Subgrid Scale Modeling for Large Eddy Simulation of Buoyant Turbulent Flows

Niranjan Shrinivas Ghaisas
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By Niranjan Shrinivas Ghaisas

Entitled
SUBGRID SCALE MODELING FOR LARGE EDDY SIMULATION OF BUOYANT TURBULENT FLOWS

For the degree of Doctor of Philosophy

Is approved by the final examining committee:

Steven H. Frankel
Chair

Jun Chen

Carl R. Wassgren

Jie Shen

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Approved by Major Professor(s): Steven H. Frankel

Approved by: David C. Anderson 08/20/2013
Head of the Graduate Program Date
SUBGRID SCALE MODELING FOR LARGE EDDY SIMULATION OF
BUOYANT TURBULENT FLOWS

A Dissertation
Submitted to the Faculty
of
Purdue University
by
Niranjan S. Ghaisas

In Partial Fulfillment of the
Requirements for the Degree
of
Doctor of Philosophy

December 2013
Purdue University
West Lafayette, Indiana
To my family.
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5.18 Correlation coefficients $\rho(\tau_{ij}, \tau_{ij}^{mod})$, where the subscripts $ij$ denote either 11-, 13- or 33- components, and the superscript $mod$ denotes any one among GM, Smagorinsky, Vreman and Sigma models. All 19 data sets, with fixed grid-filter size $\bar{\Delta} / \delta = 4$.

5.19 Correlation coefficients $\rho(\tau_{ij}, \tau_{ij}^{mod})$, where the subscripts $ij$ denote either 11-, 13- or 33- components, and the superscript $mod$ denotes any one among GM, Smagorinsky, Vreman and Sigma models. Varying grid-filter size $\bar{\Delta} / \delta$, and correlations extracted from (a) stationary passive scalar data set 3, and (b) decaying active scalar data set 14.

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ABSTRACT

Ghaisas, Niranjan S. Ph.D., Purdue University, December 2013. Subgrid scale modeling for large eddy simulation of buoyant turbulent flows. Major Professor: Steven H. Frankel, School of Mechanical Engineering.

Buoyancy effects due to small density differences commonly exist in turbulent fluid flows occurring in nature and in engineering applications. The large eddy simulation (LES) technique, which is being increasingly used for simulating buoyant turbulent flows, requires accurate modeling of the subgrid scale (SGS) momentum and buoyancy fluxes. This thesis presents a series of LES and direct numerical simulation (DNS) studies towards a priori and a posteriori evaluation of existing SGS models, and development of new SGS models for the buoyancy flux. This thesis also presents the application of LES, in elucidating qualitative physical features and accurate measures of important quantities such as turbulence budgets, in a simplified flow configuration involving buoyancy effects on a turbulent flow.

Three existing LES SGS models for buoyant turbulent flows are assessed by performing LES and comparing the results to DNS data found in the literature. The test problem for which the accuracy of these existing LES SGS models is studied is the flow in a three-dimensional thermal-driven cavity. In addition to serving as an excellent test case for SGS models, this problem demonstrates interesting phenomena related to the interaction between buoyancy and wall-bounded turbulence. Particularly, the effect of buoyancy on the vertical wall boundary layer is studied.

One drawback of existing LES models is that the SGS diffusivity is dependent solely on the velocity field. A new model for the SGS diffusivity is developed, which is expected to represent the buoyancy flux more accurately. Improvements are also made to the dynamic procedure for determining the model coefficient by taking into account the contribution of the buoyant force.
DNS of a number of homogeneous non-buoyant and buoyant flow configurations is carried out using a pseudo-spectral method, which is free from numerical errors, and artifacts such as the effect of artificial boundary conditions. A well-validated and accurate DNS database is generated, and employed for a priori evaluation of various SGS models. The ability of different models to predict the orientations and magnitudes of buoyancy fluxes is evaluated, and four new models are proposed. Preliminary a posteriori evaluation indicates that these models show an improvement over existing models.

Finally, the horizontal buoyant jet configuration, which is an example of a free-shear turbulent flow affected by buoyancy, is studied using LES. A numerical investigation of this novel flow configuration aids in outlining the physical mechanisms leading to suppression and enhancement of turbulent mixing in different regions of the flow field. Qualitative and quantitative comparisons to previous experimental results are also made, demonstrating the ability of the LES technique to accurately simulate buoyancy and stratification effects in turbulent flows.
1. INTRODUCTION

1.1 Background

A vast majority of fluid flows occurring in nature and encountered in engineering applications are turbulent in nature. Turbulent flows in engineering are encountered in practically every industry - from chemical or food processing to metallurgical industry, and from aerospace to automobiles. Study of natural phenomena such as formation of cloud systems, tornadoes and cyclones in the atmosphere, and deep sea currents and coastal upwelling of nutrients in the ocean, invariably involve a study of turbulence.

While a formal definition of turbulence has not yet been established, there is a general agreement on some typical features exhibited by turbulent flows [107]. Unsteady, irregular and inherently three-dimensional motions in turbulent flows distinguish such flows from laminar flows, which are much more orderly, and may be steady and two-dimensional. Turbulent flows are also known to be highly diffusive in nature, and are much better at mixing a transported species, than laminar flows. Finally, turbulent flows are dissipative, and cannot continue in the absence of an energy production mechanism.

Any one or a combination of a velocity gradient, rotational motion, or a density gradient in a flow, can potentially act as the energy production mechanism, and can set up a cascade of length and velocity scales, leading to turbulence. Turbulence sustained by velocity gradients, in the absence of, or far away from any boundaries, is known as free-shear turbulence. The classical jet, wake and mixing layer configurations are examples of free-shear turbulent flows [86]. Density gradients in a fluid lead to volumetric forces, called buoyant forces, which can generate or inhibit turbulence. Although stratification may equally act to generate turbulent motions, the term 'stratified turbulence' is usually reserved for flows in which density gradients, or
stratification, acts to inhibit turbulent motions. This document is almost exclusively related to the interaction of buoyant forces and turbulence.

Early studies of the subject of turbulence were purely experimental and theoretical in nature. The pioneering dye-visualisation experiment of Reynolds [91] can be said to have started the study of this subject. The seminal theory proposed in a series of studies starting with Kolmogorov [57], based on three hypothesis of local isotropy and similarity, provides the most widely accepted picture of turbulence till date. The theory proposed that a turbulent flow is made up of an infinitely large number of scales between the largest scale defined by the domain of interest, and the smallest scale defined by the large scale forcing and the fluid viscosity. Based on the theory, the size of the smallest scale, the rate of energy transfer between scales, as also the rate of dissipation of energy at different scales were computed.

With the beginning of the use of computers for scientific pursuits in the 1960s, turbulent flows have been analyzed using numerical simulation tools as well. Over the years, three broad simulation principles have emerged, namely Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds’ Averaged Navier Stokes (RANS). DNS and RANS are at the two extreme ends of the spectrum. All length and time scales are resolved in DNS, while the RANS approach assumes a clear separation of length scales between a ‘mean’ and a ‘fluctuation’ [86]. The largest length scale is resolved in a RANS computation, while the effect of all smaller scales is modeled. Thus, some modeling effort is required in RANS, while absolutely no modeling is involved in DNS. On the other hand, the computational expense required to resolve all scales is very large for DNS, while it is much smaller in case of RANS. In a LES, which lies between these two extremes, most of the energy containing scales are resolved, while the effect of the remaining scales is modeled. The modeling effort, and computational expense incurred, are thus, intermediate to the modeling effort and computational expense incurred in RANS and DNS [86]. LES has been used as the primary simulation tool for studying buoyant turbulence in this document.
The equations governing LES are obtained by performing a filtering operation on the Navier-Stokes equations. This filtering operation gives rise to conservation equations for filtered velocities, species, etc., and contain unclosed terms which account for the effect of the scales left out by the filtering operation. These are called sub-grid (SGS) terms, and need to be modeled in order to obtain equation closure, and solve the filtered Navier-Stokes equations. The accuracy of a large eddy simulation depends, to a large extent, on accurate modeling of these SGS terms, more so in cases where the essential rate-controlling processes occur at small scales [87].

1.2 Objectives

This document is concerned with evaluation and improvement of SGS models for buoyant turbulent flows, as well as application of the large eddy simulation technique to problems involving interactions between turbulence and buoyancy.

The primary objective of the first part of this work will be to study some simple SGS models for buoyant turbulent flows, by conducting high order numerical simulations. Large eddy simulations will be conducted to evaluate existing SGS models a posteriori. Results from previous high fidelity DNS benchmark studies will be used for comparisons to present LES results. This part of the document will also attempt to study the physics of the test case considered, specifically emphasizing the changes induced by the presence of volumetric buoyant body forces.

Modeling for LES of buoyant flows involves modeling the unclosed terms arising in the momentum conservation equations, as well as the unclosed terms arising in the accompanying scalar transport equation. Improvements to existing SGS models for buoyant turbulent flows will be explored. The objective of this part is to improve SGS models in order to overcome deficiencies associated with modeling the unclosed terms in the scalar transport equation, and the methodology for estimating the coefficient involved in the SGS models, taking into account the contribution of the buoyancy force.
In the second part, direct numerical simulations will be conducted and employed for *a priori* studies of some sophisticated LES models. The classical concept of ‘turbulence in a box’ is extremely useful in turbulence modeling, since the behaviour of the small scales can be isolated and simulated with a high degree of accuracy and efficiency. For this reason, direct numerical simulations will be carried out in fully periodic domains with a pseudo-spectral method. The DNS data generated will be used in *a priori* studies, and the insight gained will be utilized in building simpler, more accurate, alternatives to existing SGS models for buoyant turbulent flows.

The final objective of this document will be to apply the technique of LES to study the physics of a horizontally issuing buoyant jet. This flow configuration is an idealized model for many situations of engineering or environmental interest, and involves buoyancy-turbulence interactions in a simple geometry. The objective will be to reproduce existing experimental results, and supplement the current experimentally gained knowledge of horizontal buoyant jets by large eddy simulations.

### 1.3 Overview

A broad overview of this document is presented in this section. Chapter 2 starts with a description of the governing equations for LES, which are the filtered Navier-Stokes equations. The SGS terms which arise due to the filtering operation are unclosed, and need to be modeled. An extensive review of many existing SGS models for buoyant turbulent flows is presented, and the properties of different SGS models are discussed.

