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RESIDUAL STRESS MODELS FOR LARGE EDDY SIMULATION OF STRATIFIED TURBULENT FLOWS

A Dissertation Presented

by

F. A. V. DE BRAGANÇA ALVES

Submitted to the Graduate School of the University of Massachusetts Amherst in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

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Mechanical and Industrial Engineering
DEDICATION

Ad maiorem Dei gloriam.
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Pursuing a Ph.D. in a foreign country can be especially difficult. Luckily, I was blessed with the company of many friends that made Amherst feel like home. Karl and Melanie; Pedro and Elaine; Fabrício and Gabriela; Brenno and Priscilla; Brunno, Juliana and Santiago; Camila and Maurício; Kunal and Poonam; Leandro and Camila; Carlos and Leidiane; Sara and Bernardo; all the folks at North Village and many others provided much-needed fun and light-hearted times during these demanding years. I’d also like to thank my brothers, Augusto and Fernando, and also my good friends, Diogo and Renata, for taking the time and trouble of visiting me in this Godforsaken town (I’m joking. Amherst is a nice town).

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I’ll be forever grateful to my amazing wife, Nur. It brings me to tears to think about all the work and sacrifices she has done for me and our family. This thesis would not have existed without her. I truly feel this work is as much hers as it is mine. I wish to spend the rest of my life serving you and our family. I’d also like to thank my little monsters, Maria and Cecília, for all the joy and trouble they bring me.
The residual stresses and scalar fluxes are required to close the momentum and scalar transport equations in simulations of turbulence that are not fully resolved in space. In stratified turbulence, the stress and fluxes are statistically anisotropic unless the smallest resolved length scale is smaller than the Ozmidov scale and the buoyancy Reynolds number is sufficiently high for there to exist a range of scales that is statistically isotropic. In this work, a tensorial basis set is derived analytically that potentially contains sufficient information about the anisotropic interaction between resolved and residual scales. The residual stress tensor is evaluated by filtering data from direct numerical simulations of homogeneous stratified turbulence, with unity Prandtl number, resolved on up to $8192 \times 8192 \times 4096$ grid points along with an isotropic homogeneous case resolved on $8192^3$ grid points. Five approximations for the residual stress tensor are derived by projecting the tensor onto different tensorial
basis sets. It is found that an approximation for the residual stress which is based on a combination of the rate-of-strain and a tensor related to energy redistribution is a very good starting point for models involving just two coefficients. An extension for eddy viscosity models based on a non-linear tensor is proposed and tested on flow cases with different levels of density stratification. Different eddy viscosity models are mixed with the proposed extension on LES simulations. Results confirm the inability of pure eddy viscosity models to produce the expected anisotropy. It is shown that the proposed extension improves results in all cases, especially the correct reproduction of anisotropy.
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Chapter 1
Introduction

An assumption common in many approaches to numerical simulations of turbulent flows is that it is important to compute directly the dynamics at the larger scales in length and time whereas the smaller scales are more amenable to modeling. This assumption is explicit in large eddy simulations (LES), but it underpins a wide variety of turbulence models (e.g. Kerstein, 1988; Travin et al., 2000; Martell & Perot, 2012). Sometimes the details of the modeled scales are important, such as in reacting flows, but often the primary interest is in the effects of the modeled dynamics on the larger scales. These effects are represented by the ‘residual’ stresses and fluxes, which we define formally in §2. Our purpose in this work is to model these quantities in turbulence strongly affected by a stabilizing buoyancy force, which is sometimes called ‘stratified turbulence.’

The term stratified turbulence was first applied by Lilly (1983) to flows dominated by stable density stratification. It is studied because of its potential applicability to atmospheric and oceanic flows (Riley & Lindborg, 2008). The importance of the concept of residual stresses in simulating geophysical turbulence is reflected in the fact that some of the earliest progress in large eddy simulations was made by atmospheric scientists (Smagorinsky, 1963; Lilly, 1967; Deardorff, 1970). In general, geophysical turbulent flows consist of internal waves as well as random motions possessing potential vorticity characteristic of turbulence. Our scope here is limited to turbulence dynamics.
An important tool for studying residual stresses is direct numerical simulation (DNS). In DNS, all the dynamically relevant scales of motion are resolved and so no models are required. The earliest direct numerical simulation (DNS) of stratified turbulence was by Riley et al. (1981). Since then, DNS has been used extensively to understand stratified turbulence (e.g. Riley & de Bruyn Kops, 2003; Hebert & de Bruyn Kops, 2006b,a; Almalkie & de Bruyn Kops, 2012b; Bartello & Tobias, 2013; Watanabe et al., 2016; Maffioli & Davidson, 2016), as well as high-resolution simulations that are not fully resolved but rely on filtering or a hyper-viscous term to remove the smallest scales (e.g. Diamessis et al., 2005; Lindborg, 2006; Kimura & Herring, 2012). Laboratory experiments and theoretical work have contributed also to our understanding of stratified turbulence (e.g. Lin & Pao, 1979; Spedding et al., 1996; Praud et al., 2005; Meyer & Linden, 2014; Olsthoorn & Dalziel, 2015).

The recent review of stratified turbulence by Riley & Lindborg (2012) reports several characteristics of this flow regime that are particularly relevant to residual stresses and fluxes. In particular, stratification suppresses vertical motion and, with it, some of the vortex stretching that leads to the net downscale transfer of energy on which many turbulence models are predicated. Even in the absence of mean shear, though, local vertical shearing of horizontal motions occurs spontaneously and results in down scale transfer via, e.g., Kelvin-Helmholtz instabilities. So the turbulence is three-dimensional, but highly anisotropic, even at small scales in some conditions potentially relevant to geophysical flows (de Bruyn Kops, 2015).

The importance of understanding residual stresses and fluxes in stratified turbulence depends on the length scale at which modeled simulations will be resolved. As reviewed by Riley & Lindborg (2012), it is sometimes assumed that stratified turbulence occurs with a broad range of turbulence length scales that are not directly affected by buoyancy. Implicit in this assumption is the thought that motions at length scales below the Ozmidov length scale $L_o$ are not affected by buoyancy and, if
there is sufficient scale separation between \( L_o \) and Kolmogorov length scale \( L_k \), then a classical inertial range can exist.

The scale separation between the \( L_o \) and \( L_k \) is characterized by the buoyancy Reynolds number, \( Re_b \) (Gibson, 1980; Gargett et al., 1984), which is also called the activity parameter. In direct numerical simulations with \( Re_b = O(100) \), classical turbulence scaling is not observed (de Bruyn Kops, 2015). More specifically, the kinetic energy spectrum may scale with \( \kappa^{-5/3} \), with \( \kappa \) the wave number, but the corresponding \( 2/3 \) scaling of the second order structure function, and \( 4/5 \) scaling of the third order structure function, are not observed. Therefore, it is not appropriate to justify a model for the residual stresses with the argument that the turbulence will be always approximately isotropic and homogeneous at scales below \( L_o \), although this may be the case when \( Re_b \) is sufficiently high. Note that \( Re_b \) is the order of 100 or less in many regions of the ocean (Jackson & Rehmann, 2014).

For sufficiently low \( Re_b \), characteristics of the flow at scales smaller than \( L_o \) likely require no modeling. Lalescu et al. (2013) show for unstratified turbulence that turbulent motions at scales smaller than 20 times the Kolmogorov length scale \( L_k \) are slaved to the chaotic motions of the larger scales. \( L_o/L_k = 20 \) corresponds to \( Re_b \approx 50 \). Indeed, Watanabe et al. (2016) show that wake simulations with \( Re_b \approx 50 \) and grid resolution about equal to \( L_o \) are accurate, when compared with fully resolved DNS, with no modeling of the residual scales other than a filter to maintain stability.

So if \( L_o \) is in the top of the dissipation range, that is, within a factor of 20 of \( L_k \), then modeling the residual stresses and fluxes in a simulation with resolution equal to \( L_o \) presents no problems. At the same time, a simulation with such resolution may not provide the reduction in computational expense typically sought in a modeled simulation. This point is made by Waite (2011), who then goes on to consider length scales larger than \( L_o \) for the grid spacing in simulations of stratified turbulence.
Waite’s starting point is a mechanism by which turbulence can be generated and which, as noted above, is important in stratified turbulence, namely shear instabilities between horizontal layers that spontaneously form, even in the absence of mean shear. These layers were first observed by Lin & Pao (1979), and Lilly (1983) used heuristic arguments to predict that the velocity scale of the energy containing motions will be correlated over horizontal length scale \( L_h \gg U_{rms}/N \) where \( U_{rms} \) is the root mean square (r.m.s) velocity and \( N \) is an appropriately defined buoyancy frequency, which we take here to be the Brunt-Väisälä frequency. Using similarity arguments, Billant & Chomaz (2001) define the vertical length scale of these layers as \( L_v = U/N \), where here \( U \) is the magnitude of the horizontal velocity. Waite (2011) concludes that it is important to resolve the scale \( L_b = 2\pi U_{rms}/N \). While \( L_b \) is a vertical length scale, Waite also concludes that the horizontal grid resolution must also be no greater than \( L_b \) so that the shearing mechanisms are adequately resolved in all directions and that using an anisotropic numerical grid, with finer resolution in the vertical than the horizontal, is not effective. Khani & Waite (2014) and Khani & Waite (2015) consider the Kraichnan and Smagorinsky-Lilly models (Smagorinsky, 1963; Lilly, 1967; Kraichnan, 1976) and conclude that grid spacing \( \Delta \) in all directions between 0.17 \( L_b \) and 0.47\( L_b \), depending on which model is used, is required to capture basic features of stratified turbulence. These tests, however, were made by comparing one modeled simulation to another as no DNS data were available.

As a preliminary analysis, we use DNS results to compute exactly the residual stresses and the residual scalar flux for different filter width to Ozmidov length ratios. Using tensor decompositions theorems we analyze the relationship between the residual stresses and relevant hydrodynamic quantities. We use the results of the analysis to propose a tensorial basis to form LES models that are potentially able to reproduce basic anisotropy behaviour of the flow.
This manuscript is organized as follows. In the next chapter, we introduce the governing equations solved in a Large Eddy simulation and a brief review of typically used models for the residual stress tensor. In Chapter 3 we introduce the tensorial decompositions used in the preliminary analysis. The same decomposition is also used as reasoning basis for proposed LES models. The data base of DNS data used for evaluating the tensorial and vector decompositions is described in Chapter 4, followed by analyses and discussion of the residual stresses and fluxes in the simulated flows. In Chapter 5 we present our strategy to improve existing LES models. The lessons learnt with the preliminary analysis are use to propose the addition of an extra non-linear term to eddy viscosity models. We test different eddy viscosity models with and without the proposed models extension in Large eddy simulation of flows with different level of stratification. Concluding remarks are presented in Chapter 4.10.
CHAPTER 2
LES MODELING

2.1 Mathematical Formulation

2.1.1 Governing equations

The equations of motion for a Boussinesq fluid with Cartesian coordinates \( \mathbf{x} = (x, y, z) \) are as follows:\(^1\)

\[
\begin{align*}
\nabla \cdot \mathbf{u} &= 0 \quad \text{(2.1a)} \\
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}) &= -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 \mathbf{u} + \frac{\rho}{\rho_0} \mathbf{g} \quad \text{(2.1b)} \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= k \nabla^2 \rho - w \frac{\partial \rho_s}{\partial z} \quad . \quad \text{(2.1c)}
\end{align*}
\]

with \( \nu \) the kinematic viscosity, \( w \) the vertical component of the velocity vector \( \mathbf{u} \) and \( \mathbf{g} \) the acceleration antiparallel to the \( z \) axis. The fluid density \( \rho_t \) is split in three terms: the constant reference density \( \rho_0 \), the background density \( \rho_s \) and the fluctuation \( \rho \) so that

\[
\rho_t (x, y, z, t) = \rho_0 + \rho_s (z) + \rho (x, y, z, t) \quad . \quad \text{(2.2)}
\]

Similarly, the pressure term \( p_t \) is decomposed

\[
p_t (x, y, z, t) = p_0 + p_s (z) + p (x, y, z, t) \quad \text{(2.3)}
\]

such that

\[
\frac{dp_s}{dz} = \rho_s g \quad . \quad \text{(2.4)}
\]

\(^1\)Vectors and tensor are represented in bold lower and uppercase letters, respectively. Also, the tensor product is implied by a conjunction of two vectors: \( \mathbf{u} \mathbf{u} \equiv \mathbf{u} \otimes \mathbf{u} = u_i u_j \).
2.1.2 Filtered equations

