Large Eddy Simulation: Turbulence Project

Charles Reid

April 28, 2008
List of Figures

1. A plot of experimental velocity vs. time data for a buoyant helium plume (blue) [17] plotted with the same data filtered using various filter widths $\Delta$. ................................................................. 9
2. A diagram of the experimental setup for the Sandia FLAME lab, where the velocity data on the turbulent buoyant helium plume was gathered [17]. ......................................................... 17
3. A cross-sectional view of the unstructured mesh used in the computation. .............................................. 17
4. A diagram of the simulation geometry. Cube is 3 meters on each side. ................................................. 18
5. A plot of velocity vs. time for case 1 run on a small domain and a large domain, along with the data from Sandia. ........................................................................................................ 19
6. Figure describing the general attitude of many of today’s commercial CFD software users. ................. 20
7. A plot of velocity vs. time for case 1 run on a small domain and a large domain, along with the data from Sandia. ........................................................................................................ 21
8. Velocity vs. time data for all 7 cases at a height of 200 mm above the inlet along the centerline. ....... 21
9. Velocity vs. time data for all 7 cases at a height of 600 mm above the inlet along the centerline. ....... 22
10. Velocity vs. time data for two simulations, case 1 and case 2, at heights of 400 mm (top) and 600 mm (bottom) above the inlet. ................................................................. 22
11. Velocity vs. time data for two simulations, case 1 and case 2, along with Sandia data, at heights of 400 mm (top) and 600 mm (bottom) above the inlet. ................................. 23
12. Velocity vs. time data for two simulations, case 1 and case 7, at heights of 400 mm (top) and 600 mm (bottom) above the inlet. ................................................................. 23
13. Velocity vs. time data for two simulations, case 1 and case 7, along with Sandia data, at heights of 400 mm (top) and 600 mm (bottom) above the inlet. ................................. 24

List of Tables

1. Computational time estimates for DNS at various Reynolds numbers. .................................................. 7
2. Some common filter functions in physical and spectral space; table reproduced from [10]. ................. 10
3. Case matrix for the LES parameter study. ......................................................................................... 15
1 Turbulence Concepts

Before discussing large eddy simulation and its characteristics, some general concepts related to turbulence will first be reviewed. A discussion of the physics of turbulence will lay the groundwork for large eddy simulation, and a discussion of the most common turbulence models will provide a context. The first topic for discussion will be turbulent length scales, which will lead into the Kolmogorov Hypotheses and the turbulent energy spectrum. After that, the two most common turbulence modeling methodologies, direct numerical simulation (DNS) and Reynolds-Averaged Navier Stokes (RANS), will be discussed. The issues with each will be addressed, providing a better understanding of the advantages that large eddy simulation provides.

1.1 Length Scales

A wide range of length scales of motion are clearly visible when watching any turbulent flow. There are large eddies that govern the bulk motions of the flow, but there are also many visible eddies and fluctuations that are smaller; and there are many, many more eddies and fluctuations that are too small to be visible at all. When seeing this phenomena, the first question that comes to mind is whether and how these scales can be quantified. Is there a relationship between the large and small scales? Do they have the same time and velocity scales? At some point, the scales will become small enough that their momentum will be damped out by viscosity – the point where inertial forces in an eddy shrink to the same magnitude as the viscous forces. At this point the Reynolds number, a ratio of inertial to viscous forces, is 1.

One may begin by assuming that the small-scale motions are faster than the large scale motions, which makes the two scales statistically independent. One can then perform a basic energy balance on the small scale structures (small eddies) and see that the “energy in” is provided by energy dissipating from larger scales, and the “energy out” is energy dissipated from the small scales due to viscosity. Thus, the small scale motions should only depend on two things: first, the rate at which the eddies are supplied energy from the large-scale motions (dissipation of kinetic energy, \( \varepsilon \)); and second, the viscosity (\( \nu \)). The units of dissipation and kinematic viscosity are, respectively:

\[
\varepsilon = \left[ \frac{m^2}{s^3} \right] \\
\nu = \left[ \frac{m^2}{s} \right]
\]

These quantities can be used to form length, time, and velocity scales:

\[
\eta = \left( \frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}}
\]

\[
\tau_\eta = \left( \frac{\nu}{\varepsilon} \right)^{\frac{1}{2}}
\]

\[
u_\eta = (\nu \varepsilon)^{\frac{1}{4}}
\]

The length scale \( \eta \) is called the Kolmogorov length scale, and is the smallest length scale of the flow. At this point, it would be desirable to relate this smallest scale to the largest (integral) length scale, \( L \), to get a relationship between \( \eta \) and \( L \). The connection between the two scales lies in the kinetic energy dissipation. Dissipation has units of kinetic energy per time. Thus, the kinetic energy and time quantities can be expressed in terms of the integral scale length and velocity to get \( \varepsilon \) in terms of the integral scales. This can be substituted into (1.1) to get the relation between \( \eta \) and \( L \).
Kinetic energy can be written \( K \sim U^2 \) (where \( U \) is the integral scale velocity), and an eddy turnover time can be defined as \( t \sim \frac{L}{U} \). Then the kinetic energy dissipation can be described as the kinetic energy lost during a single eddy turnover time:

\[
\varepsilon \sim \frac{U^3}{L} \tag{1.6}
\]

Plugging this result into (1.3) yields the following relationships between the large and small length, time, and velocity scales:

\[
\frac{\eta}{L} = Re^{-\frac{3}{2}} \tag{1.7}
\]

\[
\frac{\tau_{\eta}}{t} = Re^{-\frac{1}{2}} \tag{1.8}
\]

\[
\frac{u_{\eta}}{U} = Re^{-\frac{1}{4}} \tag{1.9}
\]

It is clear at this point how critical (1.6) is to the treatment of turbulence. It is also clear that the length, time, and velocity scales of small eddies are much smaller than those of large eddies. These observations will become very important in the discussion of turbulence modeling. Also, note that while the Kolmogorov scale is very small, it is nowhere near as small as the mean free path of the fluid molecules, meaning the behavior of the fluid at scales smaller than the Kolmogorov scale can be treated as a continuum. The importance of this observation will become clear in section 1.2.2.