The first part of the thesis, involving Chapters 3 and 4, is concerned mainly with a specific class of models, known as eddy-viscosity type models. Chapter 3 deals primarily with evaluation of three eddy-viscosity type models. The configuration chosen for testing these models is the thermal-driven flow in a three-dimensional confined enclosure, or a thermal-driven cavity. The numerical code used for simulations is first discussed. SGS models are evaluated by performing LES and comparing the
results obtained to benchmark DNS results in the literature. The performance of eddy-viscosity models is also compared to that of a Stretched-Vortex model, which is a representative of non-eddy-viscosity type models. The models are evaluated for differing strengths of the imposed temperature differential, which is the driving force behind convection. Based on the accuracy of our LES simulations, physics of the flow in the thermal-driven cavity is analyzed in some detail in this chapter.

A review of existing eddy-viscosity models for buoyant turbulent flows reveals that most models for SGS diffusivity are not sensitive to temperature (or scalar) fluctuations. Chapter 4 presents the derivation of a new eddy-viscosity type model for the SGS diffusivity, with explicit dependence on the temperature field. The theoretical formulation of the model is presented, followed by tests in LES of thermal-driven cavity.

The focus of the second part of this thesis, Chapter 5, is on DNS of homogeneous flows with the aim of a priori evaluation of some of the more sophisticated SGS models. A pseudo-spectral algorithm is used to conduct DNS of homogeneous flows in fully periodic cubical domains. Different flow conditions, involving isotropic non-buoyant turbulence with a transported passive scalar, as well as anisotropic buoyancy driven turbulence, are simulated. Based on this DNS data, Dynamic Structure and Gradient (non-eddy-viscosity) type models, in addition to the eddy-viscosity models, are studied in an a priori sense. Four new models are proposed, and a preliminary a posteriori study in the homogeneous configuration is also carried out.

The dynamics of a horizontal buoyant jet flow configuration is studied via LES in the last part of the thesis, in Chapter 6. This novel configuration, set up by injecting a jet of fluid heavier than the ambient, has not been widely studied previously, and is markedly different from the vertically released buoyant jet configuration. The focus of this chapter is on quantitative comparison to available experimental data, and on identification of the key physical features of the flow, brought about by the interplay between turbulence and buoyancy.

A summary of the entire work is preseneted in Chapter 7.
2. SUB-GRID SCALE MODELS FOR BUOYANT TURBULENT FLOWS

Buoyant flows are flows driven by, or affected by, density differences in a fluid. The density differences may be caused due to the presence of a component contributing to the density, such as a dissolved salt. Temperature of the fluid can also cause density differences which cause fluid motion. The equations governing large eddy simulation of turbulent flows with a buoyancy induced body force are described in the next section. The different subgrid scale models developed over the years are then described. This chapter closes with some remarks about the testing of these SGS models and outlines scope for further model development.

2.1 Governing Equations for LES

The filtered equations governing LES of an incompressible, buoyant fluid are

\[
\frac{\partial \tilde{u}_i}{\partial x_i} = 0 \tag{2.1}
\]

\[
\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} + \tilde{F}_i - \frac{\partial \tau_{ij}}{\partial x_j} \tag{2.2}
\]

\[
\frac{\partial \tilde{\phi}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\phi}}{\partial x_j} = k_{\phi} \frac{\partial^2 \tilde{\phi}}{\partial x_j \partial x_j} - \frac{\partial \tau_{j\phi}}{\partial x_j} \tag{2.3}
\]

Equations (2.1) and (2.2) are conservation equations for mass and momentum respectively. \(u_i\) denotes the velocity in the \(i\)-direction, with \(i = 1, 2, 3\) denoting the three cartesian coordinate directions. \(p\) stands for the pressure, divided by a reference density, \(\rho_0\), while \(\nu\) stands for the viscosity of the fluid. These equations employ the Boussinesq approximation, whereby density variations are neglected in all terms except for the body force term, \(F_i\). This assumption is valid for density differences smaller than about 5% of the reference density, a situation which is easily satisfied in the atmosphere, the ocean, and in some engineering situations [86]. Under the
Boussinesq approximation, the density is further assumed to be governed by a linear equation of state

\[ \rho(\phi) = \rho_0 [1 + \beta_\phi \phi], \tag{2.4} \]

where \( \phi \) is a scalar field affecting the density, and \( \beta_\phi \) is the expansion coefficient of the fluid with respect to the scalar \( \phi \). Equation (2.3) governs the conservation of this scalar field, with \( k_\phi \) denoting the molecular diffusivity of the scalar in the fluid. It may be noted that, in contrast to a ‘passive scalar’, which is simply transported by a fluid, \( \phi \) contributes to the density of the fluid, and thus influences the flow field. For this reason, this scalar can be said to be an ‘active scalar’. As mentioned above, \( \phi \) may be the concentration of a salt, a sugar, or any other substance dissolved in the fluid. The temperature of the fluid may also be considered to be the scalar, with \( \beta_\phi \) then representing the thermal expansion coefficient. The terms ‘species’, ‘thermal’, or simply, ‘scalar’, are used interchangeably in this thesis, and it should be clear that they all refer to a scalar field affecting the density via the linear equation of state, equation (2.4).

\( F_i \) in equation (2.2) denotes the volumetric body force, arising due to density differences in the fluid, and is given by

\[ F_i = g_i \frac{[\rho(\phi) - \rho_0]}{\rho_0} = g_i \beta_\phi \phi, \tag{2.5} \]

where \( g_i \) denotes the acceleration due to gravity, which is considered to act in the vertically downward, or the negative \( x_3 \) direction. Thus, \( g_i = [0, 0, -9.81] m/s^2 \). It is obvious that the body force is zero when the density equals the reference density, and that any deviation from this density, \( \Delta \rho = (\rho - \rho_0) \), induces a volumetric force on the fluid and can set up fluid flow.

The overbars on all dependent variables in (2.1)-(2.3) denote filtered, instead of actual, quantities. Application of the filtering operation described above to the Navier-Stokes equations results in the last term, in each of the momentum and scalar equations, (2.2) and (2.3), respectively. The term \( \tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \) denotes the SGS
stress tensor, while $\tau_{i\phi} = \overline{u_i\phi} - \bar{u}_i\bar{\phi}$ denotes the SGS scalar flux. LES is concerned with the modeling of these quantities, and the different SGS models used in this study are described in the next few sections.

### 2.2 Classification of SGS Models

The problem of LES modeling involves determining the subgrid stress tensor in terms of resolved quantities. LES of buoyant convection differs from LES of non-buoyant convection in that a model for the SGS scalar flux $\tau_{i\phi}$ has to be specified in addition to a model for the SGS stress tensor $\tau_{ij}$ in terms of filtered quantities. LES SGS models can broadly be classified as eddy-viscosity type models, and non-eddy-viscosity type models. Models of the eddy-viscosity type assume the gradient diffusion hypothesis for the deviatoric (i.e. traceless) part of the stress tensor,

$$\tau_{ij} - \frac{1}{3} \tau_{ii} \delta_{ij} = -2\nu_{SGS} \bar{S}_{ij}$$  \hspace{1cm} (2.6)

$$\tau_{i\phi} = -k_{SGS} \frac{\partial \bar{\phi}}{\partial x_i}.$$  \hspace{1cm} (2.7)

$\nu_{SGS}$ and $k_{SGS}$ are the SGS eddy-viscosity and SGS eddy-diffusivity respectively while $S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$ is the filtered strain-rate tensor. Eddy-viscosity type models for $\nu_{SGS}$ and $k_{SGS}$ are of the form

$$\nu_{SGS} = C \ M \ (\bar{u}_i),$$  \hspace{1cm} (2.8)

$$k_{SGS} = C_\phi \ M_\phi \ (\bar{u}_i, \bar{\phi}).$$  \hspace{1cm} (2.9)

$C$ and $C_\phi$ are the model constants, while the velocity kernel, $M$, and the scalar kernel, $M_\phi$, are functions of the resolved velocity vector, and of the resolved velocity vector and resolved scalar respectively. The velocity and scalar kernels have traditionally been assumed to be identical,

$$M \equiv M_\phi,$$  \hspace{1cm} (2.10)
for example, by Lesieur and Rogallo [60], Cabot [14] and Peng and Davidson [81].

The constants $C$ and $C_\phi$ are related through a SGS Prandtl (or Schmidt) number,

$$Pr_{SGS} = \frac{C}{C_\phi} . \tag{2.11}$$

The SGS Prandtl number can be treated as a constant or determined dynamically [81]. When treated as a constant, it is usually taken to be of the same order of magnitude as the molecular Prandtl (or Schmidt) number. The molecular Prandtl number of a fluid-scalar combination is defined as the ratio of molecular viscosity of the fluid to the molecular diffusivity of the scalar in that fluid, $Pr = \nu / k_\phi$. Values ranging from 0.3 to 0.7 have been used in previous LES of buoyant flows ([81], [124]).

Different eddy-viscosity type SGS models then differ in the choice of the kernel used, the method used to specify the constant and the relation between SGS viscosity and SGS diffusivity. Non-eddy-viscosity type models specify $\tau_{ij}$ and $\tau_{i\phi}$ directly in terms of filtered quantities without resorting to a gradient diffusion assumption,

$$\tau_{ij} = \tau_{ij} (\bar{u}_i) \tag{2.12}$$
$$\tau_{j\phi} = \tau_{j\phi} (\bar{u}_i, \bar{\phi}) \tag{2.13}.$$  

These equations should be compared to equations (2.6)-(2.7) for eddy-viscosity type models above.

A number of eddy-viscosity type models are discussed in the next section. Different approaches used to specify the model coefficients are also discussed. Section 2.4 presents some non-eddy-viscosity type models occurring in the literature. For each model, the expression for the SGS stress tensor is presented, along with the associated expression for the SGS scalar flux. In the discussion below, $\langle \ldots \rangle$ denotes a quantity filtered on the implicit grid-level filter, while $\widehat{\langle \ldots \rangle}$ denotes a quantity filtered on the test-filter.
2.3 Eddy-viscosity models

Three eddy-viscosity models, namely Smagorinsky, Vreman and Sigma models, are described in detail in this section. These models have been tested extensively in this thesis. The constant coefficient and dynamic versions of these models have been written out separately in this section. Other eddy-viscosity models, not described here in detail, include

2.3.1 Constant Coefficient Smagorinsky Model

In the classical Smagorinsky model, the SGS viscosity is given by $\nu_{SGS} = (C_S \Delta^2) |\overline{S}|$. $\Delta$ is the LES filter width, the Smagorinsky kernel $|\overline{S}| = \sqrt{2S_{ij}S_{ij}}$ is the magnitude of the filtered strain-rate tensor and $C_S$ is the model constant. The SGS diffusivity is determined via a constant SGS Prandtl number. Typical values for the coefficients are $C_S = 0.16$ and $Pr_{SGS} = 0.7$.