In this analysis the filtering operator consists of a convolution of a homogeneous isotropic filter kernel $G(r)$ with a field $\varphi$ over the spatial domain $D$:

$$\bar{\varphi}(x,t) = \int_D G(r) \varphi(x-r,t) \, dr \quad . \quad (2.5)$$

The residual of the field $\varphi$ is then defined as

$$\varphi'(x,t) \equiv \varphi(x,t) - \bar{\varphi}(x,t) \quad (2.6)$$

such that

$$\varphi(x,t) = \bar{\varphi}(x,t) + \varphi'(x,t) \quad . \quad (2.7)$$

The filter kernel has a characteristic length $\Delta$ that is roughly the smallest length scale that would be resolved in a numerical simulation in which the residual stresses are modeled. Length scales smaller than $\Delta$ are not resolved. The convolution operator is linear and, if the filter kernel is homogeneous, the filtering operator commutes with spatial derivatives. Applying the filtering operator to the equations of motion leads to

$$\nabla \cdot \bar{\mathbf{u}} = 0 \quad (2.8a)$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot \bar{\mathbf{u}} \bar{\mathbf{u}} = -\frac{1}{\rho_0} \nabla \mathbf{p}^* + \nu \nabla^2 \bar{\mathbf{u}} + \frac{\bar{\rho}}{\rho_0} \mathbf{g} - \nabla \cdot \mathbf{\tau} \quad (2.8b)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}) = k \nabla^2 \bar{\rho} - \bar{w} \frac{\partial \rho_s}{\partial z} - \nabla \cdot \mathbf{f} \quad (2.8c)$$

Here $\mathbf{\tau}$ is the anisotropic part of the residual stress tensor $\mathbf{\tau}^r$, that is,

$$\mathbf{\tau}^r \equiv \bar{\mathbf{u}} \bar{\mathbf{u}} - \bar{\mathbf{u}} \bar{\mathbf{u}} \quad , \quad (2.9)$$

$$\mathbf{\tau} = \mathbf{\tau}^r - \frac{tr(\mathbf{\tau}^r)}{3} \mathbf{I} \quad , \quad (2.10)$$
\[ p^* = \bar{p} + \rho_0 \, tr(\tau) / 3 , \]  

(2.11)

where \( tr(\tau^r) = \tau_{ii} \) is the trace of \( \tau^r \). In the filtered scalar equation, linear background stratification has been assumed and \( f \) is the scalar residual flux

\[ f = \bar{\rho} \bar{u} - \rho \bar{u} . \]  

(2.12)

The filtered equations (2.8) differs from (2.1) by the residual stress tensor \( \tau \) and the flux \( f \), which are the terms that must be modeled in simulations of Boussinesq fluid flow that are not fully resolved.

2.1.3 Kinetic energy

For a Boussinesq fluid, the kinetic energy equation is not independent of the momentum equation. Nevertheless, the equation for filtered kinetic energy provides insight into characteristics of the residual stresses. The filtered kinetic energy per unit mass \( \bar{E} \) can be decomposed as

\[ \bar{E} = E_f + k_r \]  

(2.13)

where the kinetic energy of the filtered velocity is

\[ E_f = \frac{1}{2} \bar{u} \cdot \bar{u} \]  

(2.14)

and the residual kinetic energy \( k_r \) is

\[ k_r \equiv \bar{E} - E_f = -\frac{1}{2} tr(\tau^r) . \]  

(2.15)

The dot product of (2.8b) with \( \bar{u} \) yields the transport equation for \( E_f \):

\[ \frac{D E_f}{D t} + \nabla \cdot \left( \left( \tau + \frac{p^*}{\rho_0} I - 2\nu S \right) \cdot \bar{u} \right) = -P_r - \varepsilon_f + \frac{\bar{m} \bar{g}}{\rho_0} \]  

(2.16)
where $\bar{S}$ is the filtered rate-of-strain tensor and

$$\frac{D(\cdot)}{Dt} = \frac{\partial (\cdot)}{\partial t} + \bar{u} \cdot \nabla (\cdot),$$  \hspace{1cm} (2.17)

$$\mathcal{P}_r = -\tau : \bar{S} = -\tau_{ij} \bar{S}_{ij} \quad \text{and} \quad \varepsilon_f = 2\nu \bar{S} : \bar{S}. \hspace{1cm} (2.18)$$

Here, $\mathcal{P}_r$ is the rate of energy transfer between the filtered and the residual motions and $\varepsilon_f$ is the rate of dissipation of the kinetic energy from the filtered field. The notation for $\mathcal{P}_r$ reflects its interpretation in the transport equation of $k_r$ as the production of residual kinetic energy by the filtered velocity.

In stratified flows the buoyancy force causes the transfer rate to depend on direction, which is inconvenient to analyze in terms of scalar energy. To capture directional information about the transfer from filtered to residual kinetic energy, we compute the tensor product of the velocity vector and the momentum equation to obtain the time evolution of the tensor $E = \bar{u} \bar{u} = \bar{u}_i \bar{u}_j$. The filtered energy is related to $E$ by

$$tr (E') = \sigma_i \sigma_i = 2E_f \hspace{1cm} (2.20)$$

The residual stress tensor will act on the evolution of this energy-like tensor through the term

$$- (\bar{u} (\nabla \cdot \tau) + (\nabla \cdot \tau \bar{u}) = - \left( \bar{u}_k \frac{\partial \tau_{kj}}{\partial x_k} + \frac{\partial \tau_{ki}}{\partial x_k} \bar{u}_j \right), \hspace{1cm} (2.21)$$

which can be split into conservative and dissipative terms

$$- (\bar{u} (\nabla \cdot \tau) + (\nabla \cdot \tau \bar{u}) = \nabla \cdot \mathbf{C} - \mathcal{P} , \hspace{1cm} (2.22)$$
where $C$ is the conservative third order tensor

$$C_{kij} = -\bar{\tau}_{ki}\bar{\tau}_{kj} - \tau_{ki}\bar{\tau}_{kj} \quad (2.23)$$

and

$$\mathcal{P} = -\left( \tau \cdot \nabla \bar{u} + (\nabla \bar{u})^T \cdot \tau \right) \quad (2.24)$$

Where $(\nabla \bar{u})^T$ is the transpose of the filtered velocity gradient $\nabla \bar{u}$.

Next consider the trace of $\mathcal{P}$,

$$tr\left( \mathcal{P} \right) = -\tau_{ij} \frac{\partial \bar{u}_j}{\partial x_i} - \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j}$$

$$= -2\tau_{ij} \bar{S}_{ij} - \tau_{ij} \bar{W}_{ij} + \tau_{ij} \bar{W}_{ij}$$

$$= -2\tau_{ij} \bar{S}_{ij}$$

$$= 2P_r . \quad (2.25)$$

$\bar{W}$ is the filtered rate-of-rotation tensor, which is the anti-symmetric part of the velocity gradient. $P_r$ is the transfer rate from filtered to residual energy by the residual stresses, and is introduced in (2.16) and (2.18). Importantly, $\mathcal{P}$ provides directional information, that is, how energy transfers between the components of $u$.

Of interest is the component of $\mathcal{P}$ that describes redistribution of filtered kinetic energy among the velocity components. To isolate this, we split $\mathcal{P}$ into isotropic and anisotropic parts,

$$\mathcal{P} = \frac{2P_r}{3} I + \mathcal{R} , \quad (2.26)$$

from which

$$\mathcal{R} \equiv \mathcal{P} - \frac{2P_r}{3} I . \quad (2.27)$$

The tensor $\mathcal{R}$ isolates all of the directional information about the energy transfer rates. Although it may appear to quantify the anisotropy of the energy transfer between the filtered and residual scales, no term related to it appears in the energy
budget equation (2.16) because the tensor has a null trace. In fact, this tensor does not transfer any energy between the filtered and residual motions, but redistributes energy among the filtered velocity components. In other words, anisotropic energy transfer from the filtered scales is equivalent to isotropic transfer of the same amount of energy while redistributing energy among the directional components. Therefore, we refer to $\mathcal{R}$ as the ‘energy redistribution tensor.’

2.2 Residual stress modeling

Traditionally, the residual stress tensor is modeled in analogy with the viscous stress tensor:

$$\tau = -2\nu_t(x, t) \overline{S},$$

where the purpose of modeling is to determine $\nu_t$.

The most common modeling for $\nu_t$ is the Smagorinsky-Lilly model (Smagorinsky, 1963; Lilly, 1967):

$$\nu_r = (c_s \Delta)^2 \overline{S},$$

where $c_s$ is a constant and $\overline{S}$ is

$$\overline{S} = \sqrt{2 \overline{S} : \overline{S}}.$$  

The Smagorinsky-Lilly model is known to have a poor correlation with the actual Residual Stress tensor, but its use is acceptable since it has the basic capability of removing energy from the resolved scales at the appropriate mean rate.

Nevertheless, with a single universal constant $c_s$, Smagorinsky-Lilly’s model is unable to predict correctly different turbulent fields in rotating or sheared flows, near solid walls or on transitional flows. To overcome that Germano et al. (1991) proposed a dynamic coefficient $c_s(x, t)$ that can vary locally in the flow. The coefficient is calculated with the aid of a test filter. The test filter operator filters the field with a
filter width $\Delta_t$ larger than the one implied by the LES simulation. Considering ($\tilde{\cdot}$) the test filter operator, eq. (2.8b) can be filtered, leading to:

$$
\frac{\partial \tilde{u}}{\partial t} + \nabla \cdot \tilde{u} \tilde{u} = -\frac{1}{\rho} \nabla \tilde{p}^{*} + \nu \nabla^2 \tilde{u} + \frac{\tilde{p}}{\rho_0} g - \nabla \cdot T
$$

where:

$$
T = \tilde{u} \tilde{u} - \tilde{u} \tilde{u} .
$$

eq. (2.31) is essentially the same as the original LES equation. The tensor $T$ can be decomposed in two parts:

$$
T = L + \tilde{\tau}^r
$$

where

$$
L = \tilde{u} \tilde{u} - \tilde{u} \tilde{u} .
$$

The tensor $L$ can be calculated directly from the filtered velocity field, then, the difference between two unknown tensor can be obtained:

$$
T - \tilde{\tau}^r = L .
$$

When Smagorinsky-Lilly model is used for both the test-filtered and filtered fields the relation becomes:

$$
2c_s \Delta^2 S \tilde{S} - 2c_s \Delta^2 \tilde{S} \tilde{S} = L .
$$

This relation is used to extract the value of $c_s$ locally. To facilitate the calculation of $c_s$, the constant is pulled out from the test filtering of the second term in the left-hand size of the equation:

$$
2c_s M = L
$$

where:

$$
M = \Delta^2 S \tilde{S} - \Delta^2 \tilde{S} \tilde{S} .
$$
Now both $\mathbf{M}$ and $\mathbf{L}$ can be calculated from the filtered velocity field.

Equation 2.37 is an overdetermined system of equations. Originally, Germano et al. (1991) contracted the whole equation with $\mathbf{S}$ to get a scalar equation, but Lilly (1992) proposed using the least squared error method to find the constant. Using the least squared error method leads to the same result as contracting eq. (2.37) with $\mathbf{M}$. Then the coefficient is given by:

$$2c_s = \frac{\mathbf{L} : \mathbf{M}}{\mathbf{M} : \mathbf{M}} = \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}}.$$  \hspace{1cm} (2.39)

Both Germano et al. (1991) and Lilly (1992) reported great variability of the coefficient when calculated through this manner, also, the coefficient can become negative on some locations of the flow, what would characterize kinetic energy backscatter, which potentially led to numerical instability. It is proposed, then, to perform averages to smooth the coefficient variation on space. That is done by making averages in any homogeneous direction of the flow. Finally, the coefficient is calculated by:

$$2c_s = \frac{\langle \mathbf{L} : \mathbf{M} \rangle^*}{\langle \mathbf{M} : \mathbf{M} \rangle^*} = \frac{\langle L_{ij} M_{ij} \rangle^*}{\langle M_{ij} M_{ij} \rangle^*}.$$  \hspace{1cm} (2.40)

The coefficient can still become negative on some locations of the flow and usually on actual LES simulations the coefficient value is clipped to zero on that cases.

The averaging solves the instability problems with the dynamic Smagorinsky models, but this restricts its application to flows with at least one homogeneous direction. Meneveau et al. (1996) developed a model that can be used for inhomogeneous flows. On his method the averaging is done along fluid-particle trajectories. A time average is used for those quantities for each particular Lagrangian particle. Meneveau et al. (1996) shows that, with a proper weight function, the time average can be done through the solution of relaxation transport equations. This model is called as Lagrangian dynamic model.
Several other models based on the eddy-viscosity assumption exists (Schumann, 1975; Porté-Agel et al., 2000; Nicoud & Ducros, 1999; Vreman, 2004) but they all suffer from a poor correlation with the residual stress tensor due to intrinsic misalignment between the filtered strain rate and the residual stress tensor. In order to achieve better representation of the residual stress tensor other functional forms for the residual stress tensor are needed (Clark et al., 1979; Bardina et al., 1980; Kosovic, 1997; Wang & Bergstrom, 2005), usually in mixed form with the eddy-viscosity model, so as to control energy dissipation rate behavior.
CHAPTER 3
MATHEMATICAL FORMULATION

With the equations of motion and filtering notation now defined, we turn to the purely mathematical exercise of decomposing the residual stress tensor into other tensors amenable to physical interpretation and further analyses. In §3.1 the decompositions are exact, as are the decompositions of the energy transfer rates in §2.1.3. In §3.2, approximations to the residual stress tensor are introduced, all of which have corresponding energy transfer rates. Lastly in this section, decompositions and approximations of the flux vector are developed in §3.2.1.

