x) + \frac{(\alpha \Delta)^2}{24} \nabla^2 f(x)
\]

Applying (13) to the terms in the dynamic model [7], \( L_{ij} \) and \( M_{ij} \) become:

\[
L_{ij} = \frac{(\alpha \Delta)^2}{12} \frac{\partial \phi_i}{\partial \xi_k} \frac{\partial \phi_j}{\partial \xi_k},
\]

and

\[
M_{ij} = 2 \Delta^2 \left[ \left( \frac{\partial \phi_i}{\partial \xi_j} - \alpha^2 \frac{\partial \phi_i}{\partial \xi_j} \right) + \frac{(\alpha \Delta)^2}{24} \frac{\partial^2}{\partial \xi_k \partial \xi_k} \left( \frac{\partial \phi_i}{\partial \xi_j} - \alpha^2 \frac{\partial \phi_i}{\partial \xi_j} \right) \right],
\]

where

\[
|\nabla| = \left[ 2 \left( \frac{\partial \phi_i}{\partial \xi_j} + \frac{(\alpha \Delta)^2}{24} \frac{\partial^2}{\partial \xi_k \partial \xi_k} \right) \right]^{1/2}.
\]

Here, the constant, \( \alpha \), is a parameter that determines the test-to-grid filter ratio, \( \frac{\Delta}{\Delta} \). (Typical values of \( \alpha \) range between 1 and 2.) The dynamic coefficient, \( C_s \), can then be determined by the standard dynamic procedure [7] using Equation 9.

The effects of this test filtering method are examined by applying (13) to the fluctuating part of the grid-resolved axial velocity component, \( u_{rms} \). Figure 2 shows an instantaneous trace of \( u_{rms} \) at the LES-grid scale, and \( u_{rms} \) test-filtered according to (13) for several different values of the test-to-grid filter ratio, \( \alpha \), along the jet centerline.

The parameter, \( \alpha \), effectively determines the amount of test filtering, or smoothing, of the grid-resolved field. In theory, increasing \( \alpha \) increases the test filter width, removing more fluctuations from the grid-resolved field. Similarly, decreasing \( \alpha \) decreases the test filter width and retains more grid-scale fluctuations. If \( \alpha \) is too small, there is not enough separation of scales between the test and grid filtered levels. This can create difficulties in computing the dynamic coefficient, \( C_s \), according to (9) [7]. However, if \( \alpha \) is too large, the accuracy of this derivative-based, approximate test filter is compromised [12]. As is evident in Figure 2, there are limitations associated with selecting an appropriate value for \( \alpha \). For \( \alpha = 1 \), the test filter has the same width as the LES grid filter and performs very little smoothing of the resolved-scale field. As \( \alpha \) is increased, the accuracy of the Taylor series-based approximation (13) quickly decreases, as manifested by the increased fluctuations observed in the test-filtered field for \( \alpha \geq 2 \).

We attempted to implement this method (Equations 14–16) for dynamic modeling of (6), (7), and (8) in our round jet LES. However, the simulation could not remain stable with the dynamic model coefficients, \( C_s, C_r, \) and \( C_m \), obtained using this method for any value of \( \alpha \). Therefore, we conclude that the limitations associated with the Taylor series-based approximate test filter (13) are not well-suited for our spherical coordinate geometry and simulation.
B. Cartesian-fitted test filtering

Another solution is to filter explicitly in physical, rather than computational, space, employing a consistent, isotropic test filter with constant test-to-grid filter ratio, \( \frac{\Delta}{\Delta} \), over the entire computational domain. This can be accomplished in the present geometry by defining the test filter as a local average of quantities over a specified region that extends the same physical distance in all three coordinate directions.