2.3.2 Dynamic Smagorinsky Model

The model coefficient in the above can be determined via a localized dynamic procedure proposed by Germano et al. [36] and modified by Lilly [61].

$$C_S^2 = -\frac{\langle L_{ij}M_{ij} \rangle}{2 \langle M_{ij}M_{ij} \rangle}, \quad (2.14)$$

where

$$L_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j, \quad M_{ij} = -2C_S^2 \left( \Delta^2 |\overline{S}| S_{ij} - \Delta^2 |\overline{S}| \overline{S}_{ij} \right).$$

This procedure was extended by Peng and Davidson [81] to determine the constant for SGS diffusivity as

$$Pr_{SGS} = \frac{C_S^2}{C_\phi^2}. \quad (2.15)$$
with
\[
C_\phi^2 = \frac{\langle \epsilon_j Q_j \rangle}{\langle Q_j Q_j \rangle},
\]
\[
\epsilon_j = \tilde{u}_j \phi - \bar{u}_j \bar{\phi}, \quad Q_j = C_\phi^2 \left( \tilde{\Delta}^2 \bar{S} \frac{\partial \bar{\phi}}{\partial x_j} - \tilde{\Delta}^2 \bar{S} \frac{\partial \bar{\phi}}{\partial x_j} \right)
\]
The dynamic Smagorinsky model yields model constants which vary rapidly in space and time and have been known to lead to stability issues unless ad-hoc clipping or filtering in homogeneous directions is applied. In the thermal-drive cavity simulations described in Chapter 3, negative values of the constants have been clipped (to zero) and all numerators and denominators in determination of the constants have been averaged over the homogeneous $x$ direction (denoted by $\langle \ldots \rangle$). Similar procedures have been used in previous LES studies (e.g. Peng and Davidson [81]).

2.3.3 Constant Coefficient Vreman Model

A relatively recent eddy-viscosity type model proposed by Vreman [114] gives the SGS eddy-viscosity as
\[
\nu_{SGS} = C_V \Pi^g,
\]
where $\Pi^g$ is defined as
\[
\Pi^g = \sqrt{\frac{B^g_\beta}{\bar{\alpha}_{kl} \bar{\alpha}_{kl}}}.
\]
with
\[
B^g_\beta = \beta^g_{11} \beta^g_{22} - \beta^g_{12} \beta^g_{12} + \beta^g_{11} \beta^g_{33} - \beta^g_{13} \beta^g_{13} + \beta^g_{22} \beta^g_{33} - \beta^g_{23} \beta^g_{23},
\]
\[
\beta^g_{ij} = \frac{3}{\bar{\alpha}_{m} \bar{\alpha}_{n}} \bar{\alpha}_{m} \bar{\alpha}_{n}, \quad \bar{\alpha}_{ij} = \frac{\partial \bar{u}_j}{\partial x_i}
\]
A value of 0.07 was proposed by Vreman for the constant $C_V$ and has been used in this model. A constant SGS Prandtl number $Pr_{SGS} = 0.7$ is used to close the system.
2.3.4 Dynamic Vreman Model

A procedure for dynamically determining the constant $C_V$ in the Vreman model was proposed by You and Moin [125] and later extended to the passive scalar case for dynamically determining the SGS Prandtl number by You and Moin [126]. This procedure is based on assumption of global equilibrium between SGS production and dissipation and yields model constants which are independent of space but weakly dependent on time,

$$C_V = -\frac{\nu}{2} \left\{ \hat{\alpha}_{ij} \hat{\alpha}_{ij} - \hat{\alpha}_{ij} \hat{\alpha}_{ij} \right\}$$

(2.18)

$$C_{\phi} = k_{\phi} \left\{ \Pi^t \frac{\partial \hat{\phi}}{\partial x_i} \frac{\partial \hat{\phi}}{\partial x_j} - \Pi^g \frac{\partial \hat{\phi}}{\partial x_i} \frac{\partial \hat{\phi}}{\partial x_j} \right\}.$$

(2.19)

The effective SGS Prandtl number with these expressions for the model coefficients is

$$Pr_{SGS} = \frac{C_V}{k_{\phi}} \left\{ \Pi^t \frac{\partial \hat{\phi}}{\partial x_i} \frac{\partial \hat{\phi}}{\partial x_j} - \Pi^g \frac{\partial \hat{\phi}}{\partial x_i} \frac{\partial \hat{\phi}}{\partial x_j} \right\}.$$

(2.20)

$\Pi^t$ is defined as

$$\Pi^t = \sqrt{\frac{B^t_\beta}{\hat{\alpha}_{kl} \hat{\alpha}_{kl}^2}},$$

(2.21)

with

$$B^t_\beta = \beta^t_{11} \beta^t_{22} - \beta^t_{12} \beta^t_{12} + \beta^t_{11} \beta^t_{33} - \beta^t_{13} \beta^t_{13} + \beta^t_{22} \beta^t_{33} - \beta^t_{23} \beta^t_{23},$$

$$\beta^t_{ij} = \sum_{m=1}^3 \frac{\Delta m}{\hat{\alpha}_{ij} \hat{\alpha}_{mj}}, \quad \hat{\alpha}_{ij} = \frac{\partial \hat{u}_j}{\partial x_i}. $$

In the above equations for $C_V$, $C_{\phi}$ and $Pr_{SGS}$, {...} denotes averaging over volume.
2.3.5 Sigma Model

A model proposed by Nicoud et al. \[72\] is based on the three singular values \((\sigma_1 > \sigma_2 > \sigma_3)\) of the filtered velocity gradient tensor.

\[
\nu_{SGS} = (C_\sigma \bar{\Delta})^2 D_\sigma, \quad D_\sigma = \frac{\sigma_3 (\sigma_1 - \sigma_2) (\sigma_2 - \sigma_3)}{\sigma_1^2}.
\] (2.22)

A value of \(C_\sigma = 1.35\), as recommended in \[72\], has been used in this study along with a constant SGS Prandtl number, \(Pr_{SGS} = 0.7\).

2.4 Non-eddy-viscosity Models

A number of non-eddy-viscosity models are described in this section. The first three, Stretched Vortex, Dynamic Structure, and Gradient type models, have been studied in this thesis. A few other families of non-eddy-viscosity models are also described for the sake of completeness.

2.4.1 Stretched Vortex Model

The Stretched Vortex model is essentially a class of non-eddy-viscosity models, assuming that the subgrid scales are composed of a number of vortex filaments. The SGS stress tensor is given by

\[
\tau_{ij} = (\delta_{ij} - e^v_i e^v_j) K
\] (2.23)

\[
\tau_{j\phi} = -\frac{\Delta}{2} K^{1/2} (\delta_{jp} - e^v_j e^v_p) \frac{\partial \bar{\phi}}{\partial x_p},
\] (2.24)

where \(\delta_{ij}\) is the Kronecker delta, \(e^v_i\) are the direction cosines of the vortex axes, \(K\) is the subgrid energy and \(\bar{\Delta}\) is the grid-filter size. Many variants of this model can be derived based on the choice of the alignment vectors (which determine \(e^v_i\)) and the shape of the spectrum (which determines \(K\)). The results of simulations reported in Misra and Pullin \[68\] and Pullin \[88\] indicate a relative insensitivity to the different variants of the Stretched Vortex family of models. Hence, as a representative of the entire family
of models, one variant - denoted as Model 1a in Misra and Pullin [68], and based on Kolmogorov energy spectrum [88] - has been selected and is described here. As an example, the specific model considered here is based on vortex axes oriented along the eigenvectors corresponding to the largest and second largest eigenvalues of the filtered strain rate tensor, $\bar{S}_{ij}$. The subgrid energy, determined based on Kolmogorov spectrum, is given by

$$
K = \begin{cases} 
\frac{3K_0 2^{2/3}}{2k_c^{2/3}} \left[ 1 - (k_c\eta)^{2/3} \right] & \text{if } k_c\eta < 1 \\
0 & \text{if } k_c\eta > 1 
\end{cases}
$$

(2.25)

where $K_0$ is the Kolmogorov prefactor, and $\epsilon$ and $\eta$ refer to the local energy dissipation and Kolmogorov length scale, respectively. $k_c$ stands for the cut-off wavenumber, and is related to the LES filter width by $k_c = \pi/\Delta$. More details can be found in Pullin [88] and references therein.

### 2.4.2 Dynamic Structure Model

The dynamic structure model for the SGS stress tensor was introduced by Pomeranin and Rutland [85], and is based on the Leonard term, $L_{ij} = \hat{u}_i \bar{u}_j - \hat{u}_i \hat{u}_j$. The SGS stress tensor is given as

$$
\tau_{ij} = 2k_{SGS} \left( \frac{L_{ij}}{L_{kk}} \right).
$$

(2.26)

An analogous model for the SGS scalar flux, proposed by Chumakov and Rutland [20], is based on the Leonard-type term for the scalar field, $L_{i\phi} = \hat{u}_i \hat{\phi} - \hat{u}_i \bar{\phi}$.

$$
\tau_{i\phi} = \frac{\theta}{\Theta} L_{i\phi} = \frac{\bar{\phi}\hat{\phi} - \bar{\phi}\hat{\bar{\phi}}}{\bar{\phi}\hat{\phi} - \hat{\phi}\hat{\bar{\phi}}} \left( \hat{u}_i \hat{\phi} - \hat{u}_i \bar{\phi} \right).
$$

(2.27)

It should be noted that there are no tunable coefficients in this model. However, the terms $k_{SGS} = \tau_{ii}/2$ and $\theta = \bar{\phi}\hat{\phi} - \bar{\phi}\hat{\bar{\phi}}$ cannot be determined from purely the resolved velocity and scalar fields, $\bar{u}_i$ and $\bar{\phi}$, respectively. To overcome this, these models require that additional transport equations for $k_{SGS}$ and $\theta$ be solved. The disadvantage with this is increased memory and computational expense, as well as
the need to model extra unclosed terms, such as the scalar dissipation and triple-correlations.