3.1 Tensor decomposition

To analyze the residual stress tensor we use the exact tensorial decomposition technique of Thompson et al. (2010). A tensor $A$ can be decomposed relative to another tensor $B$ into two parts, one orthogonal to $B$ and one coaxial with $B$,

$$A = A^{\parallel B} + A^{\perp B},$$  \hspace{1cm} (3.1)

such that

$$A^{\perp B} : B = A^{\perp B} B_{ij} = 0$$  \hspace{1cm} (3.2)

and

$$A^{\parallel B} : B = A : B.$$  \hspace{1cm} (3.3)

This decomposition is not unique because the coaxial term can assume one of two relationships to $B$:

$$A^{\parallel B}_1 = \alpha B$$  \hspace{1cm} (3.4)
or
\[
A^{//B}_2 = \alpha_0 I + \alpha_1 B + \alpha_2 B^2 .
\]  
(3.5)

The first has a linear relationship to the target tensor \( B \) so that calculating this decomposition is only a matter of finding the scalar \( \alpha \). The second is a full power-series-like expansion of \( A \) on \( B \), which, by the Cayley-Hamilton theorem, will have terms up to power two only.

The coaxial part of (3.1) in terms of \( A^{//B}_1 \) is
\[
A^{//B}_1 = \left( \frac{A : B}{B : B} \right) B .
\]  
(3.6)

For the second decomposition of (3.1), the coaxial part is obtained by extracting the diagonal elements of tensor \( B \) when written on a vector basis formed by the eigenvectors of \( A \). This operation is mathematically formalized in Thompson (2008) through a fourth order tensor \( \mathcal{L} \):
\[
A^{//B}_2 = \mathcal{L} : B = \mathcal{L}_{ijkl} B_{kl}
\]  
(3.7)

where \( \mathcal{L} \) is formed by the eigenvectors \( e^{(1)} \), \( e^{(2)} \) and \( e^{(3)} \) of \( A \):
\[
\mathcal{L} = \sum_{n=1}^{3} e^{(n)} e^{(n)} e^{(n)} e^{(n)}
\]  
\[
= \sum_{n=1}^{3} e_i^{(n)} e_j^{(n)} e_k^{(n)} e_i^{(n)}.
\]  
(3.8)

Knowing \( A^{//B}_2 \), one can solve a linear system to calculate the values of the scalar coefficients \( \alpha_0 \), \( \alpha_1 \) and \( \alpha_2 \).
Once the coaxial part of (3.1) is determined, the tensor orthogonal to $B$ is readily given by

$$A^\perp B = A - A^{\parallel B}$$  \hspace{1cm} (3.9)

It is then often of interest whether the coaxial or orthogonal term dominates $A$. One approach is to collapse each tensor to a scalar index $I$, which for the coaxial component is

$$I_{A^{\parallel B}} = \left( \frac{A : A^{\parallel B}}{A : A} \right)$$  \hspace{1cm} (3.10)

and similarly for the orthogonal component. Note, since the decomposition (3.1) is exact, that

$$I_{A^{\parallel B}} + I_{A^\perp B} = 1$$  \hspace{1cm} (3.11)

### 3.2 Residual stress approximations

Now we apply the foregoing tensor decompositions to the residual stress and consider levels of approximations that are then evaluated in §4. Applying (3.1) to the residual stress tensor yields

$$\tau = \tau^{\parallel S} + \tau^{\perp S}$$  \hspace{1cm} (3.12)

from which

$$\tau^{\parallel S}_1 = \alpha S = \left( \frac{\tau : \bar{S}}{\bar{S} : \bar{S}} \right) \bar{S}$$  \hspace{1cm} (3.13)

is one of the two possible coaxial components of $\tau$. Based on this, our first approximation for $\tau$ is

$$\tau \approx \hat{\tau}_1 \equiv \alpha S,$$  \hspace{1cm} (3.14)

that is, $\tau$ is approximated by its coaxial part. The Smagorinsky-Lilly (SL) model (Smagorinsky, 1963; Lilly, 1966) is based on this approximation with the purpose of the model being to determine $\alpha$. A number of approaches have been proposed for computing $\alpha$, including Germano’s dynamic model (Germano et al., 1991). In §4, $\alpha$
is determined for each location in space via (3.13), and so $\hat{\tau}_1$ can be thought of as the best possible isotropic eddy viscosity model.

The second type of decomposition of (3.1) leads to a non-linear relationship between the filtered stress and rate-of-strain

$$\tau \approx \hat{\tau}_2 \equiv \tau^{S} = \alpha_0 I + \alpha_1 S + \alpha_2 S^2 .$$

(3.15)

This approximation is equivalent to an anisotropic eddy viscosity model with the important caveat for this analysis being that, here, $\alpha_0$, $\alpha_1$, and $\alpha_2$ are not modeled but rather are computed at each point in space using the method outlined following (3.7) so that $\hat{\tau}_2$ is the best approximation to $\tau$ locally that can be achieved with a model for $\tau$ based only on $\overline{S}$.

Any models for $\tau$ based solely on the coaxial part of $\tau$ cannot more closely match the true residual stress than $\hat{\tau}_2$. In order to produce better models, the tensor basis must be expanded beyond $\overline{S}$. For this purpose, consider the tensor

$$P = \overline{S} \cdot W - W \cdot \overline{S} .$$

(3.16)

It is related to the energy redistribution caused by the viscous stress in a Newtonian fluid. It has the property of being orthogonal to the rate-of-strain tensor, which makes it a candidate for approximating the second term in the decomposition of $\tau$, that is, $\tau^{S}$. 

To proceed, consider the tensor relationships

$$\tau^{S} = \tau^{S/P} + \tau^{S \perp P} = \beta P + \tau^{S \perp P}$$

(3.17)

from which (3.12) becomes

$$\tau = \tau^{S} + \beta P + \tau^{S \perp P} .$$

(3.18)
This leads to the following three approximations to be evaluated as potential basis for residual stress models:

\[
\tau \approx \hat{\tau}_3 \equiv \beta \bar{P}
\] (3.19)

\[
\tau \approx \hat{\tau}_4 \equiv \tau_{1}^{\|S} + \beta \bar{P} = \alpha S + \beta \bar{P}
\] (3.20)

\[
\tau \approx \hat{\tau}_5 \equiv \tau_{2}^{\|S} + \beta \bar{P} = \alpha_0 I + \alpha_1 S + \alpha_2 S^2 + \beta \bar{P}
\] (3.21)

The last approximation is based on the same tensors as the model proposed in Kosovic (1997) and applied to stably stratified boundary layers in Kosovic & Curry (2000).

In preparation for evaluating each approximation for \(\tau\), let us define a scalar index as in (3.10). The index \(I_n\) of the \(n^{th}\) approximation at a point in space is given by

\[
I_n = \left( \begin{array}{c} \tau \cdot \hat{\tau}_n \\ \tau : \tau \end{array} \right)
\]  

(3.22)

Here \(n \in 1, 2, 3, 4, 5\) indicates one of the approximations for \(\tau\). Also, for each approximation there is a corresponding energy redistribution tensor \(R_n^*\).

### 3.2.1 Scalar residual flux approximations

We consider five approximations that might form the basis for scalar residual flux models. The first is based on the common assumption of gradient diffusion:

\[
\hat{f}_1 \equiv k_1 \nabla \bar{p} .
\] (3.23)

The second approximation we consider is

\[
\hat{f}_2 \equiv k_2 (\tau \cdot \nabla \bar{p}) .
\] (3.24)

Both models are analyzed in Chumakov (2008) for unstratified isotropic turbulence with the conclusions that \(\hat{f}_1\) is applicable only in strain-dominated areas of the flow.
but is generally misaligned with the true flux whereas \( \hat{f}_2 \) provides better alignment. The third approximation is

\[
\hat{f}_3 \equiv k_3 (\nabla^T \mathbf{u} \cdot \nabla \rho),
\]

which is related to the model of Clark et al. (1979), also known as the gradient viscosity model. The Clark approximation represents the first term in the Taylor series expansion for the scalar residual flux. It is known to provide good \textit{a priori} results but produces instability in numerical simulations caused by negative diffusion of the scalar (Chumakov, 2008). The tensor \( \nabla^T \mathbf{u} \) in the Clark approximation can be decomposed into symmetric and anti-symmetric parts, producing the two other approximations analyzed in this work:

\[
\hat{f}_4 \equiv k_4 (S \cdot \nabla \rho)
\]

and

\[
\hat{f}_5 \equiv k_5 (-\bar{W} \cdot \nabla \bar{\rho}) = \frac{k_5}{2} \bar{\omega} \times \nabla \bar{\rho},
\]

Where \( \bar{\omega} \) is the filtered vorticity vector. Note that \( \hat{f}_5 \) is orthogonal to \( \nabla \bar{\rho} \), therefore it does not diffuse the scalar and is free of the negative-diffusion problem found in the Clark approximation. The performance metric for these approximations is simply the angle between the exact and approximated flux vectors.
4.1 General approach

To understand better the relationships between the various tensors and approximations defined in §3, we turn now to high-resolution direct numerical simulations. Using DNS data to evaluate residual stresses and fluxes requires consideration of the flow dynamics represented by the simulations and the length scale of the filter relative to dynamically relevant length scales in the flow. In textbook descriptions of residual stresses, it is typically assumed that the filter scale is in the inertial range (e.g. Pope, 2000). In stratified turbulence, however, the existence and characteristics of a stratified inertial range, that is, an anisotropic inertial range at scales larger than the Ozmidov length scale, are open questions (Riley & Lindborg, 2008). So, at least for the present, there is no ‘textbook’ size for the filter to be used in this type of testing. In the analyses that follow, the first approach is simply to filter three sets of DNS data to the same grid spacing. The filter width is comparable to the Taylor micro-scale and the ratio of the filter width to the Ozmidov scale is different for each case. The characteristics of the residual stresses and fluxes are reported for this first analysis. The second approach is to vary the filter width relative to the Ozmidov length for the simulation with the largest scale separation between the Ozmidov and Kolmogorov length scales.

To proceed, let us begin by defining quantities relevant to the dynamic range and parameters of the simulations. The Ozmidov ($L_o$), Taylor ($\lambda$), and Kolmogorov ($L_k$) length scales are defined in the usual way in terms of the r.m.s. of the velocity,
the dissipation rate of turbulence kinetic energy, and the Brunt-Väisälä frequency \(N\), each of which is averaged over the entire domain. The buoyancy length scale \(L_b \equiv 2\pi U/N\), consistent with Waite’s definition. Also define \(L_h\) as the horizontal integral length of the horizontal motions computed with the method recommended in Appendix E of Comte-Bellot & Corrsin (1971). All these quantities are defined as in other papers using the same data sets (Almalkie & de Bruyn Kops, 2012b; de Bruyn Kops, 2015; Portwood et al., 2016). In addition, define the Thorpe length as the r.m.s. distance that the fluid parcels would move if the fluid were sorted to have minimum potential energy. The sorting is done separately for each column in the DNS data and then averaged to produce the domain-averaged Thorpe length \(L_T\).

The use of the Taylor length scale \(\lambda\) deserves some consideration. While Taylor (1935) mistakenly assumed that it is characteristic of dissipation scales, it has become a standard scale for locating the inertial range in unstratified turbulence because it is fairly insensitive to the details of the large scales, the statistics for which are often poor in DNS. It is used to identify the vicinity of length scales in which internal intermittency exhibits power law scaling in unstratified (Almalkie & de Bruyn Kops, 2012a) and stratified (de Bruyn Kops, 2015) turbulence. As shown in §4.2, all the simulations considered here have about the same Taylor Reynolds number.

In terms of the quantities just defined,

\[
Re_b \equiv \left(\frac{L_o}{L_k}\right)^{4/3}
\]

(4.1)

is the buoyancy Reynolds number which characterizes the dynamic range available for fully three-dimensional turbulence (Gibson, 1980; Gargett et al., 1984).

\[
Re_{h1} \equiv \left(\frac{L_h}{L_k}\right)^{4/3}
\]

(4.2)
is the scale separation between the energy-containing and dissipation length scales with the subscript notation adopted to be consistent with Almalkie & de Bruyn Kops (2012b).

\[ Fr_h \equiv \frac{2\pi u_h}{NL_h} \]

is a horizontal Froude number in which the factor of $2\pi$ has been retained in the conversion between the turbulence time scale and the corresponding frequency in order to be consistent with previous papers using the same DNS data.

### 4.2 Direct numerical simulations

The four direct numerical simulations used in the foregoing analyses are the same as those reported in de Bruyn Kops (2015) and Portwood et al. (2016). Three are of axisymmetric homogeneous stratified turbulence configured the same as those reported by Almalkie & de Bruyn Kops (2012a) but are different realizations with finer spatial resolution. The fourth is an unstratified isotropic homogeneous case with a uniform mean scalar gradient. The velocity fields are in the same series as those reported by Almalkie & de Bruyn Kops (2012a) but at higher Reynolds number. The parameters for all the simulations are given in table 1.