### 1.2 Energy Spectra

The energy spectrum of turbulence is an important concept that connects many ideas, like the multiple scales of turbulence, the Kolmogorov hypotheses, and the dependence of eddy behavior on its size and the properties of the flow. The energy spectrum is obtained by looking at the kinetic energy distribution among the different scales (or wavelengths) of turbulence in wave number space. Before proceeding with a discussion specific to turbulence, a brief overview of Fourier transforms will be presented.

#### 1.2.1 Fourier Transforms

Fourier transforms serve two important purposes in the analysis of turbulence. First, they simplify the numerical procedure of differentiation and integration by changing differential operators into algebraic operators. This can be particularly useful for the governing equations of turbulence, such as the Navier-Stokes equations. Second, they provide a physical interpretation - a spectra produced from a Fourier transform can give information about turbulent length scales (in the form of frequencies). The Fourier transform of a function \( f(t) \) is \( \hat{f}(\kappa) \). It is defined as:

\[
\mathfrak{F} \left( f(x) \right) = \hat{f}(\kappa) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x') e^{-i\kappa x'} dx' \tag{1.10}
\]

This transforms the function \( f(x) \) into wave space, so that instead of being a function of position \( x \), it is now a function of the wave number \( \kappa \). A Fourier transform does not correspond to a function’s location - it corresponds to a function’s periodic behavior. For example, the Fourier transform of \( f(x) = \sin(x) \) produces a peak at \( \kappa = 1 \), because the periodic behavior of \( f(x) \) corresponds to a wave number of 1. The usefulness of the Fourier transform
is manifested in signal processing. It can provide a clear picture of how the signal behaves over time, even when the data are very noisy and no trends are immediately obvious.

Applying this idea of wavelengths and periodic behavior over time can help to visualize the energy cascade from large scales to small scales in turbulence. Large eddies will have larger characteristic times, so their frequencies (inverse times) will be lower - this corresponds to low wave numbers. Smaller eddies will have much shorter characteristic times, and thus larger frequencies and larger wave numbers. Taking the Fourier transform of the kinetic energy of a turbulent flow is a common technique that results in a spectrum that is common among turbulent flows (just as the process of the energy cascade is common to all turbulent flows). The spectrum of kinetic energy can reveal things like the rate of kinetic energy dissipation (among other things).

Next, the Fourier transform of the $n^{th}$ derivative $f^{(n)}(x)$ of the function $f(x)$ can be expressed as [10]:

$$\hat{f}^{(n)}(\kappa) = (i\kappa)^n \hat{f}(\kappa)$$

Calculating the Fourier transform of a function’s derivative is as simple as multiplying the Fourier transform by $i\kappa$ – a simple algebraic operation. Upon taking the inverse Fourier transform, one gets the derivative of the original function, that is, $f'(x)$ in $x$ space. The ease with which one can calculate derivatives is greatly simplified. This gives rise to “spectral methods” and “pseudo-spectral methods”, techniques which deal with the Fourier transforms of governing equations rather than with the governing equations themselves. These methods are important turbulence modeling techniques, and are of particular importance in large eddy simulation.

1.2.2 Kolmogorov Hypotheses

In 1941, Kolmorov advanced three hypotheses about the nature of turbulence at different length scales [5]. The first is Kolmogorov’s hypothesis of local isotropy, which states that when the Reynolds number is large enough, the small scale fluctuations in the turbulent velocity are statistically homogeneous (they are not a function of position or time) and statistically isotropic (homogeneous and invariant with respect to rotations or reflections of coordinate system). Local isotropy refers to isotropy only on small scales. This hypothesis is extremely important and useful. It dictates that directional information about the geometry and boundary conditions, which affects the large scale motions, is lost as that motion cascades to smaller scales. Smaller than a certain length scale, the behavior of the small scales is independent of the system geometry or boundary conditions, given a high enough Reynolds number.

Kolmogorov continues with two additional similarity hypotheses. The first Kolmogorov similarity hypothesis states that, for locally isotropic turbulence, the small scale velocity fluctuations have a universal form uniquely determined by the energy dissipation rate $\varepsilon$ and the viscosity $\nu$. This is an extension of the hypothesis of local isotropy. The statical universality of the turbulence in a system depends on two processes – energy transfer from large scales, and viscous dissipation. The two parameters that govern these processes are the dissipation rate and the viscosity.

The second similarity hypothesis states that, given a large enough Reynolds number, the turbulent velocity of intermediate length scales (length scales small compared to the integral length scale $L$, but large compared to the Kolmogorov length scale $\eta$) is uniquely determined by the energy dissipation rate $\varepsilon$ and does not depend on viscosity $\nu$. This completes a picture of the mechanism of turbulent energy transport. According to the first two hypotheses, the energy contained in large scale motions cascades into smaller and smaller scales until all directional information is lost. The velocity fluctuations at these small scales are uniquely determined by the dissipation rate and the viscosity. Now, using the second similarity hypothesis, the dissipation of energy by viscosity occurs only at small scales – the smallest scales of motion in the fluid serve as a kinetic energy sink. This sink does not occur at any intermediate length scales in the flow.
1.2.3 The Spectrum of Turbulence

Using the three Kolmogorov hypotheses, a clear picture of the energy spectrum can be formulated. Low wave numbers correspond to the largest eddies (since the wavelength of a wavenumber $\kappa$ is given by $l = \frac{2\pi}{\kappa}$), intermediate wave numbers correspond to an intermediate range of eddy sizes (these occur in the inertial subrange defined by the second Kolmogorov similarity hypothesis), and finally, high wave numbers correspond to the smallest scales of motion. From Kolmogorov’s second similarity hypothesis [5], one can obtain the Kolmogorov energy spectrum, as derived by Pope [10]:

$$E(\kappa) = C\varepsilon^{\frac{4}{3}}\kappa^{-\frac{5}{3}}$$

(1.12)

where $C$ is a universal constant. This energy spectrum describes the inertial subrange of the kinetic energy spectrum, which consists of the scales of the flow that depend only on the dissipation rate of kinetic energy and not on the viscosity.

1.3 Turbulence Modeling

1.3.1 Direct Numerical Simulation

Direct Numerical Simulation (DNS) is a turbulence modeling technique by which the Navier-Stokes equations are solved exactly, and all of the scales of turbulence are resolved. Equation (1.7) demonstrates how quickly this range grows with increasing Reynolds number. This massive growth in the number of scales that need to be resolved with increasing Reynolds number has severely limited the applications of DNS. In addition, incorporating any additional complexities into the simulation, such as chemical reactions or inhomogeneity, can quickly complicate the numerical algorithms and make the computational cost of a DNS simulation unrealistic.