### 2.4.3 Gradient Models

The Gradient family of models [73, 67, 65, 66], is also referred to as non-linear model (e.g. [63]) or Clark model (e.g. [19]). It is based on terms $G_{ij}$ and $G_{i\phi}$, composed of products of derivatives of the resolved velocity and scalar fields,

\[
G_{ij} = \frac{\Delta^2}{12} \frac{\partial \bar{u}_i}{\partial x_k} \frac{\partial \bar{u}_j}{\partial x_k},
\]

\[
G_{i\phi} = \frac{\Delta^2}{12} \frac{\partial \bar{u}_i}{\partial x_k} \frac{\partial \bar{\phi}}{\partial x_k}.
\]

The expressions for SGS stress tensor and SGS scalar flux are [67, 66]

\[
\tau_{ij} = 2k_{SGS} \left( \frac{G_{ij}}{G_{kk}} \right), \quad \tau_{i\phi} = C_G \Delta^2 \sqrt{k_{SGS}} \sqrt{\theta} \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right).
\]

It may again be noted, that the terms $k_{SGS}$ and $\theta$ need to be solved for via additional transport equations. A modified form, termed Modulated Gradient Model (MGM), substituting algebraic expressions for $k_{SGS}$ and $\theta$ has been proposed by Lu and Porté-Agel [65, 66]. The expressions under MGM are

\[
\tau_{ij} = 8\bar{\Delta}^2 \left( \frac{G_{ij}}{G_{kk}} \right) \left( \frac{G_{ij}}{G_{kk}} \right) H(P)
\]

\[
\tau_{i\phi} = C_M \bar{\Delta}^2 \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right) \left( \frac{G_{ij}}{|G_{kk}|} \right) \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right) H(P) H(P)
\]

where $H(x)$ represents the heaviside function, and $P$ and $P_\theta$ are SGS momentum and scalar production terms respectively.

### 2.4.4 Similarity Models

Similarity, or scale-similarity models are based on the observation that flow fields at scales of consecutive sizes have some similarity. This leads to the assumption that the Leonard stress, obtained by filtering at the test-filter level, i.e. $L_{ij} = \tilde{u}_i\tilde{u}_j - \tilde{u}_i \tilde{u}_j$,
serve as a model for the SGS stress, obtained by filtering at the grid-filter level, i.e. \( \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \). The model proposed by Liu et al. [63] for SGS stress tensor, and studied among others by Okong’o and Bellan [73] for the SGS scalar flux, is

\[
\tau_{ij} = c L_{ij} \\
\tau_{i\phi} = c L_{i\phi}.
\]  

(2.33)

(2.34)

Variants with constant and dynamically determined coefficients, as well as various types of backscatter control mechanisms have been studied in the literature, e.g. [104, 63, 64, 73].

### 2.4.5 Tensorial Eddy-viscosity Models

Eddy-viscosity models are based on a linear constitutive relation between the SGS stresses and strains, via an eddy-viscosity or an eddy-diffusivity. In comparison to this, tensorial eddy-viscosity models are based on generalized quadratic constitutive relations, which lead to additional terms for the deviatoric part of the SGS stress tensor, and for the SGS scalar flux. The SGS stress tensor is given by [118]

\[
\tau_{ij} - \frac{1}{3} \tau_{kk} = -C_S \beta_{ij} - C_W \gamma_{ij} - C_N \eta_{ij},
\]

(2.35)

where \( \beta_{ij} \) is related linearly to the strain-rate tensor \( \bar{S}_{ij} \), \( \gamma_{ij} \) to the product \( \bar{S}_{ik} \bar{\Omega}_{kj} \) and \( \eta_{ij} \) to the product \( \bar{S}_{ik} \bar{S}_{kj} \). This model has also been extended for SGS scalar flux, based on a generalized form of the gradient-diffusion hypothesis, by Wang et al. [119].

### 2.4.6 Mixed Models

Models built by combining a multiple of the above ideas are termed mixed models. The most widely used mixed models add an eddy-viscosity term to a scale-similarity term [63]. Mixed models combining Gradient and eddy-viscosity terms have also been used (e.g. [67]). Mixed models have been applied to a variety of LES studies
[127, 115, 5, 124, 102], with very accurate results. However, the major disadvantage with mixed models is related to specifying the coefficients in front of each of the terms, so as to control their relative importance.

### 2.4.7 Other Approaches

In addition to the models outlined above, a number of other approaches to LES modeling have been developed. These include implicit LES, regularization, and estimation models. Implicit LES are simulations carried out without an explicit subgrid-scale model; however, the errors introduced by the numerical discretization method are manipulated so as to provide additional dissipation required to stabilize the simulations [45]. Regularization models [38, 18, 111] modify the non-linear convective terms, instead of adding diffusion-like terms, as in conventional eddy-viscosity models. A final methodology for LES modeling involves computing the nonlinear terms ($\overline{u_i u_j}$ and $\overline{u_i \phi}$) directly, by estimating the full velocity field, instead of the resolved, or filtered, velocity field. Estimation [28], approximate deconvolution [105], and fractal non-linear [11, 13] models are examples of these approaches.

### 2.5 Closing Remarks

A large number of models for the subgrid terms in turbulent flows, have been developed over the years. However, an optimum model which provides accurate structure of the instantaneous flow field, allows for both forward-cascade (transfer of energy from large scales to small scales), as well as backward-scatter (transfer from small scales to large scales) of energy, while at the same time providing adequate dissipation for numerical stability, remains elusive. This thesis will be concerned with evaluation of various properties of a few of the above described models. The Smagorinsky, Vreman and Sigma eddy-viscosity models will be evaluated by performing large eddy simulation of thermal-driven cavity in Chapter 3, and comparing the results with results from DNS. The eddy-viscosity based models described above are all based on
the assumption that the velocity and scalar kernels are identical (equation (2.10)). This assumption implies that the SGS diffusivity is dependent only on the resolved velocity field, and not dependent explicitly on the resolved temperature field. An obvious improvement over the existing models involves developing a kernel which is sensitive to both, the resolved velocity and resolved temperature fields. Development and evaluation of such a model based on a more sensitive kernel is presented in Chapter 4. The eddy-viscosity models will again be evaluated, in comparison to Dynamic Structure and Gradient models, in an a priori sense, in Chapter 5.
3. LARGE EDDY SIMULATION OF THERMAL DRIVEN CAVITY:
EVALUATION OF SUBGRID SCALE MODELS AND FLOW PHYSICS

3.1 Introduction

Large eddy simulation (LES) of buoyant turbulent flows requires accurate modeling of the subgrid scale (SGS) stresses as well as the SGS heat flux. It is well known that turbulent flows driven by temperature differences (or any other scalar contributing to the density) are characterized by a high degree of spatial and temporal intermittency. Thus, LES of buoyant turbulent flows require SGS models which are not overly dissipative and dynamically adjust in time and space to local instantaneous flow conditions. Many SGS models have been developed over the years, and have been reviewed in detail in Chapter 2. Three eddy-viscosity models and one non-eddy-viscosity type of model are considered in this study. The earliest SGS model developed was the Smagorinsky [103] eddy-viscosity model. The recently developed SGS models from Vreman [114] and Nicoud et al. [72] employ the so called Vreman and Sigma kernels, respectively. These kernels have been shown to be superior at adjusting to local flow conditions compared to the traditional Smagorinsky kernel. A localized dynamic procedure (Lilly [61]), which adjusts the value of the model constant to local flow conditions, is often used in order to make up for the lack of variability of the Smagorinsky kernel. However, this dynamic procedure requires averaging over homogeneous directions (if any) and/or ad-hoc clipping in order to ensure numerical stability. The Vreman and Sigma kernels allow use of global dynamic procedures, such as in You and Moin [126], which are relatively more stable and can be applied even in flows without a homogeneous direction. The Stretched Vortex family (Misra and Pullin [68], Pullin [88], etc.), a non-eddy-viscosity type family of models, is another
class of models which, for similar reasons, could be potentially useful in simulating buoyant turbulent flows.

Accurate LES modeling of turbulent flows requires accurate numerical solvers in addition to a good SGS model. Modeling the convective term is especially challenging since schemes that reduce unphysical oscillations via upwinding tend to introduce excessive numerical dissipation and vice-versa (Herrmann et al. [47]). Modeling the scalar advection term is even more challenging due to the constraint that the scalar be bounded between a certain minimum and maximum value. The use of a high-order Weighted Essentially Non-Oscillatory (WENO) scheme for LES of turbulent flows has been established by Shetty et al. [99] but it does not guarantee that the scalar boundedness constraint will be satisfied. Hence, the use of the WENO scheme for the scalar advection term needs to be established for a particular problem by determining the occurrence and extent of scalar unboundedness.

Similar to the two-dimensional lid driven cavity problem [e.g. 42], flow in a two-dimensional square cavity with heated and cooled vertical walls has been a classic test case and benchmark problem for numerical schemes. The non-dimensional parameter characterizing the applied temperature difference between the two vertical walls is the Rayleigh number. The two-dimensional version has been studied numerically, among others, by De Vahl Davis and Jones [24] and by Wan et al. [117] for small Rayleigh numbers, and by P. [76], Xin and Le Quéré [122], and Le Quéré and Behnia [59] for larger Rayleigh numbers. Direct numerical simulations (DNS) of the flow in a three-dimensional rectangular cavity of aspect ratio 4 at high values of Rayleigh number were carried out by Trias et al. [108], Trias et al. [109], and Trias et al. [110]. The reduced horizontal extent of this configuration results in a flow structure that is significantly different from that observed in a cubical cavity. LES of the differentially heated cavity problem have been reported previously in a two-dimensional configuration by Sergent et al. [96] and in three-dimensional configurations by Peng and Davidson ([80] and [81]), Barbagli and Davidson [6] and Salat et al. [92]. In particular, Peng and Davidson [81] carried out computations in a cubical cavity us-
ing a second-order finite-volume method and dynamic variants of the Smagorinsky model. A combined experimental, DNS and LES study of the cubical configuration was reported in Salat et al. [92]. Although a Chebyshev spectral method was used for the DNS, the LES were carried out using a second-order finite-volume numerical method. Thus, these previous LES have been carried out in 2D or 3D cubical configurations, having employed low-order methods. Turning to non-cubical configurations, the flow in a tall cavity of aspect ratio 5:1 was studied by Barhaghi and Davidson [6]. The SGS models used included the classical constant coefficient and dynamic Smagorinsky models, and the wall adapting local eddy-viscosity (WALE) model of Nicoud and Ducros [71]. Trias et al. [111] carried out LES in a cavity of aspect ratio 4 using the regularization modeling approach, which seeks to modify the non-linear convective terms rather than model the SGS terms appearing in the filtered Navier-Stokes equations. Regularization modeling has also been applied to simulate other buoyancy driven flows, e.g. [90].