All the simulations are solutions to (2.1) with the addition of a forcing term in the momentum equations (c.f. (1b) in Almalkie & de Bruyn Kops, 2012b). The stratified cases are forced to be statistically stationary using the deterministic schema denoted ‘Rf’ by Rao & de Bruyn Kops (2011). Briefly, energy is added to the horizontal velocity components at the small horizontal wave numbers to maintain a prescribed spectrum for the horizontal kinetic energy. The target spectrum was determined by using a stochastic forcing technique similar to that of Lindborg (2006). A very small amount of energy is also added randomly to the horizontal components of velocity at small vertical wave numbers to induce shear instabilities. The forcing is applied until statistical stationarity is observed and then maintained for approximately one large-
eddy turnover time to assure convergence, as discussed by Almalkie & de Bruyn Kops (2012b). The unstratified case is forced using the method of Overholt & Pope (1998) with the target spectrum being Pope’s model spectrum with his $p_0 = 2$ and his $c_L = 6.78$ (Pope, 2000, equation (6.247)). In all cases, a steady scalar field consisting of a uniform gradient maintains the scalar fields statistically stationary. In (2.1) the stationary scalar field is denoted $\rho_s(z)$ to indicate density, but in the isotropic case the scalar is passive.

All the simulations are solved with a Fourier spectral method fully dealiased by truncation so that the maximum wave number magnitude after truncation is $\kappa_{max}$. The nonlinear terms are computed in real space and advanced in Fourier space with the third-order Adams-Bashforth algorithm as recommended by Durran (1991). The linear terms are advanced in time exactly in Fourier space. The resolution requirements meet or exceed those for DNS reviewed in §3 of Almalkie & de Bruyn Kops (2012a).

In addition to table 1, information about the stratified simulations is in table 1 and figure 1 of Portwood et al. (2016). In particular, the turbulence Froude and

<table>
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<th>Parameter</th>
<th>F3</th>
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</table>

Table 4.1: Direct numerical simulation parameters
Reynolds number, used by Brethouwer et al. (2007) to discuss regimes of stratified turbulence, are given there. All three of the simulations are significantly affected by stratification, even in the dissipation range (de Bruyn Kops, 2015), and cases F2 and F3 are in the regime termed ‘strongly stratified’ by Brethouwer et al. (2007). Since this term is used more broadly in the geophysical literature, Portwood et al. follow Falder et al. (2016) and refer to this specific regime as the ‘layered anisotropic stratified turbulence’ (LAST) regime. Since the stratified cases are all forced with the same target spectrum, and since the kinematic viscosity is the same in all cases, the only difference in input parameters among the three cases is $N$. The larger scales in the three simulations are very different from each other, though, as is evident from the two-dimensional spectra in the appendix of Almalkie & de Bruyn Kops (2012b), and these differences cause the integral length scale, the Taylor length scale and related quantities to vary among the simulations. The reason for using these three stratified data sets for this study, though, is that the Taylor lengths are comparable among the three cases and provide a convenient reference for filtering, as discussed in §4.1. The unstratified case, R4, is designed to have roughly the same value of $\lambda$ as the stratified cases.

4.3 Filtered fields

An isotropic homogeneous Gaussian filter, as described in Pope (2000, table 13.2), with characteristic width $\Delta$ is applied to the DNS fields to produce the filtered fields for analysis; other filters are considered in Appendix A. For the first set of analysis, $\Delta$ is 64 times the grid spacing $\delta$ and is nearly equal to $\lambda$ in all cases. Relationships between the length scales in the fully resolved and filtered fields are shown in table 2. Note from the table that ratios $L_b/\Delta$ overlap with those tested by Khani & Waite (2014) and Khani & Waite (2015). Also note that $\Delta/\delta = 64$, if implemented in a modeled simulation, would result in that simulation requiring a factor of $2 \times 10^5$
fewer grid points than the DNS, and, therefore, a significant reduction in computation effort.

The three-dimensional Gaussian filter is convenient for this type of study because it is easily implemented exactly in Fourier space to within the resolution of the DNS. So the residual stresses and fluxes analyzed in this study have almost no truncation error due to filtering. Further discussion on the advantage of using the Gaussian filter over other types is presented in Appendix A, along with comparisons to the box and spectral cut-off filters.

### 4.4 Preferred directions of tensors

Because it is the directionality of the buoyancy force that causes stratification, we begin our analyses by examining the preferred directions of the second order tensors and vectors defined in §3. Since the cases with stratification are axisymmetric around the vertical direction, and the unstratified case is isotropic, there is no preferred direction on the $xy$-plane. All tensors analyzed are symmetric so their eigenvectors are real and orthogonal to each other. Thus, significant information about the directional preference of each tensor is contained in its extremal eigenvector, that is, the vector related to the eigenvalue with the greatest absolute value. The p.d.f. of the vertical

<table>
<thead>
<tr>
<th></th>
<th>F3</th>
<th>F2</th>
<th>F1</th>
<th>R4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filter width to grid spacing</td>
<td>$\Delta/\delta$</td>
<td>64</td>
<td>64</td>
<td>64</td>
</tr>
<tr>
<td>Kolmogorov length to filter width</td>
<td>$L_k/\Delta$</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>Taylor length to filter width</td>
<td>$\lambda/\Delta$</td>
<td>0.96</td>
<td>0.94</td>
<td>0.92</td>
</tr>
<tr>
<td>Ozmidov length to filter width</td>
<td>$L_o/\Delta$</td>
<td>0.16</td>
<td>0.43</td>
<td>1.27</td>
</tr>
<tr>
<td>Thorpe length to filter width</td>
<td>$L_T/\Delta$</td>
<td>0.21</td>
<td>0.54</td>
<td>1.76</td>
</tr>
<tr>
<td>Buoyancy length to filter width</td>
<td>$L_b/\Delta$</td>
<td>5.85</td>
<td>11.22</td>
<td>23.15</td>
</tr>
</tbody>
</table>

Table 4.2: Filtering parameters
component $e_z$ of the normalized extremal eigenvectors for $\boldsymbol{\tau}$, $\mathcal{S}$, $\mathcal{P}$ and $\mathcal{R}$ are shown in figure 4.1. Each p.d.f. is computed from every $\vec{x}$ location in the filtered fields.

The vertical component of an eigenvector of a statistically isotropic tensor is uniformly distributed. This is the case for all the tensors in the unstratified simulation $R4$. Departure from this distribution is quite pronounced for all of stratified cases for the tensors considered. The extremal eigenvector of the residual stress tensor increasingly aligns with the horizontal plane as stratification is increased. There is also a less pronounced trend for it to align perpendicular to the horizontal plane, which is indicated by the small peak at $e_z = 1$ for $F3$ case in figure 4.1 (a). The rate-of-strain tensor tends toward aligning at 45 degrees to the horizontal, which is consistent with
the existence of horizontal shear layers. The tensor $\mathbf{P}$, which is introduced in §3 precisely to provide directional information to approximations for $\mathbf{\tau}$, has a distribution for the direction of the extremal eigenvector qualitatively similar to that of $\mathbf{\tau}$, that is, preference to align with the horizontal and the vertical directions, but in this case the vertical preference is stronger than the horizontal. The p.d.f. for the energy redistribution tensor $\mathbf{R}$ is similar to that of $\mathbf{S}$ in that it tends toward alignment 45 degrees from the horizontal.

The energy redistribution tensor, $\mathbf{R}$, warrants closer examination. The p.d.f. follows broadly the same trend as that of $\mathbf{S}$, namely a tendency to align more strongly with 45 degrees from the horizontal with increasing stratification. The trend is not as pronounced as it is for $\mathbf{S}$, however, to the extent that the least strongly stratified case (F1) is almost statistically indistinguishable from the isotropic case (R4). Portwood et al. (2016) report that F1 is dominated by space-filling turbulence with few regions of layered turbulence yet de Bruyn Kops (2015) shows that there is no classical inertial range. Together, these results suggest that the redistribution of energy among the filtered velocity components by the residual stresses is very nearly isotropic, even if the turbulence is not consistent with isotropic homogeneous turbulence, provided that the turbulence is space filling.

The preferred direction of vector quantities can be expressed by the p.d.f. of the sine of the angle $\theta$ between the vector and the horizontal plane. This is plotted in figure 4.2 for several vectors of interest. For the isotropic homogeneous case, the directions of the scalar residual flux and the gradient of the filtered fluctuating scalar gradient are roughly uniformly distributed but with a bias toward being aligned antiparallel with the mean scalar gradient. This is consistent with the ramp-cliff structure discussed in Warhaft (2000), and the bias also exists in the presence of stratification. The direction of the vorticity vector is uniformly distributed in the isotropic homogeneous case.
Figure 4.2: Probability distribution function of angle between vector and horizontal plane for: (a) residual scalar flux \( \mathbf{f} \), (b) \(-\nabla \bar{\rho}\), (c) filtered vorticity \( \vec{\omega} \).
When stratification is imposed, the preferred direction of the vectors changes markedly. As stratification gets stronger, the scalar residual flux vector tends to align with the horizontal. Note that the vector terms in (2.12) are functions of the velocity vector. Therefore the direction of the scalar residual flux will be related to that of velocity. Since stratification imposes restriction on movements in the vertical direction, the scalar residual flux will also be restricted in the vertical direction.

Unlike the residual flux, the gradient of the filtered fluctuating density aligns with the vertical, both upwards and downwards. Note that the gradient of the total density field is predominantly downward as one would expect. Vorticity, which plays an important role in reorienting scalar gradients, aligns with the horizontal plane. This is consistent with the presence of horizontal shear layers, which tend to align the vorticity with the horizontal.

### 4.5 Approximations for residual stresses

Five approximations, identified with the subscripts $n \in \{1, 2, 3, 4, 5\}$, for the residual stress tensor are introduced in §3.2, and the indices $I_n$ are introduced to represent how well $\tau$ is approximated by its projections on the tensor basis set given by $\hat{\tau}_n$. The p.d.f.s of these indices are plotted in figure 4.3 for each filtered DNS case. Also included are indices for the approximations applied to a randomly generated symmetric traceless statistically isotropic tensor.

The results for the best possible Smagorinsky-Lilly-type eddy viscosity approximation are shown in figure 4.3 (a). Recall that here we are not evaluating models, but approximations to the tensor given by its projection on a tensor basis set, and so $\alpha$ in the figure is computed directly from the DNS data via (3.13), and similarly for the coefficients required for the other panels in the figure. For the isotropic homogeneous case and the least strongly stratified case, the simple eddy viscosity approximation agrees somewhat better with the residual stress tensor from the DNS
Figure 4.3: Probability density function of index value for: (a) \( \hat{\tau}_1 = \alpha \mathbf{S} \); (b) \( \hat{\tau}_2 = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{S} + \alpha_2 \mathbf{S}^2 \); (c) \( \hat{\tau}_3 = \beta \mathbf{P} \); (d) \( \hat{\tau}_4 = \alpha \mathbf{S} + \beta \mathbf{P} \); (e) \( \hat{\tau}_5 = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{S} + \alpha_2 \mathbf{S}^2 + \beta \mathbf{P} \)
than it does with the randomly generated stress tensor. For cases F2 and F3, though, the approximation is worse than for the randomly generated stress tensor.

At first this might be disappointing until one realizes that departure from random implies the existence of information. The character of this information is already suggested by figure 4.1, namely that the residual stress and filtered rate of strain tensors are increasingly misaligned with increasing stratification strength, and that a tensor orthogonal to $\mathbf{S}$, such as $\mathbf{P}$, must be included to improve the approximation of $\mathbf{\tau}$. Indeed, one can see from the figure that $\hat{\mathbf{\tau}}_2$, which is the highest order approximation possible in terms of just $\mathbf{S}$, is not very good and that $\hat{\mathbf{\tau}}_3$, which includes no information about the rate-of-strain, is much better, at least in terms of the index $I_3$.

While the distribution of $I_3$ suggests that $\hat{\mathbf{\tau}}_3$ may be the basis for a good model, recall that this cannot be the case because stress components orthogonal to $\mathbf{S}$ transfer zero energy to the residual scales. Therefore, $\mathbf{S}$, or a tensor coaxial to it, must be included in any effective model. $\hat{\mathbf{\tau}}_4$ is the simplest approximation involving $\mathbf{S}$ that predicts fairly well the residual stress tensor while transferring the correct amount of energy to the residual scales. To see that the transfer rate must be correct, consider the production of residual kinetic energy by approximation $\hat{\mathbf{\tau}}_4$

$$\mathcal{P}_{r4} \equiv \hat{\mathbf{\tau}}_4 : \mathbf{S} = (\alpha \mathbf{S} + \beta \mathbf{P}) : \mathbf{S} = \left( \frac{\mathbf{\tau} : \mathbf{S}}{\mathbf{S} : \mathbf{S}} \right) \mathbf{S} : \mathbf{S} = \mathbf{\tau} : \mathbf{S} = \mathcal{P}_r .$$

Finally, by combining the best possible approximation of $\mathbf{\tau}$ in terms of $\mathbf{S}$ with the approximation in terms of $\mathbf{P}$, we arrive at $\hat{\mathbf{\tau}}_5$. From figure 4.1 (e) we conclude that this tensorial basis set has excellent potential to approximate the residual stress tensor.