The computational cost of a DNS simulation is determined by how much of the high wave number portion of the energy spectrum will be truncated. This fixes the the maximum wave number $\kappa_{\text{max}}$, which in turn fixes the necessary number of grid nodes $N^3$ [10]. $N^3$ is a function of the Reynolds number; as Reynolds number increases, the number of total nodes increases as:

$$N^3 \sim Re_L^{9/4}$$

(1.13)

Where $Re_L$ is defined as:

$$Re_L = \frac{K^{\frac{4}{3}}L}{\nu}$$

(1.14)

where $K$ is the kinetic energy of the system, $L$ is the integral length scale, and $\nu$ is the dynamic viscosity. In addition to the spatial discretization dependence on Reynolds number, there is also a time discretization dependence on Reynolds number via the Courant number. The total number of floating point operations that a computer must perform for a spatial domain of $N^3$ and for $M$ time steps is:

$$N^3M \sim Re_L^3$$

(1.15)

Equations (1.13), (1.14), and (1.15) are derived in detail in [10]. Table 9.1 from [10] is reproduced in part below in Table 1.3.1 to give a better idea of how the computational cost scales with Reynolds number. This table provides estimates of the computational time for DNS of isotropic turbulence for various Reynolds numbers. The CPU time is for a computer with 1 giga flop computational power (1 billion calculations per second), assuming 1,000 operations per mode per step.
Table 1: Computational time estimates for DNS at various Reynolds numbers.

<table>
<thead>
<tr>
<th>$Re_L$</th>
<th>$N$</th>
<th>$N^3$</th>
<th>$M$</th>
<th>$N^4M$</th>
<th>CPU Time</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>94</td>
<td>104</td>
<td>$1.1 \times 10^6$</td>
<td>$1.2 \times 10^3$</td>
<td>$1.3 \times 10^9$</td>
<td>20 minutes</td>
<td></td>
</tr>
<tr>
<td>375</td>
<td>214</td>
<td>$1.0 \times 10^7$</td>
<td>$3.3 \times 10^3$</td>
<td>$3.2 \times 10^{10}$</td>
<td>9 hours</td>
<td></td>
</tr>
<tr>
<td>1,500</td>
<td>498</td>
<td>$1.2 \times 10^8$</td>
<td>$9.2 \times 10^3$</td>
<td>$1.1 \times 10^{12}$</td>
<td>13 days</td>
<td></td>
</tr>
<tr>
<td>6,000</td>
<td>1,260</td>
<td>$2.0 \times 10^9$</td>
<td>$2.6 \times 10^4$</td>
<td>$5.2 \times 10^{13}$</td>
<td>20 months</td>
<td></td>
</tr>
<tr>
<td>24,000</td>
<td>3,360</td>
<td>$3.8 \times 10^{10}$</td>
<td>$7.4 \times 10^4$</td>
<td>$2.8 \times 10^{15}$</td>
<td>90 years</td>
<td></td>
</tr>
<tr>
<td>96,000</td>
<td>3,360</td>
<td>$7.8 \times 10^{11}$</td>
<td>$2.1 \times 10^5$</td>
<td>$1.6 \times 10^{17}$</td>
<td>5,000 years</td>
<td></td>
</tr>
</tbody>
</table>

While the computational cost of DNS is a significant disadvantage, it provides many valuable advantages over other simulation methods and over experimental methods. It provides volumes of information not accessible through traditional experimental methods. Because it resolves all length scales, the flow is not modeled - the simulation accurately represents the physics of turbulence. However, much of the computational cost is spent resolving the dissipation range (99.98% of the resolved modes have wave numbers in the dissipation range [10]). It will be shown shortly that large eddy simulation will eliminate this issue while maintaining the large-scale accuracy of DNS.

### 1.3.2 Reynolds-Averaged Navier Stokes

The Reynolds-Averaged Navier Stokes (RANS) models are the most common for practical engineering flow calculations. The technique consists of splitting up the velocity of the fluid into a time-averaged and a fluctuating (“turbulent”) component. The result of this, called Reynolds decomposition, is then substituted into the Navier Stokes equations. The decomposed Navier Stokes equations are nearly identical, except for a single term, called the Reynolds-stress tensor, which contains all of effects of turbulence for all length scales. The Reynolds-decomposed velocity is:

$$ u_i = \overline{U_i} + U_i' $$ (1.16)

Substituting this into the Navier Stokes equation yields the Reynolds-Averaged Navier Stokes equation:

$$ \frac{\partial \overline{U_i}}{\partial t} + \frac{\partial (\overline{U_i} \overline{U_j})}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \overline{U_i}}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (\overline{U_i' U_j'}) $$ (1.17)

Note that the time-averaged value of the fluctuating part of the velocity is zero. The last term in (1.17) (the Reynolds stress tensor) presents a closure problem, and must be modeled. This is, in fact, a problem central to turbulence modeling.

The most common model for this term is the eddy viscosity model, which originates from the analogy of interaction of eddies to molecular interaction. Molecules interacting with one another create viscosity; thus, the eddy interactions are assumed to create a "turbulent viscosity". The analogy made by Boussinesq was the rate of strain relation for a Newtonian fluid - that the rate of strain is proportional to the velocity gradient. Using this gradient transport idea, the deviatoric Reynolds stress tensor can be modeled as [14]:

$$ \tau_{ij}^d = -\nu_t (\nabla \mathbf{u} + \nabla^T \mathbf{u}) $$ (1.18)

where $\tau_{ij}^d$ is the deviator of $\tau_{ij}$:

$$ \tau_{ij}^d = \tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} $$ (1.19)
and \( \tau_{ij} \) is the Reynolds stress tensor:

\[
\tau_{ij} = U_i' U_j' = U_i U_j - \frac{1}{3} \tau_{kk} \delta_{ij}
\]

Thus, plugging (1.19) and (1.20) into (1.18) yields:

\[
\left( U_i' U_j' \right) - \frac{1}{3} \tau_{kk} \delta_{ij} = -\nu_t \left( \frac{\partial U_i'}{\partial x_j} + \frac{\partial U_j'}{\partial x_i} \right) \tag{1.21}
\]

\[
= -2\nu_t S_{ij} \tag{1.22}
\]

where \( S_{ij} \) is defined as:

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \tag{1.23}
\]