In this study, LES are conducted in order to test the suitability of four relatively recent SGS models for buoyant turbulent flows. We have used the configuration and results of Trias et al. [109] and [110] as benchmarks. A previously developed high-order numerical framework (Shetty et al. [99]) based on the WENO convective scheme has been used for the simulations. The numerical scheme has also been tested by comparing predictions to the two-dimensional thermal driven cavity results of Wan et al. [117]. This is followed by 3D simulation results at two values of the Rayleigh number based on the cavity height, $Ra = 6.4 \times 10^8$ and $Ra = 2.0 \times 10^9$. The effect of using the WENO scheme for the scalar advection equation on scalar boundedness is discussed. The WENO scalar convective scheme is further established by comparing to results obtained using the BQUICK scheme for the scalar connective term. The accuracy of our simulations allows a detailed examination of the flow features in the thermal driven cavity. Features such as the inhomogeneity of turbulence, wave and vortical interactions, and budget of the turbulent kinetic energy are studied to further
our understanding of the flow physics. Hence, this study addresses SGS modeling and numerical methods issues, as well as resolved flow physics.

3.2 Governing Equations and Numerical Methodology

3.2.1 LES Equations

The filtered equations governing LES of an incompressible, buoyant fluid are

\[
\frac{\partial \bar{u}_i}{\partial x_i} = 0 \tag{3.1}
\]

\[
\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{Pr}{\sqrt{Ra}} \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + Pr \bar{T} \delta_{i3} - \frac{\partial \tau_{ij}}{\partial x_j} \tag{3.2}
\]

\[
\frac{\partial \bar{T}}{\partial t} + \bar{u}_j \frac{\partial \bar{T}}{\partial x_j} = \frac{1}{\sqrt{Ra}} \frac{\partial^2 \bar{T}}{\partial x_j \partial x_j} - \frac{\partial \tau_{jT}}{\partial x_j}. \tag{3.3}
\]

These equations employ the Boussinesq approximation where density variations are neglected in all terms except for the body force term. For the thermal driven cavity problem, the height of the cavity \( L_z \) and the temperature difference between two vertical walls \( \Delta T \) can be considered to be typical length and temperature scales. The above equations have been non-dimensionalized with these length and temperature scales, and with \( \sqrt{Ra} k_T / L_z \) as the velocity scale. The non-dimensional parameters governing the flow are the Rayleigh number \( (Ra) \) and the Prandtl number \( (Pr) \),

\[
Ra = \frac{g \beta \Delta T L_z^3}{\nu k_T}, \quad Pr = \frac{\nu}{k_T}, \tag{3.4}
\]

where \( g \), \( \beta \), \( k_T \) and \( \nu \) denote the gravitational acceleration, thermal expansion coefficient, thermal diffusivity, and viscosity respectively. \( \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \) denotes the SGS stress tensor while \( \tau_{jT} = \bar{u}_j \bar{T} - \bar{u}_j \bar{T} \) denotes the SGS thermal flux.

Four LES SGS model combinations have been considered in this study. These include three eddy-viscosity models based on the Smagorinsky, Vreman and Sigma kernels and one non-eddy-viscosity type model from the Stretched Vortex family. The Smagorinsky kernel is coupled with the localized dynamic procedure of Lilly [61] for determining the constant, the Vreman kernel with the global dynamic procedure of
You and Moin [126], while the Sigma kernel uses a fixed value of the model constant. In addition, the constant coefficient versions of the Smagorinsky and Vreman models are also considered briefly. The models have been described in Chapter 2, and a summary is given in Table 3.1.

3.2.2 Numerical Methodology

A high-order LES code, developed and validated previously by Shetty et al. [99], was extended to perform LES of buoyant turbulent flows. The main features of the numerical methods employed in the code are briefly described here. More details may be found in [99] and references therein.

For spatial discretization, the convective and advective terms are discretized using a 5th-order WENO scheme (Jiang and Shu [51]), while viscous terms are discretized using the standard 4th-order central difference scheme. High-order accuracy of the spatial discretization is maintained even at the boundaries by using three layers of ghost nodes. The values at the ghost nodes are updated using a Stokes flow boundary condition (Morinishi et al. [69]).

Ensuring a divergence-free velocity field which satisfies the continuity equation presents the most significant challenge in incompressible flow simulation. The fractional step method with a projection algorithm is used in the current study. A low storage 3rd-order Runge-Kutta scheme has been used which advances the solution to the next time step over four stages (Gokarn et al. [44]). In each stage, velocities are updated treating all terms except the pressure term explicitly. A Poisson equation for the pressure is then solved using the multi-grid solver MUDPACK (Adams [1]). This pressure solution is then used to correct the velocities and ensure that the continuity equation is satisfied at each stage of the Runge-Kutta method.

The code also features capabilities such as test filtering operations for dynamic SGS models, near-wall grid stretching and shared memory OpenMP parallelism. Typ-
Table 3.1. Summary of LES SGS models evaluated in thermal-driven cavity.

<table>
<thead>
<tr>
<th>Model</th>
<th>Label</th>
<th>Kernel</th>
<th>Model Constant</th>
<th>$Pr_{SGS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant Smagorinsky</td>
<td>Coefficient</td>
<td>CSM</td>
<td>$</td>
<td>\bar{S}</td>
</tr>
<tr>
<td>Dynamic Smagorinsky</td>
<td>DSM</td>
<td>$</td>
<td>\bar{S}</td>
<td>$</td>
</tr>
<tr>
<td>Constant Vreman</td>
<td>Coefficient</td>
<td>VM</td>
<td>$\Pi^g$, eq. (2.17)</td>
<td>$C_V = 0.07$</td>
</tr>
<tr>
<td>Dynamic Vreman</td>
<td>DVM</td>
<td>$\Pi^g$, eq. (2.17)</td>
<td>global dynamic procedure</td>
<td>global dynamic procedure</td>
</tr>
<tr>
<td>Sigma</td>
<td>Sigma</td>
<td>$D_\sigma$, eq. (2.22)</td>
<td>$C_\sigma = 1.35$</td>
<td>$Pr_{SGS} = 0.7$</td>
</tr>
<tr>
<td>Stretched Vortex</td>
<td>SVM</td>
<td></td>
<td>eqs. (2.23)-(2.24)</td>
<td></td>
</tr>
</tbody>
</table>
ical simulations are carried out on multicore Linux machines, making use of up to 24 processors.

Tests carried out on a two-dimensional Taylor Green Vortex (TGV) problem with periodic boundary conditions demonstrated that the overall accuracy of the algorithm was 5th-order in space and 3rd-order in time, consistent with the schemes used. Further details may be found in Shetty et al. [99].

3.3 Results

3.3.1 Validation of Numerical Method

As a first level of validation, the above described numerical scheme was implemented in two dimensions and used to simulate natural convection in a square cavity. A schematic of the simulation domain and boundary conditions applied is shown in Figure 3.1a. Simulations were carried out for Rayleigh numbers over the entire laminar range from $10^3$ to $10^8$ and the results were found to be in excellent agreement with those reported in a benchmark by Wan et al. [117]. Figures 3.1b-d show the results at three highest Rayleigh numbers in the laminar range. The lines over which the velocity and temperature profiles have been obtained have been marked in Figure 3.1a for clarity. It should be noted that the values reported in Figure 3.1 have been non-dimensionalized with the scales used by Wan et al. [117], which are different from the scales used to non-dimensionalize the governing equations (1) – (3.3).

3.3.2 LES of 3D Thermal Driven Cavity

A systematic study of different LES SGS models is now presented in the context of turbulent convection in the three-dimensional thermal driven cavity depicted in Figure 3.2. A rectangular box oriented along the coordinate axes is subjected to heating along the left ($y = 0$) vertical wall and cooling along the right ($y = L_y$) vertical wall, while adiabatic boundary conditions are maintained at the top ($z = L_z$).
Figure 3.1. (a) Schematic of the 2D simulation domain. Comparison of (b) vertical velocity, (c) horizontal velocity and (d) temperature profiles with benchmark results of Wan et al. [117] for a thermal driven square cavity with Rayleigh numbers in the laminar range. Solid lines: present results; Filled square symbols: benchmark results from [117]. Results non-dimensionalized with the scales used in [117].
and bottom ($z = 0$) horizontal walls. No-slip velocity conditions are imposed on all four of these $y$ and $z$ direction walls. Finally, periodic boundary conditions are imposed in the transverse direction ($x = 0$ and $x = L_x$ walls).

Physical and numerical simulation parameters used in the studies are specified in Table 3.2. Two computational meshes were used consisting of $64 \times 64 \times 128$ and $96 \times 96 \times 192$ grid points in the $x$, $y$ and $z$ directions respectively. The grid points were equally spaced in the periodic $x$ direction, while in order to better resolve the near-wall features of the flow, a smooth grid stretching function was used, which clustered more points near the horizontal and vertical walls than near the center of the cavity in the $y$-$z$ plane. The grid stretching function used was [99]

$$
y = h \frac{(\beta + 2\alpha) \left[(\beta + 1) / (\beta - 1)\right]^{(\eta-\alpha)/(1-\alpha)} - \beta + 2\alpha}{(2\alpha + 1) \left\{1 + [(\beta + 1) / (\beta - 1)]^{(\eta-\alpha)/(1-\alpha)}\right\}},
$$

Figure 3.2. Schematic of the 3D thermal driven cavity problem.
where \( \eta \) and \( y \) denote the locations of the corresponding points on the uniform (un-stretched) and stretched grids respectively. \( h \) denotes the grid spacing in the \( y \) direction on the uniform grid. The same function was used to cluster points near the vertical walls in the \( z \) direction as well. The values of the stretching parameters \( \alpha \) and \( \beta \) are reported in Table 3.2.