Suppose we want to filter a grid-scale quantity, \( \mathbf{f}(x) \), at a physical location \((r, \theta, \phi)\) on the spherical coordinate grid. We define the shape of the test filter as a cube centered over \((r, \theta, \phi)\) having length \( l = \Delta \). The test filter width, \( \Delta \), is defined in terms of physical units as twice the local LES grid-filter width, i.e.

\[
\Delta = 2r^2 \sin \theta \Delta r \Delta \theta \Delta \phi^{(1/3)}.
\]  

Next, we convert the physical position described by \((r, \theta, \phi)\) into the equivalent position \((x, y, z)\) in Cartesian coordinates via the transformation:

\[
\begin{align*}
x &= r \cos \theta \\
y &= r \sin \theta \cos \phi \\
z &= r \sin \theta \sin \phi.
\end{align*}
\]

We can then determine the extent of the test filter (i.e. the `edges' of the cube) in the \( x \)-direction according to:

\[
\begin{align*}
x^+ &= x + \frac{\Delta}{2} \\
x^- &= x - \frac{\Delta}{2}
\end{align*}
\]

and similarly for the \( y \)- and \( z \)-directions. To locate the positions of the cube edges on the spherical coordinate grid, the locations \( x^+, x^-, y^+, y^-, z^+, z^- \) are transformed back into their spherical coordinate equivalents to obtain the locations \((r^1, \theta^1, \phi^1), (r^2, \theta^2, \phi^2), ..., (r^{27}, \theta^{27}, \phi^{27})\). Then 3D linear interpolation is performed to evaluate \( \mathbf{f}(x) \) at each of the 27 \((r^i, \theta^i, \phi^i)\) locations. Finally, \( \mathbf{f}(x) \) at \((r, \theta, \phi)\) is computed using Simpson’s rule for numerical integration.

By performing this intermediate mapping onto Cartesian coordinates, we can ensure that the test filter has the same physical dimension, \( \Delta \) (defined according to Equation 17, in all three coordinate directions, \((r, \theta, \phi)\)), and guarantee that the test filtering volumes are convex. We also maintain a constant test-to-grid filter ratio, \( \frac{\Delta}{\Delta} \), throughout the entire domain. The Cartesian-fitted test filter performs very well in test filtering grid-resolved quantities for the dynamic procedure (Equations 9–11) and is used in all simulation runs presented in this paper.
C. Lagrangian averaging of dynamic coefficients

The round jet lacks an appropriate homogeneous direction over which to perform the spatial averaging (i.e., \( \langle L_{ij}M_{ij} \rangle \) and \( \langle M_{ij}M_{ij} \rangle \)) required to stabilize the dynamic coefficients, \( C_s, C_r, \) and \( C_m [7] \). Therefore, we implement the Lagrangian dynamic procedure (see [13] for details), where \( L_{ij}M_{ij} \) and \( M_{ij}M_{ij} \) are averaged along fluid particle path lines over a specified time scale, \( T \). Figure 3 shows time traces of \( L_{ij}M_{ij} \) and \( M_{ij}M_{ij} \), evaluated locally and Lagrangian-averaged over one eddy turnover time, \( \delta/U_c \). It can be seen that averaging over the local eddy turnover time, \( \delta/U_c \), is sufficient to constrain \( L_{ij}M_{ij} \) and \( M_{ij}M_{ij} \) to positive values and stabilize the dynamic coefficient.

V. Results

For each scalar flux model, the simulation is run for 350 non-dimensional time units, corresponding to approximately two domain flow-through times. (One domain flow-through time is defined as the non-dimensional time required for a fluid particle at the inflow boundary to reach the outflow boundary 45\( D \) downstream.) Then, 160 three-dimensional data fields, separated by \( 1.5D/U_o \), are collected and used for computing the statistics.

A. Instantaneous velocity and concentration fields

Instantaneous spatial contours of axial velocity, \( u/U_o \), are shown in Figure 4. The corresponding spatial contours for the scalar concentration, \( C \), are shown in Figure 5 for the eddy diffusivity model (7), and Figure 6 for the mixed model (8).