The \( \frac{1}{3} \tau_{kk} \delta_{ij} \) term can then be incorporated into the pressure gradient term and the Reynolds stress tensor can be grouped with the molecular viscosity term. This makes the RANS equation:

\[
\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial}{\partial x_i} \left( p + \frac{1}{3} \tau_{kk} \delta_{ij} \right) + (v + \nu_t) \frac{\partial^2 U_i}{\partial x_i \partial x_j} \tag{1.24}
\]

This casts turbulence as a diffusion-driven process with an enhanced diffusivity, \( \nu_t \). However, the turbulent viscosity is now the term that requires closure. Using scale analysis, a turbulent viscosity will scale like \( UL_t \), where \( L_t \) is a length scale of the turbulence. An early turbulent viscosity model, the Prandtl mixing length model [11], obtains the length scale from a “mixing length” that is empirical and related to the flow configuration. It obtains a velocity profile from the mixing length times the velocity gradient. This one-equation model is very crude and grows increasingly less accurate as the flow becomes more complex.

The weakness in this model led to the development of further models. The two that will be briefly covered here are the \( k - \varepsilon \) and \( k - \omega \) models. These two-equation models are based on expressing velocity using kinetic energy, and expressing the length scale using a second quantity such that \( Z \sim K^n L^n \). This allows the turbulent viscosity to be expressed in terms of these two quantities \( K \) and \( Z \). The transport equations for these two quantities comprise the two equations for the model. There is a large body of literature describing these two equation models (c.f. [10] [19]), so only a cursory explanation will be presented here.

The \( k - \varepsilon \) model is based on the quantities \( K \), the kinetic energy, and \( \varepsilon \), the turbulent kinetic energy dissipation. The \( k - \omega \) model is based on the quantities \( K \) and \( \omega \), the dissipation of kinetic energy per unit kinetic energy \( K \omega \) (the inverse of the time scale on which dissipation of kinetic energy occurs). A transport equation is constructed for both, consisting of transport terms for production, dissipation, dispersion (turbulent transport), convection, and diffusion of the quantity of interest. When the model is implemented, for example in a computational fluid dynamics (CFD) code, these transport equations are solved, along with the Navier-Stokes equations, to yield the correct quantities for \( K \) and \( \varepsilon \) or \( \omega \), which are arranged to form \( U \) and \( L \) for the turbulent diffusivity model.

1.4 Part 1 in Summary

In the preceding sections some important groundwork has been laid for a discussion of large eddy simulation. Many ideas in large eddy simulation are direct extensions of ideas brought up in Section 1; many others are direct analogs. Although Part 1 contains a large body of information related to the foundations of turbulence, and not to large eddy simulation, a thorough understanding of these concepts is critical to understanding large eddy simulation.
2 Large Eddy Simulation

Large eddy simulation (LES) is a turbulence modeling technique based on separation of large scales from small scales. Unlike RANS, LES resolves large scale motions of the turbulent flow, producing more accurate results. However, unlike DNS, LES does not resolve small scales of the flow (also called the subgrid scales). It resorts to subgrid models to account for turbulent motions below a cutoff length. The first topic to be covered will be the technique that LES uses to separate the large and small scales; this technique will be applied to the governing equations, and a discussion will follow of the subgrid turbulence model. In the discussion that follows, complexities such as variable fluid properties, chemical reactions, or other multiphysics will be ignored.

2.1 Filtering: Separation of Scales

Filtering is a technique to reduce the fluctuation in a quantity. In the case of turbulence, the fluctuations (random noise) in some quantity of interest $Z$ are due to the small-scale turbulence. Hence, filtering separates the bulk motions of the large scales from the fluctuations due to the small scales. In spectral space, components of $Z$ greater than a specific cut-off frequency are truncated. In physical space, this corresponds to a weighted averaging over a given volume. The parameter controlling how much of $Z$ is truncated (and thus modeled) is the filter width $\Delta$. It is one of the most important parameters in an LES model, as it affects almost every aspect of the simulation. The wider a filter is, the more information is truncated. As the filter grows to an infinite width, every scale of motion is modeled, because every fluctuation is filtered out (this is analogous to, but not the same as, RANS; it will be shown that decomposition of $Z$ in LES is not the same as the decomposition of $Z$ in RANS). As the filter width shrinks to zero, no motions are modeled (this is the same as DNS). Figure 1 illustrates the effect of the filter width.

2.1.1 Spatial Filtering

There are several different types of filtering; the type of filtering used in an LES simulation depends largely on the flow. Spatial filtering is the conventional approach to filters in large eddy simulation [10] [14] [4] [12] [13]. The spatial filtering operation, as defined by Leonard [6], is:

![Figure 1: A plot of experimental velocity vs. time data for a buoyant helium plume (blue) [17] plotted with the same data filtered using various filter widths $\Delta$.](image-url)
The function \( G \) is called the \textit{filter function}, also called the \textit{filter kernel}. To represent the filtered property \( Z \) in spectral space, suppose that \( Z \) has the Fourier transform:

\[
\hat{Z}(\kappa) = \mathfrak{F} (Z(x))
\]

Then the filtered property \( \hat{Z} \) in spectral space can be written as:

\[
\hat{Z}(\kappa) = \hat{G}(\kappa) \hat{U}(\kappa)
\]

where

\[
\hat{G}(\kappa) = 2\pi \mathfrak{F} (G(x))
\]

There are several common filter functions; these include:

- Gaussian filter, which has the same second moment as a Gaussian bell curve;
- Top-hat or box filter, which looks like a box in physical space (but in spectral space looks like a Gaussian with a sinusoid at either end; and
- Sharp spectral filter, which looks like a Gaussian with a sinusoid at either end in physical space but is a step function in spectral space (i.e. any wave numbers above a cutoff wave number are completely truncated, and any wave numbers below the cutoff wave number are not damped or modified at all)

These functions are given in Table 2.1.1, which is a reproduction in part of Table 13.2 from [10].

Table 2: Some common filter functions in physical and spectral space; table reproduced from [10].