The simulations were carried out for 500 non-dimensional time units, for the flow to achieve statistical stationarity, and for a further 1000 time units, over which, time averages of velocities, temperature, and other relevant quantities were collected. This time period was found to be sufficient for all the statistics considered in this study to converge. Statistical averaging was carried out over time, the homogeneous \( x \) direction and also made use of anti-symmetry of all velocities and temperature around the volumetric centroid of the cavity (Trias et al. [109]). In order to ensure that the size of the computational domain in the periodic direction \( (L_x) \) is adequate, simulations were repeated with two additional domain sizes in the periodic direction. All statistically averaged quantities were found to be identical for the three cavity sizes. This method of justifying the size of the cavity in the periodic direction is similar to the one used by Barhaghi and Davidson [6]. The results from Direct Numerical Simulations (DNS) of this problem reported in [108], [109], and [110] are used as benchmarks. Profiles of first-order turbulent statistics, viz. mean velocity and temperature, are presented in Section 3.3.4 while a comparison of the second order statistics (components of the Reynolds stress tensor and velocity-temperature correlations) is presented in Section 3.3.5.

### 3.3.3 Instantaneous Flow

The driving force behind convection in the thermal driven cavity is the temperature difference applied between the two vertical walls. Fluid near the hot wall becomes warmer and rises, while fluid near the cold wall cools and sinks. Fluid parcels accelerating upwards along the hot wall, and downwards along the cold wall, turn as they
Table 3.2. Physical and numerical parameters for thermal-driven cavity simulations.

<table>
<thead>
<tr>
<th>$Ra; Pr$</th>
<th>Domain $(L_x \times L_y \times L_z)$</th>
<th>Grid Size $(N_x \times N_y \times N_z)$</th>
<th>Grid Stretching Parameters [99]</th>
<th>Time Step</th>
<th>Total Time</th>
<th>Statistics collected from time onward</th>
</tr>
</thead>
<tbody>
<tr>
<td>$6.4 \times 10^8; 0.7$</td>
<td>$2 \times 0.25 \times 1$</td>
<td>$64 \times 64 \times 128$</td>
<td>$\alpha = 0.5; \beta = 1.2$</td>
<td>$10^{-2}$</td>
<td>1500</td>
<td>500</td>
</tr>
<tr>
<td>$2.0 \times 10^9; 0.7$</td>
<td>$1 \times 0.25 \times 1$</td>
<td>$64 \times 64 \times 128; 96 \times 96 \times 192$</td>
<td>$\alpha = 0.5; \beta = 1.2$</td>
<td>$10^{-2}$</td>
<td>1500</td>
<td>500</td>
</tr>
</tbody>
</table>
encounter the top and bottom walls respectively. This sets up a flow with the principle direction as shown in Figure 3.2. Figure 3.3 shows an instantanous snapshots, representative of the flow in the thermal cavity after the flow has achieved its statistically stationary state. The iso-temperature surfaces in Figure 3.3a indicate that the flow around the mid-vertical region is much more organised and structured, than near the top-left and bottom-right corners. The $\lambda_2$ iso-surfaces depicted in Figure 3.3b show that the small-scale structures associated with turbulence are concentrated in the downstream regions of the vertical boundary layers, near the top and bottom walls. These observations are consistent with the previous DNS studies [110].

3.3.4 Mean Velocity and Temperature Profiles

Detailed comparisons of profiles of different quantities are presented in this and the next subsection. Figure 3.4 shows nine different vertical locations along the thermal cavity, ranging from $z = 0.1$ to $z = 0.9$ in increments of 0.1. Profiles of mean vertical velocity and mean temperature at these nine different vertical locations along the thermal cavity in the region near the hot wall are shown in Figures 3.5 and 3.6 for the two Rayleigh numbers considered.

The constant coefficient Smagorinsky and constant coefficient Vreman models, which are the simplest possible versions of those respective classes of models, are unable to predict the mean profiles accurately. It can be seen from Figures 3.5 and 3.6 that the peaks of the velocity profiles predicted by the constant coefficient Smagorinsky model are farther away from the wall than obtained from DNS, while the predicted temperature gradients at the wall are smaller than those obtained from DNS. Thus, the constant coefficient Smagorinsky model with $C_S = 0.16$ can be inferred to be too diffusive. The constant coefficient Vreman model with $C_V = 0.07$ was found to be unstable. Application of the dynamic procedure to the Vreman model yielded a constant ($C_V \approx 0.9$ at $Ra = 6.4 \times 10^8$; $C_V \approx 0.6$ at $Ra = 2.0 \times 10^9$) which was one order of magnitude larger than the constant value used here. In other words,
Figure 3.3. Instantaneous snapshot of the flow at $Ra = 2.0 \times 10^9$ on a $96 \times 96 \times 192$ grid using Sigma model. Iso-surfaces of (a) temperature from $-0.45$ to $0.45$ in increments of $0.1$ and (b) $\lambda_2 = -0.5$ [50] colored with vorticity magnitude. For plotting purposes, the domain in the periodic direction has been truncated to $x \in [0.75, 1]$. 
Figure 3.4. Schematic of the $y - z$ plane of the thermal cavity displaying locations at which profiles of mean velocity, mean temperature and turbulent fluctuations are compared to DNS results.
Figure 3.5. Profiles of (a) mean velocity $\langle W \rangle$ and (b) mean temperature $\langle T \rangle$ along horizontal coordinate near the wall at nine vertical locations $z = 0.1$ to $z = 0.9$ in increments of 0.1 for $Ra = 6.4 \times 10^8$. Square symbols: DNS of Trias et al. [109], dash-dotted line: Constant Coefficient Smagorinsky Model, solid line: Dynamic Vreman Model. Abscissa is $4y$ and each vertical subdivision is 0.2 units for $\langle W \rangle$ and 0.5 units for $\langle T \rangle$. 
Figure 3.6. Profiles of (a) mean velocity $\langle W \rangle$ and (b) mean temperature $\langle T \rangle$ along horizontal coordinate near the wall at nine vertical locations $z = 0.1$ to $z = 0.9$ in increments of 0.1 for $Ra = 2.0 \times 10^9$. Square symbols: DNS of Trias et al. [109], dash-dotted line: Constant Coefficient Smagorinsky Model, solid line: Dynamic Vreman Model. Abscissa is $4y$ and each vertical subdivision is 0.2 units for $\langle W \rangle$ and 0.5 units for $\langle T \rangle$. 
with the present high-order method, a larger value of model coefficient was found to be necessary for the Vreman model to yield stable simulations. A similar trend has been observed in Shetty et al. [99], where simulation at higher Reynolds number could not be carried out with the constant coefficient Vreman model, and the dynamic procedure predicted higher values for the constant $C_V$.

Contrasting the predictions of these constant coefficient models, the dynamic Smagorinsky and dynamic Vreman models predict the near-wall mean profiles accurately. The near-wall profiles of mean vertical velocity and mean temperature obtained using the dynamic Vreman model are shown in Figures 3.5 and 3.6. Very similar profiles are obtained using the dynamic Smagorinsky, Sigma and Stretched Vortex models, and have not been shown here since they overlie the DVM results almost exactly and would be indistinguishable from these results. Thus, these four models are able to predict mean profiles accurately in the near-wall region.

Predictions of these four models are examined away from the walls in Figure 3.7 and 3.8, which show profiles of mean velocities and temperature over the entire width of the thermal cavity at two vertical locations: $z = 0.5$ and $z = 0.8$. These locations have been marked by dashed horizontal lines in Figure 3.4. At the mid-vertical location ($z = 0.5$), LES predictions using all models match the DNS results for both values of $Ra$. At the off-center location ($z = 0.8$), the dynamic Smagorinsky, Sigma and Stretched Vortex models are accurate at $Ra = 6.4 \times 10^8$, but show some discrepancies with the DNS data at $Ra = 2.0 \times 10^9$. The dynamic Vreman model however shows discrepancies at both Rayleigh numbers away from the walls at $z = 0.8$.

### 3.3.5 Second-order Turbulent Statistics

Since the constant coefficient versions of Smagorinsky and Vreman models failed to predict the mean velocities and temperature accurately, their performance with regard to predicting second-order statistics is not considered. The remaining four
Figure 3.7. Mean vertical velocity (left panel) and temperature (right panel) profiles for $Ra = 6.4 \times 10^8$, at (a,b) $z = 0.5$, and (c,d) $z = 0.8$. 
Figure 3.8. Mean vertical velocity (left panel) and temperature (right panel) profiles for $Ra = 2.0 \times 10^9$, at (a,b) $z = 0.5$, and (c,d) $z = 0.8$. 
LES SGS models are evaluated with regard to their ability to predict second-order turbulent statistics in this section.

The relevant turbulent statistics can be grouped into velocity and temperature RMS quantities (viz. $u_{rms}$, $v_{rms}$, $w_{rms}$ and $T_{rms}$) and velocity-velocity or velocity-temperature cross-correlations (viz. $\langle v'w' \rangle$, $\langle v'T' \rangle$ and $\langle w'T' \rangle$). Profiles of these turbulent statistics obtained using the four models are compared to DNS results in Figures 3.9 and 3.10 for $Ra = 6.4 \times 10^8$. Figure 3.9 shows results at the mid-vertical location ($z = 0.5$), where turbulent fluctuations are much smaller than at off-center locations, such as those depicted in Figure 3.10 ($z = 0.8$). Also, due to the assumed flow symmetry about the center of the cavity, the abscissa on Figure 3.9 ranges from $[0, 0.125]$ instead of $[0, 0.25]$ on Figure 3.10.

It can be seen that the dynamic Smagorinsky, Sigma and Stretched Vortex models are excellent at predicting the turbulent statistics at both vertical locations, $z = 0.5$ and $z = 0.8$. The dynamic Vreman model on the other hand severely under-predicts the turbulent fluctuations. Further, the Stretched Vortex and Sigma models are slightly better than the dynamic Smagorinsky model.