B. Mean quantities and profiles

The mean centerline axial velocity in the self-similar region of a round turbulent jet is expected to follow the relation [14]:

\[
\frac{U_c}{U_o} = B_u \left( \frac{x - x_o}{D} \right)^{-1},
\]

where \( x \) is the axial coordinate, \( U_c \) is the centerline axial velocity, \( U_o \) is the initial axial velocity at the jet exit, \( B_u \) is a proportionality constant, and \( x_o \) is the virtual origin of the jet. Figure 7 shows the mean centerline axial velocity for the turbulent jet. The \( 1/x \) expected decay rate is plotted for comparison. The LES results agree well with the expected centerline decay rate. For \( Sc = 1 \), the mean centerline scalar concentration is expected to follow a similar decay rate as the centerline axial velocity and can be described by [14]:

\[
C \approx \frac{1}{x}
\]
The centerline concentration decay for the eddy diffusivity (7) and mixed (8) models are shown in Figure 8. The $C = 1/x$ curve is also plotted for comparison. Both models follow the shape of the expected $C = 1/x$ curve fairly well. The mixed model initially predicts a faster centerline concentration decay rate compared to the eddy diffusivity model. However, starting near $x = 10D$ and continuing to the end of the domain, the trends reverse and the eddy diffusivity model predicts the faster decay rate.

The radial velocity profile of a round turbulent jet is approximated by [14]:

$$\frac{U}{U_c} = \exp(-K_u \eta^2),$$

where $\eta = y/(x - x_0)$. Here, $y$ is the radial coordinate, $x$ is the axial coordinate, and $K_u$ is a constant that can be determined by a least-squares fit to the data. Similarly, the radial concentration profile can be approximated by:

$$\frac{C}{C_0} = \exp(-K_c \eta^2).$$

Radial profiles of axial velocity and scalar concentration at downstream location $x = 20D$ are presented in Figures 9 and 10, respectively.

A Gaussian-like profile shape is observed for both axial velocity (Figure 9) and scalar concentration (Figure 10). Profiles of the scalar concentration, $C/C_0$, for both scalar flux models are wider than the velocity profile. As seen in Figure 10, the mixed model has a slightly wider concentration profile than the eddy diffusivity model, suggesting that the mixed model predicts a faster spreading rate for $C$. This observation somewhat contradicts the slower centerline concentration decay rate (compared to the eddy
Figure 6. Instantaneous spatial contours of scalar concentration, $C$, for the mixed model.

Figure 7. Mean centerline decay of axial velocity, $U_c$.

diffusivity model) predicted by the mixed model in Figure 8. Further analysis is needed to fully explain these results.

C. Growth rates of velocity and scalar concentration

The velocity half-width, $\delta_{0.5,u}$, is defined as the radial position, $y$, at which the axial velocity, $u$, satisfies the relation:

$$u = 0.5U_c$$

(27)

The scalar concentration half-width, $\delta_{0.5,C}$, is defined analogously as the radial position at which the scalar concentration, $C$, satisfies:

$$C = 0.5C_0$$

(28)

The velocity and scalar half-widths are described by the relations:

$$\delta_{0.5,u} = \beta_u(x - x_o)$$

(29)

and

$$\delta_{0.5,C} = \beta_C(x - x_o).$$

(30)

$\beta_u$ and $\beta_C$ are constants determined by least-squares fits to the data, and describe the growth rates of the velocity and scalar profiles, respectively.

In Figure 11, the velocity half-width, $\delta_{0.5,u}$, as well as the scalar half-width, $\delta_{0.5,C}$, for both scalar models are plotted for the first 35 diameters of the domain. We observe that $\delta_{0.5,u}$ is linear, as expected.
Figure 8. Mean centerline decay of scalar concentration, $C_0$.