<table>
<thead>
<tr>
<th>Name</th>
<th>Filter function</th>
<th>Transfer function</th>
</tr>
</thead>
<tbody>
<tr>
<td>General</td>
<td>( G(r) )</td>
<td>( \hat{G}(\kappa) = \int_{-\infty}^{\infty} e^{-i\kappa r} G(r) dr )</td>
</tr>
<tr>
<td>Box</td>
<td>( \frac{1}{\Delta} ) ( H \left( \frac{1}{2} \Delta -</td>
<td>r</td>
</tr>
<tr>
<td>Gaussian</td>
<td>( \left( \frac{6}{\pi \Delta^2} \right)^{\frac{3}{4}} ) ( \exp \left( -6 \frac{r^2}{\Delta^2} \right) ) ( \exp \left( -\frac{\kappa^2 \Delta^2}{24} \right) )</td>
<td></td>
</tr>
<tr>
<td>Sharp Spectral</td>
<td>( \frac{\sin \left( \frac{\pi r}{\Delta} \right)}{\pi r} )</td>
<td>( H (\kappa_C -</td>
</tr>
</tbody>
</table>

2.1.2 Temporal Filtering

It was mentioned earlier that spatial filtering is the most common type of filtering. There is another type of filtering, temporal filtering, that will be discussed because it addresses some important issues with spatial filtering, although it is not as common. Temporal filtering provides a more natural link between RANS and LES. It also provides a significant advantage in data analysis. Frisch, in his book on turbulence, stated, “Most experimental data on
fully developed turbulence are obtained in the time domain and then recast into the space domain via the Taylor hypothesis” [2]. Using time-filtering eliminates the need to recast the data into a spatial domain. There are several other additional advantages to using a temporal filter [12]. Superficially, temporal filtering looks the same as spatial filtering. A property $Z$ that is time filtered is defined as:

$$\bar{Z}(t) = \int_{-\infty}^{t} f(t')G(t' - t)dt'$$  \hspace{1cm} (2.5)

This has the same form as (2.1). However, upon further investigation, one discovers that the individual terms in the time-filtered governing equations are not Galilean-invariant (that is, the values of the terms will change based on the frame of reference). Several different approaches have been taken to circumvent this, including casting the temporal filter in a Lagrangian frame of reference [7] and in an Eulerian frame of reference [12]. The terms in the spatially filtered governing equations, in contrast, are naturally Galilean-invariant [16].

For the sake of brevity, the following sections will discuss filters only in the context of spatial filters. This is done primarily due to convention in the approach to filters in large eddy simulation, but also because it will bypass problems stemming from the Galilean invariance of temporally-filtered governing equations. For a more detailed treatment of time filters, see [12] and [13].

### 2.2 Filtered Navier Stokes Equations

At this point, the concept of filtering can be applied to the velocity field, and the velocity can be decomposed into its filtered and residual parts:

$$u_i = \bar{u}_i + u'_i$$  \hspace{1cm} (2.6)

where $\bar{u}_i$ is the filtered part of the velocity and $u'_i$ is the residual (or subgrid) part. In RANS the Reynolds decomposition of the velocity (1.16) was applied to the Navier Stokes equations to yield the Reynolds-averaged Navier Stokes equations (1.17); similarly the decomposition of the velocity into its filtered and residual parts is now applied to the Navier Stokes equations. This yields:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + v \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} (2.7)

It should be recognized that the non-linear $\bar{u}_i u_j$ term is not the same as $\bar{u}_i \bar{u}_j$. In order to put $\bar{u}_i u_j$ in terms of the filtered velocities, the decomposed velocity $\bar{u}_i + u'_i$ is substituted into the term to get:

$$\bar{u}_i u_j = (\bar{u}_i + u'_i) (\bar{u}_j + u'_j)$$

$$= (\bar{u}_i \bar{u}_j) + (\bar{u}_i u'_j) + (u'_i \bar{u}_j) + (u'_i u'_j)$$  \hspace{1cm} (2.8)

Two primary approaches can be taken to combine this result with (2.7). The first approach, of [6], puts everything in terms of the filtered variables:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + v \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} (2.9)

where $\tau_{ij}$ is an additional term representing the small scale, subgrid turbulence, and (for this approach) it is:
\[
\tau_{ij} = \left( u_i' u_j' \right) + \frac{1}{R_{ij}} \left( u_i u_j' + u_i' u_j \right) + \frac{1}{L_{ij}} \left( u_i \bar{u}_j - \bar{u}_i u_j \right)
\]

(2.10)

where the Reynolds subgrid stress tensor \( R_{ij} \) represents interactions of residual scales with other residual scales, the cross-strain stress tensor \( C_{ij} \) represents cross-strains between the large and small scales, and the Leonard tensor \( L_{ij} \) represents strain due to interactions among the large scales. Using this approach to split up the non-linear term, the Navier Stokes equations become:

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (u_i' u_j')
\]

(2.11)

However, one issue with this approach is that \( u_i u_j \) requires a grid twice as fine in the \( i \) and \( j \) directions as the grid for \( \bar{u}_i \). This issue is resolved by using the second approach: leaving the double-filtered term \( \bar{u}_i \bar{u}_j \) in the non-linear term and getting a slightly different form of the Navier Stokes equation.

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (u_i' u_j')
\]

(2.12)

Note that (2.11) and (2.12) look very similar to (1.17). They are very different, however, and it is extremely important to understand and recognize the differences. Reynolds decomposition decomposes velocity into a time-averaged and a time-fluctuating component, and the average of this fluctuating component is zero. Conversely, large eddy simulation decomposes velocity into its filtered and subgrid parts - the filtered part is not an average, but rather the motions of the fluid that are representative of the large-scale motions (the low frequencies in the energy spectrum). Furthermore, a filtered residual is not equal to zero - that is, \( u_j' \neq 0 \).

The last term in (2.11) and (2.12) is called the subgrid stress tensor. While it looks very similar to the Reynolds stress tensor in (1.17), it represents only the subgrid scale turbulence – the rest of the turbulence (the large-scale turbulence) is resolved. Because the small scale turbulence is not resolved, it must be modeled; common subgrid models are the subject of 2.3.

### 2.3 Subgrid Model

*The energy cascade is then viewed solely as an energy loss of the large-scales due to an artificial viscosity arising from subgrid-scale motions.*


Leonard alludes to the most common and the most immediately obvious method of modeling the subgrid scale turbulence – an eddy viscosity model. (1.18) can be used as the proposed viscosity model, replacing \( \nu_t \) with \( \nu_{sgs} \).