Figures 3.11 and 3.12 show the turbulent statistics at mid-vertical ($z = 0.5$) and off-center ($z = 0.9$) locations respectively for $Ra = 2.0 \times 10^9$. At the mid-vertical location (Figure 3.11), the behavior of the models is similar to their behavior at lower $Ra$. The dynamic Smagorinsky, Sigma and Stretched Vortex models predict the turbulent statistics closely while the dynamic Vreman model fails to do so. At the off-center location, the dynamic Smagorinsky, Sigma and Stretched Vortex models under-predict the turbulent fluctuations in the region $y \in [0, 0.1]$ and are acceptable over the rest of the $y$ region. Figure 3.12 shows that while the dynamic Vreman model continues to under-predict the turbulent statistics, it is able to capture the shape of the profiles of turbulent statistics.

Results of LES simulations at $Ra = 2.0 \times 10^9$ using a finer grid ($96 \times 96 \times 192$) with Sigma model are shown in Figure 3.13. Increasing the resolution shows a definite improvement in the prediction of turbulent statistics over the entire region.
Figure 3.9. Second order turbulent statistics at mid-vertical location $z = 0.5$ for $Ra = 6.4 \times 10^8$: (a-d) RMS quantities and (e-g) cross-correlations.
Figure 3.10. Second order turbulent statistics at off-center location $z = 0.8$ for $Ra = 6.4 \times 10^8$: (a-d) RMS quantities and (e-g) cross-correlations.
Figure 3.11. Second order turbulent statistics at mid-vertical location $z = 0.8$ for $Ra = 2.0 \times 10^9$: (a-d) RMS quantities and (e-g) cross-correlations.
Figure 3.12. Second order turbulent statistics at off-center location $z = 0.9$ for $Ra = 2.0 \times 10^9$: (a-d) RMS quantities and (e-g) cross-correlations.
$y \in [0, 0.25]$. A similar improvement in LES results is seen on using a finer grid with
dynamic Smagorinsky and Stretched Vortex models, and has not been shown. Thus, a
finer grid is required for simulating turbulent natural convection at a higher Rayleigh
number. In order to quantify the near-wall resolution of the simulations, the value of
the first grid point in the $y$ direction expressed in terms of non-dimensional wall units
is plotted in Figure 3.14. The viscous length scale, $\delta_\nu$, used for this normalization is
given by

$$
\delta_\nu = \left[ \frac{\sqrt{Ra}}{Pr} \frac{\partial \langle W \rangle}{\partial y} \bigg|_{y=0} \right]^{-1/2}.
$$

(3.6)

Figure 3.14 shows that the first grid point in the $y$ direction is at a maximum distance
of $y_1^+ \approx 2.9$ for $Ra = 6.4 \times 10^8$ on the $64 \times 64 \times 128$ grid, and for $Ra = 2.0 \times 10^9$ on
the $96 \times 96 \times 192$ grid, while $y_1^+ \approx 4.4$ for $Ra = 2.0 \times 10^9$ on the $64 \times 64 \times 128$ grid.
This suggests that a resolution of $y_1^+ \approx 2.9$ is adequate for simulation of turbulent
natural convection in the present context.

### 3.3.6 Discussion

Results of LES of the thermal driven cavity have been shown in the previous three
subsections. It should be noted that the simulations were not stable without the SGS
models. Further, as stated in Section 3.3.5, simulations with constant coefficient
Vreman model with $C_V = 0.07$ were not stable, and that the dynamic procedure,
which resulted in stable simulations, yielded larger values for the coefficient. These
observations may be related to the fact that the use of high-order finite difference
schemes for discretization of the Navier-Stokes equations on non-uniform grids does
not necessarily satisfy exact mass, momentum and energy conservation [112]. Thus,
although SGS models should ideally act to improve the accuracy of the results without
affecting numerical stability, we observe that for the present high-order approach,
SGS models also help in overcoming stability issues related to conservation. Similar
observations were made by Shetty et al. [99] for their (non-buoyant) lid-driven cavity
problem using the high-order numerical scheme on non-uniform grids.
Figure 3.13. Second order turbulent statistics at off-center location $z = 0.9$ for $Ra = 2.0 \times 10^9$ on a finer $96 \times 96 \times 192$ grid. (a-d) RMS quantities and (e-g) cross-correlations.
Figure 3.14. Spacing of the first grid point in the $y$ direction, expressed in terms of wall units, for different values of $Ra$ and different grid sizes, using Sigma model.
The results indicate that the dynamic Smagorinsky, Sigma and Stretched Vortex models yield almost identical results throughout the thermal cavity at both the Rayleigh numbers. This is remarkable since the underlying assumptions are completely different. Dynamic Smagorinsky and Sigma models are of the eddy-viscosity family, while the Stretched Vortex is a non-eddy-viscosity model. The dynamic Smagorinsky model employs a localized dynamic procedure to determine the model coefficient, while the Sigma model uses a constant coefficient. The Smagorinsky kernel is not very sensitive to the resolved flow, as can be seen from the fact that results improve dramatically on application of the dynamic procedure. The accuracy of the Sigma model on the other hand can be attributed entirely to its kernel, thus clearly demonstrating its superiority over the Smagorinsky kernel.

The Vreman kernel is supposed to be superior to the Smagorinsky kernel since it yields vanishing eddy-viscosity in locally laminar regions. However, this is not borne out by our present LES results. The poor performance of the dynamic Vreman model could be related to the dynamic procedure. In the current simulations, the global dynamic procedure of You and Moin [126] has been used for both velocity and temperature, which yields spatially constant values of $C_V$ and $Pr_{SGS}$. It was observed that the $Pr_{SGS}$ computed oscillated around $Pr_{SGS} \approx 13.3$ for $Ra = 6.4 \times 10^8$ and around $Pr_{SGS} \approx 6.4$ for $Ra = 2.0 \times 10^9$. These values are much higher than the conventional value of $Pr_{SGS} \approx 0.7$. Although the conventional value is ad-hoc, and not based on any physical reasoning, it was observed that the value gives good results with Sigma model. Also, the $Pr_{SGS}$ computed by the dynamic Smagorinsky model is of order $Pr_{SGS} \approx 1$. Thus, simulations with $Pr_{SGS} = 0.7$ and $C_V$ computed using the global dynamic procedure, equation (2.18), were carried out. Simulations were also carried out on a finer grid of size $96 \times 96 \times 192$ with the dynamic procedure applied for both $C_V$, equation (2.18), and $Pr_{SGS}$, equation (2.20). The results of these two simulations are presented in Figure 3.15. However, no definite conclusions can be drawn regarding the behavior of the dynamic Vreman model from these results. The results seem to indicate that the Vreman kernel coupled with the global dynamic
procedure is not suitable for simulating turbulent natural convective flows. Further tests with other dynamic procedures and other eddy-diffusivity closure models are needed in order to ascertain the suitability of Vreman kernel to buoyant turbulent flows.

3.3.7 Role of Scalar Advective Scheme

The role of the advective scheme used for the scalar (temperature) equation is established in this section. As mentioned earlier, the use of WENO schemes in general requires unphysical clipping in order to maintain scalar boundedness. However, it was observed that no such clipping was required in any of the present simulations. It should be noted that the present simulations were started from a sufficiently diffuse initial state without very sharp gradients, since the initial state is irrelevant in our present simulations where we are interested in the statistically stationary turbulent state of the thermal cavity.

It has been mentioned in literature [47] that in addition to causing violation of scalar bounds, the WENO scheme is dissipative in nature. Herrmann et al. [47] showed that the BQUICK scheme was much better at preserving scalar variance while maintaining scalar boundedness than the 3rd order WENO scheme in a finite volume framework. In order to further establish the validity of our numerical solver, computations have been carried out with the scalar convective term discretized using BQUICK instead of WENO scheme. Dynamic Smagorinsky and dynamic Vreman models were tested with this scalar convective scheme at the two Rayleigh numbers. The results of simulations using BQUICK are compared to those obtained using WENO in Figure 3.16. It is seen that the scalar statistics obtained using the 5th order WENO scheme in our finite difference framework are very close to those obtained using BQUICK. The results of BQUICK and 5th order WENO are almost identical. Thus, the accuracy or discrepancies of the present simulation results can be attributed
Figure 3.15. Second order turbulent statistics at off-center location $z = 0.9$ for $Ra = 2.0 \times 10^9$ on a finer $96 \times 96 \times 192$ grid. (a-d) RMS quantities and (e-g) cross-correlations.
3.4 Characterization of Turbulence in the Thermal Driven Cavity

The previous section indicates that our LES simulations are accurate and can predict both mean quantities as well as fluctuating turbulent statistics over the entire cavity at $Ra = 6.4 \times 10^8$. A detailed study of the features of turbulence in the
thermal driven cavity at this Rayleigh number is presented in this section, following a similar presentation for the flow in a lid-driven cubical cavity by Bouffanais et al. [10]. Several features such as inhomogeneity, interaction between wave and vortical motions, and the turbulent kinetic energy (TKE) budget are examined qualitatively and quantitatively using the LES results obtained from Sigma model.

3.4.1 Inhomogeneity

Turbulence in the thermal driven cavity is expected to be inhomogeneous due to the presence of two vertical walls which maintain a temperature difference and two horizontal walls which confine the flow. A time averaged measure, \( \langle \delta \rangle \), can be developed to quantify the extent of this inhomogeneity, following Bouffanais et al. [10],

\[
\langle \delta \rangle = \frac{\langle \epsilon \rangle}{\nu} - \langle \omega_i \omega_i \rangle = 2 \frac{\partial^2 \langle u_i' u_j' \rangle}{\partial x_i \partial x_j}.
\]  

(3.7)

\( \langle \epsilon \rangle \) denotes the TKE dissipation while \( \langle \omega_i \omega_i \rangle \) denotes the time average of the fluctuating enstrophy. Homogeneous regions are marked by a value of \( \langle \delta \rangle \) equal to zero, since the Reynolds stress tensor does not vary in space in homogeneous turbulence. The degree of departure from zero of this quantity marks the extent of inhomogeneity.

Homogeneous and highly inhomogeneous regions in the thermal cavity can be clearly identified from contours of \( \langle \delta \rangle / \langle \delta \rangle_{\text{max}} \) plotted in Figure 3.17. The contours have been blanked in regions where the measure satisfies the criterion \( \langle \delta \rangle / \langle \delta \rangle_{\text{max}} < 0.01 \).