### 4.6 Approximations for energy redistribution

While in many approaches to turbulence simulation it is the momentum equation that requires a closure model in the form of an approximation for the residual stress
tensor, very often more attention is given to the energetics of models than to accurate approximation of the stress tensor itself. In this section we analyze the energy transfer rates resulting from each of the approximations for $\tau$. From equations analogous to (4.4), all of the approximations except $\hat{\tau}_3$ result in correct energy transfer from filtered to residual scales. Recall from §3 that this transfer rate can be represented as an isotropic production rate of residual kinetic energy plus a resolved-scale redistribution of energy described by the redistribution tensor $\mathcal{R}$.

As with the tensors analyzed in §4.4, the properties of $\mathcal{R}$ allow the directionality of the tensor to be described by the vertical component $e_z$ of the extremal eigenvector. P.d.f.s of this quantity are shown in figure 4.4. As expected, for the isotropic case R4, $e_z$ has uniform distribution. Stratification biases the extremal eigenvector toward 45 degrees from the horizontal consistent with horizontal shear being important in layered turbulence. In the case with space-filling turbulence (F1), the p.d.f. of the extremal eigenvector of $\mathcal{R}$ departs only modestly from that in the unstratified cases.

Considering now the approximations for $\mathcal{R}$, all the approximations for $\tau$ produce the correct statistical redistribution of energy for the isotropic case R4 because all tensors are isotropic. For the two more strongly stratified cases, F2 and F3, both of the approximations involving $\mathcal{P}$ redistribute energy quite accurately (statistically), but the full expansion of $\tau$ in terms of $\mathcal{S}$ ($\hat{\tau}_2$) redistributes energy quite well in light of how poorly it represents $\tau$. The simple Smagorinsky-Lilly-like type approximation $\hat{\tau}_1$ does not capture the energy redistribution at all well. For case F1, the energy redistribution tensor is almost isotropic, therefore any of the approximations captures it fairly well, although the simplest approximation departs somewhat from the correct directions.
Figure 4.4: P.d.f.s of vertical component $e_z$ of the extremal eigenvector of the energy redistribution tensor $\mathcal{R}_n^*$ produced by each approximation $n$ for: (a) F3, (b) F2, (c) F1 and (d) R4.
4.7 Scalar residual flux approximations

Figure 4.5 shows the angle between the scalar residual flux and approximations for it. For the two first approximations, the results for the isotropic case are similar to those of Chumakov (2008); there is a better alignment with the second approximation tested. While that still holds with density stratification, the scalar residual flux tends to be more likely perpendicular to the approximations, and this trend gets stronger with increased stratification. The results for $\hat{f}_4$ is qualitatively similar to that of the Clark approximation. The last approximation also shows good alignment with the scalar residual flux for every case, more persistently as stratification gets stronger. Approximations $\hat{f}_3$, $\hat{f}_4$ and $\hat{f}_5$ produces much better results than $\hat{f}_1$ and $\hat{f}_2$.

It is interesting to consider $\nabla \rho$, shown in figure 4.5 (a), in the context of available potential energy (APE) and mixing. APE is the portion of potential energy that can be converted to kinetic energy due to the volumetric constraint imposed by conservation of mass (Lorenz, 1955). Mixing due to molecular diffusion irreversibly converts APE to background potential energy. In the limit of high Péclet number, APE is proportional to the square of the perturbation density if the mean density profile is linear (Holliday & McIntyre, 1981). By multiplying (2.8c) by $\bar{\rho}$, we arrive at the time evolution equation for $\bar{\rho}^2$, which is proportional to the local APE of the filtered field. The term in this equation related to mixing is $\mathbf{f} \cdot \nabla \bar{\rho}$. Therefore, accurate alignment between a model for the residual flux and $\nabla \bar{\rho}$ is very important if the model is to predict mixing in the residual field.

4.8 The effect of filter width

In the preceding analyses, there is an underlying hypothesis that the alignment of the tensors and vectors are determined solely by the ratio of length between the filter width and the Ozmidov length. In this respect, cases F2 and F3 are qualitatively different from case F1 because F1 is dominated by space filling turbulence whereas
Figure 4.5: Probability distribution function of cosine of the angle between the density residual flux $\mathbf{f}$ and: (a) $\hat{\mathbf{f}}_1 = k_1 \nabla \tilde{\rho}$; (b) $\hat{\mathbf{f}}_2 = k_2 \mathbf{\tau} \cdot \nabla \tilde{\rho}$; (c) $\hat{\mathbf{f}}_3 = k_3 \nabla^T \mathbf{\bar{u}} \cdot \nabla \tilde{\rho}$; (d) $\hat{\mathbf{f}}_4 = k_4 \mathbf{S} \cdot \nabla \tilde{\rho}$ and (e) $\hat{\mathbf{f}}_5 = \frac{k_5}{2} \mathbf{\omega} \times \nabla \tilde{\rho}$.
Table 4.3: Filtering parameters for different filter widths in case F1.

<table>
<thead>
<tr>
<th></th>
<th>F2</th>
<th>F1N(\frac{1}{2})</th>
<th>F1</th>
<th>F1N2</th>
<th>F1N4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filter width to grid spacing</td>
<td>(\Delta/\delta)</td>
<td>64</td>
<td>32</td>
<td>64</td>
<td>128</td>
</tr>
<tr>
<td>Kolmogorov length to filter width</td>
<td>(L_k/\Delta)</td>
<td>0.022</td>
<td>0.044</td>
<td>0.022</td>
<td>0.011</td>
</tr>
<tr>
<td>Taylor length to filter width</td>
<td>(\lambda/\Delta)</td>
<td>0.94</td>
<td>1.84</td>
<td>0.92</td>
<td>0.46</td>
</tr>
<tr>
<td>Ozmidov length to filter width</td>
<td>(L_o/\Delta)</td>
<td>0.43</td>
<td>2.55</td>
<td>1.27</td>
<td>0.64</td>
</tr>
<tr>
<td>Thorpe length to filter width</td>
<td>(L_T/\Delta)</td>
<td>0.54</td>
<td>3.52</td>
<td>1.76</td>
<td>0.88</td>
</tr>
<tr>
<td>Buoyancy length to filter width</td>
<td>(L_b/\Delta)</td>
<td>11.22</td>
<td>46.29</td>
<td>23.15</td>
<td>11.57</td>
</tr>
</tbody>
</table>

F2 and F3 are dominated by layered or comparatively quiescent regions (Portwood et al., 2016). To better isolate the effect of the filter width to Ozmidov length ratio, three additional filter widths are considered for case F1. The variants are denoted F1N\(\frac{1}{2}\), F1N2 and F1N4, the details of which are tabulated in table 3.

The p.d.f.s of the vertical component of the extremal eigenvectors for \(\tau\), \(S\), \(P\) and \(R\) are shown in figure 4.6 for all the variants of F1 and for F2. Panels (a) and (c) of the figure suggest that the orientation of \(\tau\) and \(P\) depends significantly on the filter width relative to the Ozmidov scale so that case F1N4 is qualitatively similar to case F2. Panel (b) and (d), however, support our hypothesis that the fraction of the domain exhibiting layering is important to the alignments of \(S\) and \(R\) because none of the variants of F1 is similar to F2 for these tensors.

The preferred direction of the vectors of interest are shown in figure 4.7. As with the residual stress tensor, the scalar residual flux shows qualitatively similar results for F2 and for the case F1N4 for which the filter width is larger than the Ozmidov length. The same happens for the direction of the gradient of the density field. The alignment of the vorticity vector, though, is profoundly different in cases F1N4 and F2. In case F2, local vertical shear in F2 tends to align the vorticity vector with the horizontal plane, and there is no equivalent mechanism in case F1 even when \(\Delta/L_o\)
Figure 4.6: Probability distribution function of vertical component $e_z$ of the extremal eigenvector for (a) $\tau$, (b) $\mathbf{S}$, (c) $\mathbf{P}$ and (d) $\mathbf{R}$. Along the top axis is shown the angle of the eigenvector to the horizontal plane.
is comparable. Therefore, any model based on approximation $\hat{f}_5$ will be sensitive to the turbulence regimes in the flow.

### 4.9 Different Filter Kernels

In simulations of fluid flows, the numerical method inherently filters the flow. This is most obvious in large-eddy simulations but it is true in other simulations, including DNS. The characteristics of the implied filtering operation are not known, but it is assumed that the filter diminishes high frequencies while preserving the large scale motions. In this analysis, the effects of the implicit filtering operation are represented by an explicit Gaussian filter. So it is important to investigate whether the results
presented previously depend qualitatively on the type of filter. In this appendix, we consider the Gaussian, box average and spectral cutoff filters as defined in Pope (2000). In all cases, filtering is computed in Fourier space and is exact because each filter type can be written in terms of a transfer function in Fourier space; our DNS represent the flows in terms of infinite Fourier series with all except a finite number of the amplitudes identically zero and so these transfer functions are exact.

The characteristics of the Gaussian, box average, and spectral cutoff filters can be understood by observing their transfer functions. The spectral cutoff eliminates entirely the frequencies above a particular wave number. The Gaussian filter is rather compact and exponentially approaches a complete elimination of high frequency variations. The box average filter is the least compact of the three filters in Fourier space, but nevertheless diminishes the small scales. In real space the order of compactness is reversed. Importantly, the spectral cutoff filter is not positive semi-definite and can lead to unphysical flow characteristics such as negative residual kinetic energy or negative residual scalar concentration. Because the Gaussian filter is compact both in physical space and in Fourier space, it is used for all the analyses in this work except those presented in this section.

The analyses of §4.4 are repeated with different filter kernels as shown in figure 4.8. The filtered strain rate tensor \( \mathbf{S} \) and tensor \( \mathbf{P} \) behaves almost exactly the same way for the three filters. The residual stress tensor is slightly different with the spectral cutoff filter but there is no qualitative difference. The energy redistribution tensor \( \mathbf{R} \) is almost the same with the box and Gaussian filters whereas the spectral cutoff filter results in a somewhat different distribution for the direction of the extremal eigenvector but does not contradict the conclusions from §4.4; again we note from its transfer function the spectral cutoff filter can produce unphysical results and so no great weight should be given to the results with that filter.
Figure 4.8: Probability distribution function of vertical component of the extremal eigenvector for (a) \( \tau \), (b) \( \overline{S} \), (c) \( \overline{P} \) and (d) \( \mathcal{R} \) for different filter kernels. Along the top axis is shown the angle of the eigenvector to the horizontal plane.
The analyses of §4.5 are repeated for different filter kernels with the results shown in figure 4.9. The spectral cutoff filter does not significantly affect $\hat{\tau}_1$ but introduces significant randomness into the other approximations. This is not surprising given that this filter kernel is not positive definite. Importantly, the conclusions drawn in §4.5 are insensitive to which of the positive-definite filters (Gaussian or box) are used.

The preferred direction for energy the redistribution $\mathbf{R}$ with the spectral cutoff and box filters are shown in figure 4.10. The results for the Gaussian filter is shown in figure 4.4(a). For this measure, although the filter does quantitatively change the results, the conclusions drawn from figure 4.4 are not affected by the details of the filter.

### 4.10 Conclusions from preliminary analysis

Large-eddy and other types of turbulence simulations depend on models for the effects of the residual scales on the filtered scales. If these models are tensor-based, the first step in model development is finding the minimum set of tensors on which the models must be based in order to reproduce basic properties of the residual stress tensor. In our nomenclature, modeling involves finding the coefficients by which to weight the tensors. In this analysis the optimal coefficients are computed exactly from direct numerical simulation data and we call the optimally weighted tensor combinations “approximations” with the goal of finding a minimal tensorial basis set that contains the necessary information to be a potentially good starting point for modeling the residual stresses and scalar flux in stably stratified turbulence.

The buoyancy force inherent in stratified turbulence causes anisotropy. It is, therefore, not surprising that an isotropic eddy viscosity assumption does not approximate the residual stresses at all well even though it is able to ensure the correct transfer of energy from the filtered to the residual scales. In fact, a statistically isotropic randomly generated tensor with zero trace is a more promising starting point for
Figure 4.9: Probability density function of index value for: (a) $\hat{\tau}_1 = \alpha \mathbf{S}$; (b) $\hat{\tau}_2 = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{S} + \alpha_2 \mathbf{S}^2$; (c) $\hat{\tau}_3 = \beta \mathbf{P}$; (d) $\hat{\tau}_4 = \alpha \mathbf{S} + \beta \mathbf{P}$; (e) $\hat{\tau}_5 = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{S} + \alpha_2 \mathbf{S}^2 + \beta \mathbf{P}$ for different filter kernels
Figure 4.10: P.d.f.s of vertical component $e_z$ of the extremal eigenvector of the energy redistribution tensor $\mathcal{R}_n^*$ produced by each approximation $n$ for: (a) Box filter, (b) Spectral cutoff filter.

modeling the residual stresses. Even a full expansion of the filtered rate-of-strain tensor $\mathcal{S}$ is not able to reproduce basic characteristics of the residual stress tensor $\tau$. This is because in stratified turbulence the two tensors are systematically misaligned with the extremal eigenvector of $\tau$ tending to align with the horizontal while that of $\mathcal{S}$ tending to align $45^\circ$ from the horizontal. Therefore, the filtered strain rate tensor is inherently unable to reproduce the correct anisotropy, regardless of how the eddy viscosity coefficient is computed in a model. A tensor that is orthogonal to $\mathcal{S}$ is required as part of the tensorial basis set for an effective model. Such a tensor should be able to reproduce the anisotropic transfer of energy, \textit{due to the residual motions}, between the filtered velocity components. Analysis of the kinetic energy equation reveals a candidate for this tensor which, when combined with $\mathcal{S}$, yields an excellent approximation to $\tau$ involving three independent coefficients and a very good approximation using two.