Using scale analysis, the subgrid scale viscosity can be expressed as

\[
\nu_{sgs} \sim \frac{l_0}{t_0}
\]

(2.13)

Thus, the closure problem now lies in finding \( l_0 \) and \( t_0 \). Models resolving the closure problem of the subgrid viscosity can be classified in three groups [14]:

1. Models using global characteristics of the resolved scales. Assumptions must be made in order to obtain the global characteristics of the resolved scales used in these models.
2. Models using characteristics of the region near the cutoff frequency $\kappa_c$, where the resolved scales interact with the subgrid scales. Generally, these models are more accurate than models using global characteristics because they are based on more relevant local information.

3. Models for quantities specific to the subgrid scales, such as the subgrid scale kinetic energy. These are more accurate than either of the former because no assumptions must be made about the interaction between the resolved scales and the subgrid scales.

Several subgrid models will be presented in the context of these categories. The Smagorinsky model, first proposed by Smagorinsky in an epic 1962 paper [15], is still the most common subgrid model in use; it falls into the first category. Several other models, including the dynamic Smagorinsky model and a one-equation model for the subgrid kinetic energy $k_{sgs}$, will be discussed in the context of the three classifications above.

2.3.1 Smagorinsky Subgrid Model

The Smagorinsky subgrid model was first proposed by Smagorinsky in 1962 [15], though it was formulated in a significantly different way than is presented here. The model proposes an eddy viscosity for (1.18) in the form:

$$v_{sgs} = (C_s \Delta)^2 \mathcal{S}$$

$$= (C_s \Delta)^2 (2\mathcal{S}_{ij}\mathcal{S}_{ij})^2$$

where $C_s$ is the Smagorinsky constant, $\Delta$ is the filter width, and $\mathcal{S}$ is the characteristic filtered rate of strain. The filtered rate of strain $\mathcal{S}_{ij}$ is defined in a manner analogous to (1.23):

$$\mathcal{S}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

The derivation of this form is given in detail by Sagaut [14]. The Kolmogorov local isotropy hypothesis is applied (see Section 1.2.2), as is the Kolmogorov form of the energy spectrum (given in Section 1.2.3). In addition, it is assumed that the energy cascade is a continuous process that does not change with time – in other words, there is no accumulation of energy at any scale. Sagaut [14] calls this the “local equilibrium hypothesis”. Thus, a global average dissipation rate of kinetic energy $\langle \varepsilon \rangle$ (which is constant at every point in the flow) can be combined with the characteristic cutoff filter width $\Delta$, which is the physical space analog to a cutoff frequency $\kappa_c$ in spectral space, in a scaling analysis to yield:

$$v_{sgs} \sim \langle \varepsilon \rangle^{\frac{1}{3}} (\Delta)^{\frac{4}{3}}$$

At this point it is clear why the Smagorinsky subgrid model falls into the first category above - it depends on the global properties of the flow through the global dissipation rate of kinetic energy $\langle \varepsilon \rangle$. The local equilibrium hypothesis must be made in order to obtain the subgrid turbulent viscosity (2.14). The local equilibrium hypothesis, however, is only reasonable for isotropic homogeneous turbulence, since it is the only type of turbulence that lends itself to a theoretical analysis.

Sagaut [9] lists several reasons why the Smagorinsky model is unsuccessful; these reasons include:

- The ratio of $L/\Delta$ is too low for the theory behind the Smagorinsky model to apply.
- The Smagorinsky coefficient is not constant, but depends on the ratio $\Delta/\eta$, which changes locally.
2.3.2 Dynamic Smagorinsky Subgrid Model

In 1991, Germano [3] proposed a dynamic eddy viscosity model, in which the Smagorinsky constant $C_s$ is a function of position and time. His new methodology was to use two filter functions, a grid filter function $G$ and a coarser (i.e. wider filter width) test filter function $\tilde{G}$, which yields the overall filter function $\tilde{G}$. First, the grid filter is applied to the Navier Stokes equations to yield (2.11). Next, the test filter is applied to yield:

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}(T_{ij})$$  \hfill (2.18)

where the residual stress tensor $T_{ij}$ is:

$$T_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j$$  \hfill (2.19)

Using these expressions, after some manipulation the expression for the dynamic Smagorinsky constant is given as:

$$C_s(y,t)^2 = -\frac{1}{2} \left( \frac{<L_{kl}S_{kl}>}{\Delta^2 <|S|S_{mn}S_{mn}> - \Delta^2 <|S|S_{pq}S_{pq}>} \right)$$  \hfill (2.20)

where $L$ relates the resolved turbulent stress $L_{ij}$, which is the same as in (2.10) and can be calculated explicitly, to the subgrid-scale stresses at the test and grid scales, $T_{ij}$ and $\tau_{ij}$. Now, using (1.18) and (2.14), the subgrid stress tensor becomes:

$$\tau_{ij}^d = -\left( \frac{<L_{kl}S_{kl}>}{\left( \Delta \right)^2 <|S|S_{mn}S_{mn}> - <|S|S_{pq}S_{pq}>} \right) S$$  \hfill (2.21)

The method was tested against DNS data for two cases a priori, and was then implemented in LES simulations of the same cases. The authors saw better agreement with experimental data in the LES simulation using the dynamic Smagorinsky model than in the a priori analysis of DNS data.

2.3.3 Structure Function Model

A different subgrid model that fits into the second category given above is the structure function model [8]. It differs from models of type 1 in that it does not depend on global properties of the flow, but instead depends only on the rate of kinetic energy dissipation at the specific cutoff length scale (or, in this formulation, the cutoff wavelength $\kappa_c$). The kinetic energy at the cutoff frequency $E(\kappa)$ is evaluated using the structure function of the velocity field (see Appendix G in [10]), which is used to calculate the dissipation (a term in an assumed energy spectrum). The expression for the subgrid viscosity, as derived in [14], becomes:

$$\nu_{sgs} (x, \Lambda, t) = 0.105 \Delta \sqrt{F_2 (x, \Lambda, t)}$$  \hfill (2.22)

where $F_2 (x, \Lambda, t)$ is the part of the velocity structure function calculated only from the resolved scales. This model, unlike the Smagorinsky model, depends on the spatial location $x$ and on time. However, it runs into a problem in that the spatial information is local, but the frequency information is not – so the evaluation of the energy at
the cutoff frequency may be inaccurate for the same reasons the Smagorinsky model is inaccurate due to the local isotropy hypothesis – the model will not account for variations in the energy spectrum.