Figure 9. Radial profile of axial velocity at $x = 20D$

by Equation 29. Through a least-squares fit of $\delta_{0.5, u}$ in the range $15D < x < 32D$, the growth rate of the velocity profile, $\beta_u$ in Equation 29, is found to be $\beta_u = 0.113$. This is larger than the growth rates observed by others [9,15,16], which fall in the range $\delta_{0.5, u} \approx 0.08 - 0.09$. However, $\delta_{0.5, u}$ has also been found to vary depending on simulation parameters such as: grid selection, inflow, outflow, and lateral boundary conditions, as well as experimental conditions [9,15,17]. Therefore, we conclude that our computed axial velocity growth rate, $\beta_u = 0.113$, is reasonable, and that the scaling of the velocity field is accurately represented by the LES.

The scalar half-width, $\delta_{0.5, C}$, is larger than the velocity half-width, $\delta_{0.5, u}$, for both the eddy diffusivity and mixed models, as evident in Figure 11. Here, it can be seen that $\delta_{0.5, C}$ for the mixed model (hereafter referred to as $\delta_{C, \text{mix}}$) is larger than $\delta_{0.5, C}$ for the eddy diffusivity model (hereafter referred to as $\delta_{C, \text{ED}}$). Least-squares fitting of $\delta_{C, \text{ED}}$ and $\delta_{C, \text{mix}}$ in the range $15D < x < 32D$ find growth rates $\beta_{C, \text{ED}} = 0.129$ for the eddy diffusivity model, and $\beta_{C, \text{mix}} = 0.139$ for the mixed model. These observations are consistent with the wider radial concentration profile observed for the mixed model in Figure 10.

D. Scalar concentration fluctuations

The root mean square (rms) of the resolved scale scalar fluctuations is defined by

$$C_{rms} \equiv \left[ \langle (C - \langle C \rangle)^2 \rangle \right]^{1/2},$$

where $\langle \rangle$ denotes averaging. The rms of scalar fluctuations, $C_{rms}$, along the jet centerline, scaled by the local centerline concentration, $C_0$, is shown in Figure 12. Plots for both the eddy diffusivity and mixed models
agree with trends that have been observed in previous studies [15, 17]. The scalar fluctuation rms is zero at the inflow and increases with downstream distance as the jet undergoes transition to turbulence. In the self-similarity region, i.e. $x > 20D$, $C_{rms}/C_0$ should asymptote to a constant value if the scalar fluctuations are self-similar [15, 17]. This trend has been observed experimentally [17], but has not been reproduced numerically [15, 16]. Here, we find that $C_{rms}/C_0$ along the centerline oscillates between values of 0.2 and 0.3 in the similarity region. These findings are consistent with the numerical results of [15] and [16], as well as the experimental value of $C_{rms}/C_0 = 0.237$ quoted by Dowling and Dimotakis [17] for a round jet at $Re_D = 16,000$.

Figure 13 shows radial profiles of $C_{rms}/C_0$ as a function of $\eta$, averaged over the self-similarity region $20D < x < 35D$. The rms of the scalar fluctuation peaks just off the jet centerline, near $\eta = 0.7$, and decreases with $\eta$ as the outer boundary of the jet is approached. Again, these trends are similar to those reported in previous studies [15–17].

In Figures 12 and 13, we observe that the eddy diffusivity and mixed models give similar results for $C_{rms}/C_0$, both along the centerline (Figure 12) and in radial profiles (Figure 13). It is interesting to note that although the two scalar flux models predict different centerline concentration decay and concentration profile growth rates, as seen in Figures 8, 10, and 11, both models produce statistically similar fluctuating scalar fields.
VI. Dynamic model coefficients

In Figure 14 we show the variation of $C_s$, the dynamic coefficient for $\tau_{ij}$ in Equation 6, along the centerline of the jet. $C_s$ is small near the inflow region, where the flow is mostly laminar. Then, after approximately $5D$, $C_s$ quickly increases as the jet undergoes transition to turbulence. For $x > 10D$, the coefficient, $C_s$, takes on values between 0.12–0.16.