The eddy diffusion approximation for the scalar residual flux is not appropriate for strongly stratified flows because the flux is most often perpendicular to the gradient of the scalar. Including the residual stress tensor in the approximation of the scalar flux results in only a slight improvement. Approximations of the type introduced by Clark
et al. (1979), which involve either the filtered rate-of-strain or filtered vorticity, are effective because they include tensors that are statistically aligned with the residual flux.

Turbulence in stratified flows can form in various regimes depending on strength of the inertial force relative to that of the buoyancy force. The ratio of the forces is the Froude number $Fr$. When $Fr$ is very small, and the Reynolds number sufficiently high, turbulence tends to form in layers. Falder et al. (2016) refer to this regime as the “layered anisotropic stratified turbulence” (LAST) regime to distinguish it from stratified turbulence in general. When $Fr$ is larger, but buoyancy forces are still important, then highly anisotropic space-filling turbulence can form, as it does in one of the three stratified flow cases considered for this study. The preferred alignment of some tensors depends on whether the turbulence is layered or space filling while the alignment of other tensors does not. We conclude, therefore, that the tensorial basis for any effective model must be capable of capturing the anisotropy in both regimes, and the approximations for residual stress and flux that we present meet this requirement.

Finally, we note again that the coefficients in each of our approximations are optimally determined from the fully resolved simulations. Effective models require approximating these coefficients. Effective models, however, must be based on tensors that are able to reproduce the characteristics of the modeled term. We have determined a minimum tensorial basis for potentially effective two and three coefficient models for the residual stress plus an additional coefficient to well-approximate the scalar residual flux.
CHAPTER 5
EXTENDING EDDY-VISCOSITY MODELS

Accurately reproducing the residual stress tensor is a difficult task. Because of that, most of current LES modeling efforts aim not at faithfully reproducing the residual stress tensor itself, but solely its interaction with the filtered fields, mainly the energy transfer from large to small scales. In fluid flows where turbulence is locally isotropic at the filter scale, a simple eddy viscosity assumption is sufficient to reproduce this desired behaviour. Our preliminary analysis shows that for stratified turbulence, if the filter width is above the Ozmidov length scale, the eddy-viscosity assumption is inherently unable to reproduce the correct anisotropy.

Our proposal is to develop and test LES models that are capable of reproducing basic anisotropic behaviour of stratified turbulence.

5.1 Modeling strategy

Using the decomposition defined in Chapter 3 we decompose the residual stress tensor in

$$\tau = \tau^S + \tau^S$$  \hspace{1cm} (5.1)

This decomposition is based on the double dot operator, which serves as a inner product for the vector space formed by symmetric traceless tensors. Conveniently, this inner product is the operator that produces the isotropic energy transfer between the large and small scales. Therefore, we can attribute specific roles for each parts of the tensor: the part that is proportional to the strain rate is the part responsible for the
isotropic energy transfer, while the orthogonal-to-the-strain-rate part is responsible to reproduce the energy redistribution on the flow.

τ∥S should be modeled with either a linear or non-linear relationship to \( \bar{S} \). Our preliminary analysis suggests using the tensorial basis set formed by \( \bar{S} \) and \( \bar{P} \) as the simplest yet accurate model for the residual stress tensor. The closure problem then becomes:

\[
\begin{align*}
\tau^\parallel S &= \nu_t \bar{S} \quad (5.2) \\
\tau^\perp S &\approx \beta \bar{P} \quad (5.3)
\end{align*}
\]

where \( \nu_t \) and \( \beta \) need to be modeled\(^1\). Equation 5.2 is equivalent to the well-known eddy-viscosity model. It is also advantageous to use this tensorial basis set because, since the two terms are independent, we can directly expand already developed eddy-viscosity models with the second term, without the need for rethinking eddy-viscosity modeling.

Simple dimensional analysis dictates that \( \beta \) must have dimensions of \( \ell^2 \). The most obvious choice for \( \ell \) is the filter width \( \Delta \). Then, eq. (5.3) is rewritten as

\[
\tau^\perp S \approx C_\beta \Delta^2 \bar{P} \quad (5.4)
\]

where \( C_\beta \) is an non-dimensional coefficient that must be modeled.

### 5.2 Estimation of the coefficient \( C_\beta \)

Using the filtered DNS cases F3, F2 and F1, described in table 4.2, we calculate \( C_\beta \) as:

\(^1\)Alternatively, \( \tau^\parallel S \) can be rewritten as \( \tau^\parallel S = \frac{2\nu_\tau}{\bar{S}^2} \bar{S} \), where instead of the eddy-viscosity, the production term \( P_r \) would be modeled directly.
The probability distribution function of the coefficient is shown in figure 5.1. The most probable value for the coefficient was found to be close to 0.1 and did not vary for the different cases analyzed. We note that, for a LES model utilizing this tensor to perform accurately, it is important to accurately reproduce the correct coefficient value mainly in areas where the norm of the tensor has larger values since those areas will be strongly affected by the residual stress model. Therefore, as shown in figure 5.1(b), we also analyze the probability distribution function of the coefficient conditioned on areas where the norm of the tensor is greater than two standard deviations from its mean value. On those areas, the deviation of the coefficient is even smaller than that for the full field. We conclude that, for the cases analyzed, the coefficient can reasonably be considered constant. The estimated value calculated from the filtered DNS analyzed is $C_\beta \approx 0.093 \pm 0.014$.

Although the analysis performed suggests a constant coefficient is adequate for the flow cases studied, there is no guarantee that that should hold for any class of flows. Boundary conditions, such as no-slip conditions, usually affect coefficient values for
residual stress models. Because of that, we proceed to explore options for calculating $C_\beta$ dynamically.

### 5.2.1 Using Germano’s identity to calculate $C_\beta$ dynamically

In order to calculate dynamically the coefficient for the tensor $P$ we use Germano’s identity, described in equation 2.35. For the tensorial basis proposed, the identity becomes:

$$C_\beta \Delta_t^2 P^* - 2c_s \Delta_t^2 \tilde{S} \tilde{S} - C_\beta \Delta^2 \tilde{P} + 2c_s \Delta^2 \tilde{S} \tilde{S} = L . \quad (5.6)$$

where $L = \tilde{u} u - \tilde{u} \tilde{u}$, $P^* = \tilde{S} \cdot \tilde{W} - \tilde{W} \cdot \tilde{S}$ and $C(\tilde{\cdot})$ is the test filter operator with width $\Delta_t$, usually taken to be $2\Delta$.

We propose two manners to extract the coefficient from the identity.

#### 5.2.1.1 Based on Lilly’s dynamic model

The first one follows the same reasoning presented in Germano’s and Lilly’s (Germano et al., 1991; Lilly, 1992) approach for calculating the dynamic Smagorinsky coefficient $c_s$. In their approach, the coefficients are extracted from the filtering operator. Then, Germano’s identity becomes:

$$L \approx 2c_s M + C_\beta M_P , \quad (5.7)$$

where $M$ is the same quantity of the original Lilly’s model (defined in equation 2.38) and $M_P = \Delta_t^2 P^* - \Delta^2 \tilde{P}$.

Similarly to Lilly’s model, the equations for the coefficients are overdetermined. Since the tensor basis used for the model is orthogonal by construction, the coefficients $c_s$ and $C_\beta$ must be independent of each other. We use this fact as a justification to minimize each component of the model independently, albeit not being consistent with
equation 5.7. Therefore, the coefficient $c_s$ is calculated in the exact same manner as in Lilly’s models (equation 2.39) and $C_\beta$ is calculated through:

$$C_\beta \approx \frac{L : M_P}{M_P : M_P}.$$  \hspace{1cm} (5.8)

As stated before, this manner of calculating the coefficients carries the same inconsistencies as the original Germano’s dynamic Smagorinsky model. To address these inconsistencies Piomelli & Liu (1995) proposed a localization procedure that removes the mathematical inconsistency to any desired order of accuracy in time. Our second method for calculation of $C_\beta$ is based on this model.

5.2.1.2 Based on Piomelli’s dynamic model

Piomelli & Liu (1995) main proposal is to use an approximation for the coefficient that is enclosed in the filtering operation. The approximation for the coefficient at a given time and local is estimated based on a time-backward extrapolation scheme. Applying Piomelli’s idea to the current model proposed, equation 5.6 is recast as:

$$C_\beta \Delta_t^2 P^* - 2c_s \Delta_t^2 \tilde{S} \tilde{S} = L + \frac{C_\beta^* \Delta^2 P}{\Delta_t \Delta_t} - 2c_s^* \Delta^2 \tilde{S} \tilde{S} = L^* \hspace{1cm} (5.9)$$

where on the right side an estimation for the coefficients, denoted by $c_s^*$ and $C_\beta^*$ and assumed to be known, are used. Since $c_s^*$ and $C_\beta^*$ are known, and since by construction $P^*$ is orthogonal to $\tilde{S}$, the coefficients $c_s$ and $C_\beta$ can be exactly calculated locally:

$$c_s = -\frac{1}{2\tilde{S} \Delta_t^2} \frac{L^* : \tilde{S}}{\tilde{S} : S} \hspace{1cm} (5.10)$$

and

$$C_\beta = \frac{1}{\Delta_t^2} \frac{P^* : P^*}{P^* : P^*} \hspace{1cm} (5.11)$$
For a first order approximation, the estimation for the coefficients at time-step $n$ are given by:

$$c^*_s = e^{n-1}_s + \Delta t \left( \frac{\partial c_s}{\partial t} \right)_{n-1} = e^{n-1}_s + \frac{t_n - t_{n-1}}{t_{n-1} - t_{n-2}} (e^{n-1}_s - e^{n-2}_s)$$

(5.12)

and

$$C^*_\beta = C^{n-1}_\beta + \Delta t \left( \frac{\partial C_\beta}{\partial t} \right)_{n-1} = C^{n-1}_\beta + \frac{t_n - t_{n-1}}{t_{n-1} - t_{n-2}} (C^{n-1}_\beta - C^{n-2}_\beta).$$

(5.13)

5.3 LES models combinations to be tested

We have laid out three possibilities for modeling the part of the residual stress tensor that is orthogonal to the strain rate tensor. The first one simply uses a constant coefficient and the others utilize Germano’s identity to calculate the coefficient dynamically. Dynamic calculation of the coefficient demands filtering operations, which are done through numerical convolution and greatly increases the computational cost of the model. Therefore, we argue that it is only reasonable to use the dynamic approach for the calculation of $\beta$ when one is already using a dynamic model for the eddy viscosity. On the other hand, the constant-coefficient model for $\beta$ can be used with either dynamic or non-dynamic eddy viscosity models.

On the next section, we proceed to test different combinations of eddy viscosity models and $\tau^\perp_S$ models. For a non-dynamic eddy viscosity model, we ruled out the classical Smagorinsky model and decided to use Vreman’s model (Vreman, 2004). Although the cases analyzed are homogenous, stable density stratification produces three dynamically distinct regions in the flow. Portwood et al. (2016) characterize them as quiescent flow, intermittent turbulent layers, and turbulent patches. In initial LES test simulations for the most strongly stratified case F3, the Smagorinsky model was over-dissipative and failed to predict an eddy viscosity field that is consistent with the three dynamically distinct regions of the flow. Vreman’s model, on the other
hand, was able to auto-tune the eddy viscosity in a manner consistent with those regions. Indeed, the model was constructed precisely to have the intrinsic ability to vanish the eddy viscosity for flow types with zero theoretical subgrid dissipation.

The eddy viscosity proposed by Vreman (2004) is the following:

\[ \nu_t = c_v \sqrt{ \frac{B_\gamma}{\alpha_{ij} \alpha_{ij}} } , \]  

(5.14)

with

\[ \alpha_{ij} = \frac{\partial \tilde{\pi}_j}{\partial x_i} , \]  

(5.15)

\[ \gamma_{ij} = \Delta^2 \alpha_{ki} \alpha_{kj} , \]  

(5.16)

\[ B_\gamma = \gamma_{11} \gamma_{22} - \gamma_{12}^2 + \gamma_{11} \gamma_{33} - \gamma_{13}^2 + \gamma_{22} \gamma_{33} - \gamma_{23}^2 . \]  

(5.17)

The model constant \( c_v \) is related to the Smagorinsky constant \( C_S \) by \( c_v \approx 2.5 C_S^2 \).

When the default value of \( C_S \approx 0.17 \) is used, the constant becomes \( c_v \approx 0.072 \).