2.3.4 One-Equation Subgrid Kinetic Energy Model

The third type of subgrid model, based on quantities specific to the subgrid scales, can be considered analogous to the two-equation RANS models. It is a one-equation model for the subgrid kinetic energy, $k_{sgs}$. The subgrid model of Yoshizawa [20] is a common one-equation subgrid model. The equation for the subgrid kinetic energy (from [20] and [1]) is given as:

$$\frac{\partial k_{sgs}}{\partial t} + \frac{\partial}{\partial x_j} \left( u_j k_{sgs} \right) = \frac{\partial}{\partial x_j} \left[ (u + v_{sgs}) \frac{\partial k_{sgs}}{\partial x_j} \right] + P_{k_{sgs}} - C_\epsilon \frac{k_{sgs}^2}{\Delta} P_{k_{sgs}} = 2v_{sgs} \mathcal{S}_{ij} \mathcal{S}_{ij} \tag{2.23}$$

These quantities are then used to calculate the subgrid viscosity:

$$v_{sgs} = C_k \Delta k_{sgs} \tag{2.24}$$

Compared to the Smagorinsky and structure function models, the one-equation subgrid kinetic energy model gives a much better representation of the subgrid scales. The way (2.23) is obtained is analogous to the way the kinetic energy equation is obtained for the $k-\omega$ or $k-\epsilon$ models. First, the filtered momentum equation (for large scales) is subtracted from the unfiltered momentum equation, which yields the subgrid scale momentum equation (in terms of $u'_i$). This equation is then multiplied by $u'_i$ to yield the subgrid kinetic energy equation (equation 3.33 in [14]). Several terms are then modeled, which leads to (2.23).

3 LES Parameter Study

Part of the present work was a parameter study of a large eddy simulation of a buoyant, non-reacting, turbulent helium plume run in Star CCM+, a commercial CFD software package. Several simulations were run, each with a different model parameter changed from its default value. A case matrix is shown in 3. To induce an effect on the simulations, the values of each constant were changed by at least 75%. A discussion of the a priori expectations of the parameter effects will be saved until the simulation and experimental geometries and boundary conditions have been described.

<table>
<thead>
<tr>
<th>Case</th>
<th>Van Driest damping coeff.</th>
<th>$C_t$</th>
<th>Pseudo-turbulence spectrum size</th>
<th>$C_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1 (Base Case)</td>
<td>25</td>
<td>30</td>
<td>100</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 2</td>
<td>1</td>
<td>30</td>
<td>100</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 3</td>
<td>25</td>
<td>10</td>
<td>100</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 4</td>
<td>25</td>
<td>50</td>
<td>100</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 5</td>
<td>25</td>
<td>30</td>
<td>350</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 6</td>
<td>25</td>
<td>30</td>
<td>30</td>
<td>0.17</td>
</tr>
<tr>
<td>Case 7</td>
<td>25</td>
<td>30</td>
<td>100</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Case 1 was the default or base case - it was run using only the default values for the LES parameters. Subsequent cases adjusted a single parameter value.
The Van Driest damping function coefficient, part of the Van Driest damping function, affects the selection of the filter width by the LES solver in Star CCM+. The filter width is calculated as:

\[
\Delta = f_v C_s V^{1/3}
\]

where \(C_s\) is the Smagorinsky constant, \(V\) is the cell volume, and \(f_v\) is the Van Driest damping function, defined as:

\[
f_v = 1 - \exp \left( \frac{y^+}{A} \right)
\]

\(A\) is the Van Driest damping coefficient (the parameter being varied for case 2), and \(y^+\) is the dimensionless distance from the wall:

\[
y^+ = \frac{u^* d}{\nu}
\]

\(u^*\) is the friction velocity from the instantaneous wall shear stress at the nearest wall face, \(d\) is the distance from the wall, and \(\nu\) is the kinematic viscosity.

\(C_t\) is the time constant, used to calculate a subgrid time scale. The time scale is computed as:

\[
T = \frac{C_t}{S}
\]

where \(S\) is the characteristic filtered rate of strain as defined in (2.14).

The pseudo-turbulence spectrum is a set of random numbers used to define an inlet or initial condition for large eddy simulation. Each number in the spectrum is used to construct an initial velocity field.

3.1 Setup

3.1.1 Experimental Setup

The experimental data for the buoyant helium plume were taken at the Fire Laboratory for Accreditation of Models by Experimentation (FLAME) lab at Sandia National Labs. The data were gathered using a pulsed UV laser to allow for measurement of optical scattering of light by acetone particles that were seeded into the flow. A high-speed camera took pictures that were then analyzed using particle image velocimetry (PIV) interrogation software called Sleuth. The experimental setup for the Sandia case is shown in Figure 2. The helium plume inlet is 1 meter in diameter, elevated 2.45 meters off the floor. There is a 0.51 meter sheet of steel surrounding the inlet so that air entrained into the helium plume is entrained radially. The helium passes through 2 layers of steel honeycomb before leaving the inlet to ensure a uniform velocity profile. The entering velocity profile is uniform to within 6%. The entering helium is at 294 K, and is composed of 96.4% helium, 1.9% oxygen, and 1.7% acetone. The entering velocity is 0.325 m/s [18].

3.1.2 Simulation Setup

The simulation of the buoyant turbulent helium plume was run in CD Adapco’s Star CCM+ CFD software. The simulation was an unsteady-state large eddy simulation model. The computational domain was 3 meters cubed, with a 1 meter inlet that was 100 mm off the ground. An unstructured computational mesh was used. Instantaneous velocity data was gathered at four points along the centerline. The points were 200 mm, 400 mm, 505 mm, and 600 mm above the inlet. The domain and the location of each of these points is depicted in Figure 4. The boundary conditions used for the simulation were periodic for each wall, a pressure outlet for the top, and a wall at the bottom.
Figure 2: A diagram of the experimental setup for the Sandia FLAME lab, where the velocity data on the turbulent buoyant helium plume was gathered [17].

Figure 3: A cross-sectional view of the unstructured mesh used in the computation.
The inlet velocity of the helium was $0.351 \, \text{m/s}$. The system was treated as an ideal gas, and the simulation was isothermal at 300 K. The entering gas was 100% helium, and the computational domain was initially 100% air. The Navier Stokes equations were solved implicitly. For the large eddy simulation model in Star CCM+, the only subgrid model available was the Smagorinsky model.