Figure 15 shows the axial variation of $C_r$, the dynamic coefficient for $\tau_{iC}$ in Equation 7, and $C_m$, the dynamic coefficient for $\tau_{iC}$ in Equation 8. Both $C_r$ and $C_m$ have trends similar to $C_s$. $C_r$, the coefficient for the eddy diffusivity model (Equation 7), is generally larger in magnitude than $C_s$. $C_m$, the coefficient for the mixed model (Equation 8), is approximately half the magnitude of $C_r$ for the majority of axial locations along the centerline. $C_m$ controls the amount of energy dissipation to the subgrid scales supplied by the eddy diffusivity part of the mixed model (8). With the addition of the Leonard-type term in the mixed model, the eddy diffusivity part of Equation 8 is required to 'model' less, and therefore the coefficient, $C_m$, is smaller.

Radial profiles of $C_s$ at different downstream locations are shown in Figure 16. The magnitude of $C_s$ is highest off the centerline of the jet, near $\eta = 0.7$, and decreases with $\eta$. The profiles appear to be self-similar closer to the jet centerline, for $\eta \leq 0.2$. As the lateral boundary of the jet is approached, the profiles vary in width, becoming narrower with increasing $x/D$.

Radial profiles of $C_r$ and $C_m$ are presented in Figure 17. The profile trends observed for $C_r$ and $C_m$ are slightly different from those seen in Figure 16 for $C_s$. Both $C_r$ and $C_m$ have wider radial profiles than $C_s$, and peak near the outer, lateral boundary of the jet for $x/D < 18$. Profiles of $C_r$ and $C_m$, like $C_s$, appear
to exhibit self-similar behavior for \( \eta \leq 0.2 \). \( C_r \), the coefficient for the eddy diffusivity model, has a wider profile shape and is larger in magnitude compared to \( C_m \), the mixed model coefficient. These results are consistent with the observation that less ‘modeling’ is required by the eddy diffusivity part of the mixed model, resulting in smaller values for \( C_m \).

VII. Conclusions and ongoing work

Subgrid scale models for subgrid scalar flux are evaluated in large eddy simulation of passive scalar mixing in a round, turbulent jet. Effects of the subgrid scalar modeling are isolated by varying the models used to close the subgrid scalar flux term while using the same modeling approach for the momentum model. We study two SGS scalar flux models based on mainstream modeling approaches: the dynamic eddy diffusivity model and the one-parameter, dynamic mixed model. Results for the velocity field and the scalar field predicted by both scalar models show good agreement with expected trends as well as results obtained by previous numerical and experimental studies (e.g., [15], [17]). The eddy diffusivity model predicts a faster centerline concentration decay rate. However, the mixed model predicts a wider concentration profile in the self-similar region of the jet. Both models predict statistically similar fluctuating scalar concentration fields.

We developed and implemented a novel, explicit test filtering method based on fitting Cartesian grids to the spherical coordinate geometry to resolve the issues associated with test filtering in a spherical coordinate system. This method ensures that the test filter is spatially isotropic, and that a constant test-to-grid filter ratio is maintained throughout the computational domain. The Cartesian-fitted test filter is found to give
Figure 16. Radial profiles of $C_s$ at different downstream locations.

Figure 17. Radial profiles of $C_r$ (-) and $C_m$ (--) at different downstream locations.

good results when used in the dynamic procedure [7] to compute the dynamic model coefficients.

Ongoing work includes further numerical studies using LES and DNS of turbulent jet mixing. Additional subgrid scalar modeling approaches are being studied and implemented in the LES. We also plan to perform experiments in the same flow configuration, using particle image velocimetry (PIV) and planar laser-induced fluorescence (PLIF) for simultaneous velocity and scalar field measurements. These combined numerical and experimental measurements will allow more comprehensive assessment and validation of subgrid scale models.

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