Besides Vreman’s model, the dynamic Smagorinsky model – in the version proposed by Lilly (1992) – and Piomelli’s localized dynamic model were used to model the part of the residual stress tensor that is in-phase with the strain rate tensor. Large-eddy simulations were run for each model with and without the addition of the constant-coefficient model for \( \tau^{i\mathcal{S}} \) based on \( \boldsymbol{P} \). For the two dynamic eddy viscosity models, additional simulations were run with the dynamic version of calculation of \( C_\beta \). The combined models used are listed below, together with shorter notations used in figures labels:

1. Vreman

2. Germano’s Dynamic Smagorinsky with Lilly’s modification (Dyn. Smag.)

3. Piomelli (Pio.)

4. Vreman + constant \( C_\beta \) (Vreman+P)
5. Germano’s Dynamic Smagorinsky with Lilly’s modification + constant $C_\beta$ ($Dyn. Smag.+P$)

6. Piomelli + constant $C_\beta$ ($Pio.+P$)

7. Dynamic Smagorinsky + dynamic $C_\beta$ ($Dyn. Smag. + dyn. P$)

8. Piomelli + dynamic $C_\beta$ ($Pio. + dyn. P$)

5.4 Testing extended eddy-viscosity models in large eddy simulations of cases F3, F2 and F1

The eight residual stress models constructed were tested in forced axisymmetric homogeneous stratified flow simulations equivalent to cases F3, F2 and F1 shown in table 4.1. The filtered fields presented in table 4.2 were used as the initial condition for the simulation. The cases are forced to be statistically stationary using the deterministic schema denoted ‘Rf’ by Rao & de Bruyn Kops (2011). Briefly, energy is added to the horizontal velocity components at the small horizontal wavenumbers to maintain a prescribed spectrum for the horizontal kinetic energy. The spectrum prescribed is the same as that from the DNS cases. A very small amount of energy is also added randomly to the horizontal components of velocity at small vertical wavenumbers to induce shear instabilities. All cases were run for a total of two integral length scales and mean values were calculated using both spatial and time averages. Time averages were performed for the duration of one integral time scale after already running the cases for one integral time scale. Similarly to the DNS simulations, the pseudospectral method was used.

5.4.1 Numerical Method

In the pseudospectral method, the equations of motions are solved in Fourier space. Non-linear terms are computed in real space and transformed back to Fourier space.
using the efficient FFTW algorithm. In order to decrease the number of Fourier transforms needed, the Navier-Stokes equations under Boussinesq’s assumptions were cast in rotational form. Under Boussinesq’s assumption, the velocity field is divergence-free, so, the equations solved numerically are reduced to following:

\[
\frac{\partial \hat{u}}{\partial t} = -\nu |\hat{k}| \hat{u} + \mathbf{n}_l \tag{5.18}
\]

and

\[
\frac{\partial \hat{\rho}}{\partial t} = -\frac{\nu}{\Pr} |\hat{k}| \hat{\rho} + n_{\ell \rho} , \tag{5.19}
\]

where

\[
\mathbf{n}_l = \mathbf{u} \times \mathbf{\omega} - ik \cdot \hat{\tau} + \frac{\hat{\rho} g}{\rho_0} - \frac{k}{k \cdot k} \left( k \cdot \left( \mathbf{u} \times \mathbf{\omega} - ik \cdot \hat{\tau} + \frac{\hat{\rho} g}{\rho_0} \right) \right) , \tag{5.20}
\]

\[
n_{\ell \rho} = -ik \cdot (\hat{u} \hat{\rho} + f) - \frac{\partial \rho_s}{\partial z} \hat{u}_{k_z} , \tag{5.21}
\]

\( \mathbf{k} \) is the wavenumber vector and ( \( \hat{\cdot} \) ) the Fourier transform operator.

All the simulations are solutions to (5.18) with the addition of a forcing term in the momentum equations. Dealias errors are prevented by truncating the fields in wavenumbers above 2/3 of the maximum wavenumber of the simulation grid. To advance the velocity and density perturbation fields in time, a third-order explicit exponential time differencing (ETD) algorithm was used (Cox & Matthews, 2002). It involves exact integration of the governing equations followed by an approximation of an integral involving only the nonlinear terms \( \mathbf{n}_l \) and \( n_{\ell \rho} \). A detailed derivation of the method is presented in appendix A.

In all cases, a Prandtl number \( \Pr \) of one was assumed. The eddy diffusion residual flux model was used for all cases:

\[
f \approx -\nu_t \nabla \rho \ , \tag{5.22}
\]
where \( \nu_t \) is the eddy viscosity as calculated by the chosen eddy viscosity model for the residual stress tensor.

The grid size was chosen so as the effective maximum wavenumber, the maximum non-truncated wavenumber, has the same value as the filter cutoff wavenumber used in table 4.2. The filter width \( \Delta \), used in the calculation of the residual stress tensor models, is assumed to be the same as the effective grid spacing \( \delta_e \) which is \( 2/3 \) of the simulation grid spacing \( \delta \). The parameters used for each flow case are summarized in table 5.1.

### 5.4.2 Simulation Results and discussion

In order to evaluate the models performance we start by analyzing how well the LES simulations reproduce – or fail to – the mean horizontal, vertical and potential energy compared to the filtered DNS cases. The horizontal kinetic energy \( E_h \), the vertical kinetic energy \( E_v \) and the potential energy \( E_p \) are defined as follow:

\[
E_h = \frac{(u_1^2 + u_2^2)}{2} ,
\]

Table 5.1: LES numerical simulation parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>F3</th>
<th>F2</th>
<th>F1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal domain size to grid spacing ( L_h/\delta )</td>
<td>192</td>
<td>192</td>
<td>192</td>
</tr>
<tr>
<td>Vertical domain size to grid spacing ( L_v/\delta )</td>
<td>24</td>
<td>48</td>
<td>96</td>
</tr>
<tr>
<td>Horizontal size to effective grid spacing ( L_h/\delta_e )</td>
<td>128</td>
<td>128</td>
<td>128</td>
</tr>
<tr>
<td>Vertical size to effective grid spacing ( L_v/\delta_e )</td>
<td>16</td>
<td>32</td>
<td>64</td>
</tr>
<tr>
<td>Effective grid spacing to Ozmidov length ( \delta_e/L_o )</td>
<td>6.25</td>
<td>2.32</td>
<td>0.79</td>
</tr>
<tr>
<td>Effective grid spacing to Buoyancy length ( \delta_e/L_b )</td>
<td>0.17</td>
<td>0.09</td>
<td>0.04</td>
</tr>
<tr>
<td>Gravity acceleration ( g_z )</td>
<td>-1.0</td>
<td>-1.0</td>
<td>-1.0</td>
</tr>
<tr>
<td>Reference density ( \rho_0 )</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Density gradient ( \frac{\partial \rho_s}{\partial z} )</td>
<td>-577.31</td>
<td>-143.86</td>
<td>-35.96</td>
</tr>
<tr>
<td>Kinematic viscosity ( \nu \times 10^{-4} )</td>
<td>1.085</td>
<td>1.085</td>
<td>1.085</td>
</tr>
</tbody>
</table>
\[ E_v = \frac{(u_3^2)}{2} \]  \hspace{1cm} (5.24)

and

\[ E_p = \frac{g}{\rho_0} \left( \frac{\partial \rho_s}{\partial z} \right)^{-1} \rho^2 . \]  \hspace{1cm} (5.25)

The anisotropy of the velocity field is measured by the ratio \( E_v/E_h \). Since the vertical motions interact directly with the potential energy, it is also informative to analyze the potential to vertical energy ratio \( E_p/E_v \).

Reproducing correctly the quantities presented above is the most basic requirements for a residual stress model. We can make a more rigorous benchmark for the models by analyzing their capability of reproducing not only the energy correctly but also each quantity of the mean energy budget equations. The energy budget equations, disregarding viscous effects, are:

\[ \frac{\partial E_h}{\partial t} = F - T_h - P - \mathcal{P}_r, \]  \hspace{1cm} (5.26)

\[ \frac{\partial E_v}{\partial t} = -T_v + P - B - \mathcal{P}_r, \]  \hspace{1cm} (5.27)

and

\[ \frac{\partial E_p}{\partial t} = -T_\rho + B - \mathcal{P}_r, \]  \hspace{1cm} (5.28)

where \( T_h, T_v \) and \( T_\rho \) are the nonlinear transfer rates, which have zero mean value; \( F \) is the prescribed forcing; \( P \) is pressure work; \( B \) is the buoyancy flux; \( \mathcal{P}_r, \mathcal{P}_r \) and \( \mathcal{P}_r \) are the energy transfer rate due to residual motions, also referred to as sub-grid scale (SGS) dissipation rates.

In the flows analyzed energy is injected solely in the horizontal motions. Pressure work provides a net source of energy for vertical motions, drawn from horizontal kinetic energy. The buoyancy flux transfers energy between vertical motion and potential energy. In the LES simulations, the residual motions will have a net effect of removing energy from each energy quantity from the flows. Since stratification
imposes anisotropy in the flow, it is also interesting to analyze the SGS dissipation anisotropy (\( \mathcal{P}_v/\mathcal{P}_h \)) produced by each model.

### 5.4.2.1 Results for case F3

The errors for each residual stress model regarding the total energy components for the most strongly stratified case is shown in figure 5.2. The tested models are listed in the vertical axis while the errors – compared to DNS values – is presented in the horizontal axis. Different data points are used for each of the total energy components analyzed.

Since in all cases the horizontal spectra are forced to prescribed values for small wavenumbers, it is expected for errors in the horizontal kinetic energy to be small for all models. Figure 5.2 shows that that is indeed the case. The three eddy viscosity models, when used without the extension proposed in this work, produce large errors in the prediction of the vertical kinetic energy. The error in the vertical kinetic energy
energy for Vreman, dynamic Smagorinsky, and Piomelli models are of $\sim 25\%$, $\sim 30\%$ and $\sim 35\%$ respectively. This error also induces large errors in the kinetic energy anisotropy $E_v/E_h$ and the potential to vertical energy ratio $E_p/E_v$.

Figure 5.2 clearly shows that the introduction of the nonlinear $\overline{P}$ tensor greatly improves all models. All the errors for the models extended with the $\overline{P}$ tensor become smaller than 10 percent. Vreman’s model and the dynamic Smagorinsky with constant value for $C_\beta$ performs markedly well. The models which calculate dynamically the coefficient $C_\beta$ did not produce better results than their version with a constant coefficient, while still producing much better results then their version without any model for $\tau_p$.

Figure 5.3 shows the errors in the components of the mean energy budget equation. Overall the errors are larger than those in the energy quantities. We note that, while for the first quantities analyzed one of the components ($E_h$) were almost fixed for all simulations, none of the energy budget elements show in figure 5.3 were

![Graph showing error (%) for different models](image-url)
fixed. Therefore, the errors propagate to all different elements of the budget equation. Therefore, reproducing exactly all the components is a much more difficult task. For the models without the extension proposed in this work, the largest errors appear in the SGS dissipation of vertical kinetic energy $P_{rv}$. When the models are extended with the constant-coefficient $P$ model, this error is reduced at the expense of a slight increase of the error in the SGS dissipation of horizontal motions. Nevertheless, the SGS dissipation anisotropy and pressure work errors are also minimized. While the proposed extension helps to reproduce the correct SGS dissipation rate anisotropy, the errors in each component of the total SGS dissipation are still significant. This indicates that the eddy viscosity part of the models still needs improvement, but that is beyond the scope of this work.

It is interesting to notice that, for the models with a dynamic calculation of $C_\beta$, the SGS dissipation rate of vertical kinetic energy $P_{rv}$, contrarily to the other cases, is under-predicted. So is the SGS dissipation rate anisotropy. Those results suggest that the calculated values for $C_\beta$ might be larger then they should be. Figure 5.4 shows the probability distribution function of the coefficient produced by each model, together with that from filtered DNS. Both methods of dynamic calculation of $C_\beta$
Figure 5.5: P.d.f.s of vertical component $e_z$ of the extremal eigenvector of the energy redistribution tensor $\mathbf{R}$, produced by different residual stress models in large eddy simulations of case F3.

indeed produce larger values. While the most probable calculated from DNS data is 0.093, for both dynamic methods it is around 0.12. We note that, overall, the values calculated using Piomelli’s approach are larger than those from Lilly’s dynamic method.

We now evaluate how well each model reproduces the correct alignment for the energy redistribution tensor $\mathbf{R}$, defined in equation 2.27. In the analysis presented in Section 4, we show that eddy viscosity models are inherently unable to reproduce the correct alignment and that adding the $\mathbf{P}$ tensor to the model tensor basis might improve the results. We were able to reproduce those results in the LES simulations, as shown in figure 5.5. The eddy viscosity models, when used with the proposed extension, produce markedly better alignment for the energy redistribution tensor, qualitatively similar to that from the filtered DNS case.

5.4.2.2 Results for case F2

We now draw our attention into the results from LES simulations of case F2. The density stratification in case F2 is weaker than that of case F3, but the grid spacing
is still larger than the Ozmidov length for the case. Therefore all resolved scales are still in the theoretical anisotropic range.