### 3.2 Expectations

Based on a thorough analysis of the Smagorinsky subgrid model, I found several recommended values for the Smagorinsky constant. They ranged from 0.10 to 0.20, with most recommended values being closer to 0.20. Many sources mentioned that the Smagorinsky model consistently overpredicts the energy dissipation [14] [9] [3]. My expectation was that the Smagorinsky constant value of 0.17 would fit the experimental data better than the Smagorinsky constant value of 0.05, since the 0.05 value was not within the recommended range of values. Also, I expected that the energy spectrum of the case with $C_s = 0.17$ would look different than the energy spectrum for $C_s = 0.05$. Because the subgrid constant would be smaller, the modeled subgrid stresses would also be smaller, which would cause fewer small scale fluctuations. This would decrease the amount of kinetic energy being removed from the large scales, so the slope of the inertial range would be smaller.

A larger or smaller filter width would also impact the simulation results, so changing a parameter that affects the filter width should have a direct impact on the simulation results. The Smagorinsky constant does affect the filter width – if the constant is larger (the default value), the filter width will be wider. This makes sense, and corresponds to an increase in the "importance" of the subgrid model. On the other hand, a decrease in the Smagorinsky constant will decrease the filter width, and make the subgrid model less important because fewer length scales are being modeled and more are being resolved.

### 3.3 Results and Discussion

Figure 5 shows the plots of velocity vs. time for case 1 and for the Sandia data at each height (200 mm, 400 mm, 505 mm, and 600 mm). There is clearly good agreement in the puffing frequencies between the simulation and the experimental data. However, the velocity magnitude of case 1 (and of all cases) is off by a significant amount. This is likely due to discrepancies between the boundaries of the simulation and the boundaries of the simulation.

The initial suspicion was that the helium plume was not spreading fast enough because the 3 meter domain was not large enough (the experimental domain was roughly 6 meters by 6 meters). A second simulation was run on a 6 meter by 6 meter domain, still 3 meters high, under the exact same conditions. The results of this simulation are plotted with the experimental data in 7 (simulation data at 400 mm, 505 mm, and 600 mm above the inlet along the centerline; due to an error in the simulation setup, no data was gathered at the point 200 mm above the inlet). It is evident from the figure that a larger domain did not resolve the problem.

The issue is likely related to the air inlet in the Sandia experimental setup - there is a flowrate of air entrained radially into the helium plume in the FLAME lab setup which is not replicated in the simulation. Also, the $0.25 \, \text{m/s}$ discrepancy in the inlet velocities, while minor, could snowball into a much larger velocity magnitude difference as
the helium is accelerated upward due to buoyancy. Finally, although extremely slight, the density differences between the experimental setup (96% helium, 1.9% air, and 1.7% acetone at 294 K) and the simulation (100% helium at 300 K, density calculated using the ideal gas law) could also contribute to the higher acceleration of the helium plume in the simulation.

The velocity plots of all seven cases at a height of 200 mm superimposed are show in Figure 8. It is clear from the figure that none of the parameters had any significant impact on the velocity profile after 200 mm. The same plot at 600 mm above the centerline (Figure 9) shows that many parameters changed had no effect even after 600 mm. However, there are two cases that stand out in particular. The first is case 7, for which the Smagorinsky constant was changed from 0.17 to 0.05. The second is case 2, for which the Van Driest damping function coefficient was changed.

The simulation data for case 1 ($C_s = 0.17$) and case 7 ($C_s = 0.05$) are plotted in Figs. 12 and 13. It is clear from these plots that the effect of changing the Smagorinsky constant to a value that is half of the very lowest recommended value in literature had almost no effect on the velocity profile, even at a height of 400 mm and 600 mm. The simulation data for case 1 ($A = 25$) and case 2 ($A = 1$), plotted in Figures 10 and 11, again show results that are not expected. The distance from the cell to the wall, in the case of the helium plume, is 1.5 meters – so $u^*$ in (3.2) should be zero, the Van Driest damping function should be 1 regardless of the value of A, and the velocity profile should look the exact same as for case 1. But as the figures show, there are some noticeable, albeit slight, differences between the velocity profiles.
3.4 Concluding Remarks

The primary conclusion from the parameter study was that the LES model in Star CCM+ did not behave as expected. While it yielded sensible results that matched the puffing frequency of the experimental data well, changing most of the parameters had no effect on the simulation results. The effect was only significant for two cases, and the effect the parameter change had for those two cases was not what was expected. Even after an in-depth analysis into the theory behind large eddy simulation, there was little clarity in the parameter study. This may be due in part to a lack of experience in analyzing simulation results, but is largely due to the lack of transparency in the LES model implemented. Further study would be warranted to gain any insight as to why these parameters did not have the effect expected.

The present work has presented turbulence concepts important to understanding large eddy simulation. It has presented a brief introduction to large eddy simulation, touching on many subjects but also leaving many more totally unexplored. Several subgrid models were analyzed, and optimally the results of the parameter study would have allowed an analysis of the primary weakness of the Smagorinsky subgrid model - that the Smagorinsky constant is not, in fact, constant. However, the results of the parameter study were not what was expected. It is a useful conclusion nonetheless, as it demonstrates, once again, that commercial CFD software is a double-edged sword; it can give sensible and useful answers, but if the user does not understand the model, those results are generally worthless (see Figure 6).

![Comic Strip](image)

Figure 6: Figure describing the general attitude of many of today’s commercial CFD software users.
Figure 7: A plot of velocity vs. time for case 1 run on a small domain and a large domain, along with the data from Sandia.

Figure 8: Velocity vs. time data for all 7 cases at a height of 200 mm above the inlet along the centerline.
Figure 9: Velocity vs. time data for all 7 cases at a height of 600 mm above the inlet along the centerline.

Figure 10: Velocity vs. time data for two simulations, case 1 and case 2, at heights of 400 mm (top) and 600 mm (bottom) above the inlet.
Figure 11: Velocity vs. time data for two simulations, case 1 and case 2, along with Sandia data, at heights of 400 mm (top) and 600 mm (bottom) above the inlet.

Figure 12: Velocity vs. time data for two simulations, case 1 and case 7, at heights of 400 mm (top) and 600 mm (bottom) above the inlet.
Figure 13: Velocity vs. time data for two simulations, case 1 and case 7, along with Sandia data, at heights of 400 mm (top) and 600 mm (bottom) above the inlet.
References