The errors in the total energy components produced by each model are shown in figure 5.6. Similarly to the F3 case, pure eddy viscosity models are unable to reproduce the correct vertical kinetic energy and, therefore, the correct anisotropy. When the models are extended with the proposed tensor, the errors are markedly reduced. The largest errors in those cases are around ten percent. We note that errors in these improved models are larger in case F2 than in case F3. At first sight, that might appear unexpected as case F3 is more strongly anisotropic, therefore theoretically more difficult to reproduce. A possible cause for the smaller errors in case F3 is the larger areas of quiescent regions. Portwood et al. (2016) shows that, in case F3, the strong stratification causes turbulence to be confined in a small highly turbulent volume patch of the flow. Therefore, provided that the residual stress models are able to "turn-off" adequately, the regions in the F3 case flow that are affected by the residual stress models are smaller than that for case F2 and the residual stress model might have a smaller impact on the mean error of the mean energy elements.

Figure 5.7 shows the error in the energy budget components for case F2. Similarly to case F3, the main improvement caused by the addition of the $\overline{P}$ tensor is a better representation of the SGS dissipation rate of vertical kinetic energy, which also improves the SGS dissipation anisotropy. We note that, for this case, the error in the SGS dissipation rate of potential energy $Pr_\rho$ was significant for most cases, suggesting improvement in the residual density flux model is needed.

Finally, figure 5.8 shows that the representation of the statistical alignment of the energy redistribution tensor is greatly improved when the proposed extension is used with different eddy viscosity models.
Figure 5.6: Error in: horizontal kinetic energy ($E_h$); vertical kinetic energy ($E_v$); potential energy ($E_p$); kinetic energy anisotropy ($E_v/E_h$); potential to vertical energy ratio ($E_p/E_v$) for different residual stress models in large eddy simulations of case F2.

Figure 5.7: Error in: mean SGS dissipation rate of horizontal kinetic energy ($\mathcal{P}_{rh}$); mean SGS dissipation rate of vertical kinetic energy ($\mathcal{P}_{rv}$); SGS dissipation anisotropy ($\mathcal{P}_{rv}/\mathcal{P}_{rh}$); mean SGS dissipation rate of potential energy ($\mathcal{P}_{rp}$); mean buoyancy flux ($B$); mean pressure work ($P$) for different residual stress models in large eddy simulations of case F2.
5.4.2.3 Results for case F1

The LES simulations for case F1 are resolved up to the theoretically isotropic scales. Therefore, while a large range of the resolved scales is anisotropic, the subgrid motions are expected to be closer to that of isotropic turbulence. Figure 5.9 shows that the largest error in the energy for the LES simulations of case F1 comes from potential energy. As expected, for pure eddy viscosity models, the error in the vertical kinetic energy is not as large as for cases F2 and F1. Still, adding the proposed extension to the eddy viscosity models improves the representation of vertical motions, which in turn improves the results for the kinetic energy anisotropy and the potential energy.

The error in the components of the energy budget equation is shown in figure 5.10. For pure eddy viscosity models, the largest error appears in the SGS dissipation rate of vertical kinetic energy $P r_v$. Again, adding the proposed extension to the models improves the reproduction of the correct anisotropy. The most significant errors for the improved models come from the SGS dissipation of potential energy, suggesting the residual density flux model needs to be improved, but that is beyond the scope of this work.
Figure 5.9: Error in: horizontal kinetic energy ($E_h$); vertical kinetic energy ($E_v$); potential energy ($E_p$); kinetic energy anisotropy ($E_v/E_h$); potential to vertical energy ratio ($E_p/E_v$) for different residual stress models in large eddy simulations of case F1.

Figure 5.10: Error in: mean SGS dissipation rate of horizontal kinetic energy ($\mathcal{P}_{rh}$); mean SGS dissipation rate of vertical kinetic energy ($\mathcal{P}_{rv}$); SGS dissipation anisotropy ($\mathcal{P}_{rv}/\mathcal{P}_{rh}$); mean SGS dissipation rate of potential energy ($\mathcal{P}_{r\rho}$); mean buoyancy flux ($B$); mean pressure work ($P$) for different residual stress models in large eddy simulations of case F1.
Figure 5.11: P.d.f.s of vertical component $e_z$ of the extremal eigenvector of the energy redistribution tensor $\mathcal{R}$ produced by different residual stress models in large eddy simulations of case F1.

Figure 5.11 shows the statistical alignment of redistribution tensor produced by the models. All models reproduce the expected nearly isotropic behavior.
CHAPTER 6
CONCLUSIONS

In this work, we analyzed the modeling of the residual stress tensor for flows subject to strong stable density stratification. We hypothesized that, if the Ozmidov length scale is not resolved in a LES simulation, then, the common hypothesis of local statistical isotropy will not hold and models for the residual stresses must accurately reproduce the correct expected anisotropy.

As a preliminary analysis, presented in Section 4, we tested our hypothesis by calculating exactly the residual stress tensor using DNS data of flows with different levels of stratification. Using tensor decomposition theorems, we exactly extracted the part of the residual stress tensor that is in-phase with the strain rate tensor $\mathbf{\mathcal{S}}$. We were able to show that any model that is based on a linear relationship with the strain rate tensor would be inherently incapable of reproducing the correct energy transfer anisotropy in flows simulations were the Ozmidov length is not resolved.

Using the same tensor decompositions we tested several levels of approximations for the residual stress tensor using both linear and non-linear relationship to $\mathbf{\mathcal{S}}$ together with a linear relationship with a tensor formed by the Lie product of $\mathbf{\mathcal{S}}$ and $\mathbf{\mathcal{W}}$, referred in the text as $\mathbf{\mathcal{P}}$. It was shown that the part of the residual stress tensor that is proportional to $\mathbf{\mathcal{P}}$ played a key role in reproducing the correct anisotropy. An approximation for $\mathbf{\tau}$ formed by a non-linear relationship to $\mathbf{\mathcal{S}}$ and a linear relationship to $\mathbf{\mathcal{P}}$ was shown to provide optimal reproduction of the true tensor. We also concluded that a linear combination of both is sufficient to reproduce the correct anisotropy of the residual stresses.
From the tensor decomposition theorems used in this work, we provided a mathematical foundation for modeling independently the parts of the residual stress tensor that is in-phase and out-of-phase with the strain rate tensor. That allowed us to focus this work exclusively in modeling the out-of-phase part of the residual stress tensor $\mathbf{\tau}^\perp \mathbf{S}$ while taking advantage of current eddy viscosity models.

In Section 5 we presented three options for modeling $\mathbf{\tau}^\perp \mathbf{S}$. In the first one, a constant coefficient is used. In the other two, the coefficient is calculated dynamically using two different approaches. We tested three different eddy viscosity models: Vreman’s model (Vreman, 2004), Germano’s dynamic Smagorinsky model with Lilly’s modification (Lilly, 1992) and Piomelli’s localized dynamic model (Piomelli & Liu, 1995). Large eddy simulations similar to the three DNS cases analyzed in Section 4 were run with both the original and extended eddy viscosity model. In all cases, the addition of the proposed extension markedly improved the results, mainly the reproduction of the correct anisotropy. Out of all eddy viscosity models tested, the most computationally inexpensive is Vreman’s model. This model, when extended with the proposed $\mathbf{\overline{P}}$ model, was able to perform as well as the other dynamic eddy viscosity models tested.

For the cases analyzed a dynamic calculation for $C_\beta$ was shown to be unnecessary. It was also shown that the proposed methods for calculating $C_\beta$ dynamically could produce values larger than the expected values. Nevertheless, dynamic calculation of $C_\beta$ could be necessary for more complex flows with different boundary conditions. Meneveau (2012) reviews several different approaches that use Germano’s identity that could potentially be helpful in developing better dynamic models for $C_\beta$ as future work.
APPENDIX

DERIVATION OF THIRD ORDER ADAPTIVE EXPOENTIAL TIME DIFFERENCING SCHEME

In this appendix, we derive a third-order adaptive explicit exponential time differencing scheme. Based on the steps provided by Cox & Matthews (2002), we start with a model ordinary differential equation:

\[
\frac{\partial u}{\partial t} = cu + F(u, t)
\]  

(A.1)

where \( c \) is a constant and \( F \) represents non-linear terms. Then, we multiply the equation by the integrating factor \( e^{-ct} \) and integrate the equation over a single time-step from \( t = t_n \) to \( t = t_{n+1} = t_n + \delta \). The result is

\[
u(t_{n+1}) = u(t_n) e^{c\delta} + e^{c\delta} \int_0^\delta e^{-c\tau} F(u(t_n + \tau), t_n + \tau) \, d\tau
\]  

(A.2)

This formula is exact. The essence of the ETD method is deriving an approximation to the integral in this equation. For that, we use a similar approach to that of the third-order Adams-Bashforth method.

Using previous time-step values for \( F \), a parabola is fitted and extrapolated to compute the integral in equation A.2. Let \( F_n \) be the value of the non-linear term at a
time-step \( n \) and \( \delta_n = t_n - t_{n-1} \), the parabola, with origin at \( t = t_n \), that fits through \( F_n, F_{n-1} \) and \( F_{n-2} \) is given by

\[
f(\tau) = \left( \frac{F_n \delta_{n-1} - (\delta_n + \delta_{n-1}) F_{n-1} + \delta_n F_{n-2}}{\delta_n^2 \delta_{n-1} + \delta_n^2 \delta_{n-1}} \right) \tau^2 + \left( \frac{(2 \delta_n \delta_{n-1} + \delta_n^2) (F_n - F_{n-1}) + \delta_n^2 (F_{n-2} - F_{n-1})}{\delta_n \delta_{n-1} (\delta_n + \delta_{n-1})} \right) \tau + F_n .
\] (A.3)

The integral in equation A.2 is then approximated by:

\[
e^{c\delta} \int_{0}^{\delta} e^{-c\tau} F(u(t_n + \tau), t_n + \tau) \, d\tau \approx e^{c\delta} \int_{0}^{\delta} e^{-c\tau} f(\tau) \, d\tau
\] (A.4)

which is amendable to exact integration.

The final equation will have the form:

\[
u_{n+1} = u_n e^{c\delta} + A(c, \delta, \delta_n, \delta_{n-1}) F_n + B(c, \delta, \delta_n, \delta_{n-1}) F_{n-1} + C(c, \delta, \delta_n, \delta_{n-1}) F_{n-2} ,
\] (A.5)

where

\[
A = \frac{c^2 \left( \delta_n^3 \left( e^{c\delta} - 1 \right) + \delta_n \left( \delta_{n-1} \left( e^{c\delta} - 1 \right) - 2\delta \right) - \delta (\delta_{n-1} + \delta) \right)}{c^3 \delta_n (\delta_n + \delta_{n-1})} + \frac{c (2 \delta_n \left( e^{c\delta} - 1 \right) + \delta_{n-1} \left( e^{c\delta} - 1 \right) - 2\delta) + 2 \left( e^{c\delta} - 1 \right)}{c^3 \delta_n (\delta_n + \delta_{n-1})},
\] (A.6)

\[
B = \frac{c^2 \delta (\delta_n + \delta_{n-1} + \delta) + c \left( \delta_n \left( -e^{c\delta} \right) - \delta_{n-1} e^{c\delta} + \delta_n + \delta_{n-1} + 2\delta \right) - 2 e^{c\delta} + 2}{c^3 \delta_n \delta_{n-1}}
\] (A.7)

and

\[
C = \frac{c^2 (-\delta)(\delta_n + \delta) + c \left( \delta_n \left( e^{c\delta} - 1 \right) - 2\delta \right) + 2 \left( e^{c\delta} - 1 \right)}{c^3 \delta_{n-1} (\delta_n + \delta_{n-1})}.
\] (A.8)

When \(|c\delta| \ll 1\) care must be taken in the evaluation of the coefficients due to large rounding errors in its numerical computation. For that cases, Taylor series for
the coefficients should be used. The coefficients using a third order approximation are then given by

\[
A \approx \frac{c^2\delta^3}{6} + \frac{c\delta^2(3\delta_n^2 + 3\delta_n\delta_{n-1} + 2\delta_n\delta + \delta_{n-1}\delta)}{6\delta_n(\delta_n + \delta_{n-1})} + \frac{\delta(6\delta_n^2 + 6\delta_n(\delta_{n-1} + \delta) + \delta(3\delta_{n-1} + 2\delta))}{6\delta_n(\delta_n + \delta_{n-1})},
\]

(A.9)

\[
B \approx -\frac{c\delta^3(\delta_n + \delta_{n-1})}{6\delta_n\delta_{n-1}} - \frac{\delta^2(3\delta_n + 3\delta_{n-1} + 2\delta)}{6\delta_n\delta_{n-1}},
\]

(A.10)

and

\[
C' \approx \frac{c\delta_n\delta^3}{6\delta_{n-1}(\delta_n + \delta_{n-1})} + \frac{\delta^2(3\delta_n + 2\delta)}{6\delta_{n-1}(\delta_n + \delta_{n-1})},
\]

(A.11)

In this work, an ETD scheme were preferred over standard integrating factor (IF) methods because, when compared to an ETD method with the same order, IF methods have larger error constants (Cox & Matthews, 2002), among other weakness, such as not preserving the fixed points of the original ODE being solved.
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