It is apparent from Figure 3.17 that the flow is more or less homogeneous in roughly the central vertical-half of the cavity, away from the horizontal walls. Further, the hot and cold jets impinging the horizontal walls near the top-left and bottom right corners respectively result in eddies being ejected towards the cavity core and cause regions of highly inhomogeneous flow.
Figure 3.17. Inhomogeneity of turbulence in the thermal driven cavity quantified by contours of $\langle \delta \rangle$. Contours have been blanked in regions with $\langle \delta \rangle / \langle \delta \rangle_{\text{max}} < 0.01$. 
3.4.2 Wave and Vortical Motions

It is known that fluid motion in the presence of stratification can be characterized by either wave or vortical motions at comparable length scales, and interaction between the two may lead to small-scale turbulent motions (e.g. Waite and Bartello [116]). These phenomena can be observed in the thermal cavity as described below. Time averaged contour plots of temperature reveal that the cavity core is stably stratified (with a non-dimensional vertical temperature gradient of roughly unity) while instantaneous contour plots reveal oscillations around the mean contour lines. Based on these observations, the presence of internal waves in the cavity core has been established by Trias et al. [108]. Fluid heated or cooled by the vertical walls accelerates vertically, and turns as it reaches the horizontal walls. This motion results in ejecting coherent vortices into the cavity core which break down into turbulence due to interactions with the internal waves.

Time series data of the resolved Nusselt number \( Nu = -\partial T / \partial y \) at nine locations \((z = 0.1 \text{ through } z = 0.9)\) along the hot wall \((y = 0)\) have been generated. Figure 3.18 shows the time series plots and corresponding Fourier transformed plots at locations \( z = 0.5 \) and \( z = 0.8 \). It is apparent that the dominant frequency at \( z = 0.5 \) is much smaller than the dominant frequency at \( z = 0.8 \). An examination of the spectral content of the signals at all nine locations reveals that low frequency waves dominate till \( z = 0.6 \), and a clear transition to high dominant frequencies occurs at \( z = 0.7, 0.8 \) and \( 0.9 \). In other words, wave motion is dominant in the core of the cavity till about \( z = 0.6 \), while turbulence is concentrated in the region near the top-left corner beyond \( z = 0.7 \). By symmetry, at the cold wall, wave motion is dominant till about \( z = 0.4 \) while turbulent fluctuations are concentrated near the bottom-right corner beyond \( z = 0.3 \).
Figure 3.18. Time series data (left panel) and power spectral density distribution (right panel) of the resolved Nusselt number at (a,b) $z = 0.5$ and (c,d) $z = 0.8$. 
3.4.3 Production and Dissipation

The TKE balance equation for a buoyant flow includes the buoyant production term $Pr \langle w'T' \rangle$ in addition to turbulent transport, production ($P = - \langle u'_k u'_k \rangle \partial \langle U_i \rangle / \partial x_k$) and dissipation ($\epsilon = 2Pr/\sqrt{Ra} \langle s'_{ij} s'_{ij} \rangle$, where $s'_{ij} = 1/2 (\partial u'_i/\partial x_j + \partial u'_j/\partial x_i)$ is the fluctuating strain rate tensor). The left hand side term is zero at statistically stationary state, while the transport term, which is responsible for redistributing turbulence over the domain, should reduce to zero on taking a global average over the entire volume (denoted by $\{ ... \}$ in the equation below),

$$\left\{ \frac{Dk}{Dt} \right\}^0 = \{ P \} + \{ \epsilon \} + \{ Pr \langle w'T' \rangle \}. \quad (3.8)$$

Similarly, the volume averaged temperature variance balance equation at statistically stationary state reads

$$\left\{ \frac{D \langle T'T' \rangle}{Dt} \right\}^0 = \{ \epsilon_T \} + \{ P_T \} - \{ \epsilon_T \}, \quad (3.9)$$

where $P_T$ and $\epsilon_T$ are defined as

$$P_T = -2 \langle u'_k T' \rangle \partial \langle T \rangle / \partial x_k, \quad \epsilon_T = \frac{2}{\sqrt{Ra}} \langle \partial T' \partial T' \rangle / \partial x_k. \quad (3.10)$$

For the $Ra = 6.4 \times 10^8$ computation using Sigma model, we have $\{ P \} = 3.47 \times 10^{-5}$, $\{ \epsilon \} = 3.63 \times 10^{-5}$, and $\{ Pr \langle w'T' \rangle \} = 0.45 \times 10^{-5}$. Thus, the global averages of production, dissipation and buoyant production balance each other serving as another level of validation of our numerical method. It may be noted that the buoyant production term is lesser in magnitude than the other two terms, but is not negligible. Volume-averaging the thermal production and dissipation terms gives $\{ P_T \} = 6.17 \times 10^{-5}$ and $\{ \epsilon_T \} = 5.66 \times 10^{-5}$, which again balance each other, differing by less than 9%.

Contours of production plotted in Figure 3.19a show that production occurs mainly in the vertical wall boundary layers and where accelerating fluid streams hit the top and bottom walls, ejecting eddies into the core. While the production term is usually observed to be positive, Figure 3.19a shows significant regions
Figure 3.19. Contours of (a) TKE production, (b) TKE dissipation, (c) thermal production and (d) thermal dissipation in the thermal cavity at $Ra = 6.4 \times 10^8$ using Sigma model.
of the thermal cavity with negative production. Concentrating on the hot wall boundary layer, the positive peak of production \( P_{\text{max}} = 1.07 \times 10^{-3} \) occurs at \((y, z) = (0.02, 0.89)\), while the negative peak \( P_{\text{min}} = -1.27 \times 10^{-4} \) occurs near the top wall at \((y, z) = (0.030, 0.993)\). The contour plots of Figure 3.19b indicate that dissipation occurs mainly at the walls at downstream locations, and peaks at \((y, z) = (0.0, 0.89)\). Thermal production, shown in Figure 3.19c, has peaks \( P_{T,\text{max}} = 1.78 \times 10^{-3}, P_{T,\text{min}} = 3.27 \times 10^{-4} \) at \((y, z) = (0.012, 0.89)\) and \((y, z) = (0.033, 0.977)\) respectively, while thermal dissipation (Figure 3.19d) again peaks at the wall, at \((y, z) = (0.0, 0.92)\). It can be seen that turbulent production and dissipation for both, the kinetic energy and the temperature variance, occur in similar regions in the thermal cavity, though the thermal quantities appear over a larger area.

### 3.4.4 Vertical Wall Boundary Layer Dynamics

The structure of the buoyant boundary layers along the vertical walls is examined in detail in this subsection. At all vertical locations, the mean vertical velocity, \( \langle W \rangle \), which is zero at the wall, \( y = 0 \), increases with \( y \), and attains a maximum some distance \( y_{\text{max}} \) in the horizontal direction, before decaying to zero near the cavity center. Two characteristic widths for the vertical wall boundary layer can be defined based on this, namely, \( y_{\text{max}} \), where the vertical velocity attains a maximum; and \( y_{\text{half}} \), further away from the wall, where the vertical velocity falls to half its peak value at \( y_{\text{max}} \). The values of \( y_{\text{max}} \) and \( y_{\text{half}} \), expressed in terms of non-dimensional wall units (i.e. normalized by the local viscous length scale, eq. (3.6)) at three different vertical locations are tabulated in Table 3.3. Also tabulated are the local Grashof numbers, \( Gr_z = g\beta\Delta T z^3/\nu^2 \).

In describing the structure of a buoyancy driven boundary layer, the region \( y \in [0, y_{\text{max}}] \) is usually referred to as the inner part, while \( y \in (y_{\text{max}}, y_{\text{half}}) \) is referred to as the outer part of the boundary layer. Figure 3.20 shows profiles of three turbulent quantities along \( y \), very close to the wall, at three vertical locations. The two vertical
Table 3.3. Vertical wall boundary layer characteristics at $Ra = 6.4 \times 10^8$ using Sigma model.

<table>
<thead>
<tr>
<th>Vertical location</th>
<th>$y_{max}^+$</th>
<th>$y_{half}^+$</th>
<th>$Gr_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z = 0.2$</td>
<td>8.65</td>
<td>19.66</td>
<td>$3.6 \times 10^6$</td>
</tr>
<tr>
<td>$z = 0.5$</td>
<td>11.46</td>
<td>24.91</td>
<td>$5.6 \times 10^7$</td>
</tr>
<tr>
<td>$z = 0.8$</td>
<td>11.28</td>
<td>22.72</td>
<td>$2.3 \times 10^8$</td>
</tr>
</tbody>
</table>

lines in Figure 3.20 mark the two characteristic boundary layer widths, viz. $y_{max}$ and $y_{half}$. All $y$ coordinates are expressed in terms of wall units. It can be seen that at all three vertical locations, the peaks of the turbulent quantities lie in the outer region of the boundary layer. This is contrary to the observation for non-buoyant boundary layers, where turbulent quantities peak in the inner part of the boundary layer, in the buffer layer [56]. Similar observations regarding the structure of the boundary layer have been made in other buoyant turbulent studies, such as a 5:1 thermal driven cavity at the cavity mid-height ($z = 0.5$) [6], and in buoyant turbulent boundary layers in infinite vertical channels [6].

There has been some ambiguity about the sign of the velocity cross-correlation, $\langle v'w' \rangle$, near the wall in a buoyant turbulent boundary layer (see introduction of [6]). Barhaghi and Davidson [6] mentioned in their thermal cavity simulations, that $\langle v'w' \rangle < 0$ close to the wall, at the cavity mid-height, while the signs at other locations along the boundary layer were not specified. Furthermore, it was also shown [6] that the sign of $\langle v'w' \rangle$ at cavity mid-height was determined by the combination of production and buoyant production. Figure 3.21a shows profiles of $\langle v'w' \rangle$ at three vertical locations, extracted from our current simulations. It can be seen that $\langle v'w' \rangle < 0$ at $z = 0.8$, but not at $z = 0.2$ and $z = 0.5$. The near-wall profiles of $P_{23}$, $B_{23}$ and $P_{23} + B_{23}$ have been plotted in Figures 3.21(b-d), corresponding to the three
Figure 3.20. Profiles of $\langle w'w' \rangle$, $\langle w'T' \rangle$ and $\langle T'T' \rangle$, depicting the structure of the boundary layer along the vertical hot wall at different vertical locations, (a) $z = 0.2$, (b) $z = 0.5$ and (c) $z = 0.8$. Solid vertical lines mark the locations $y_{\text{max}}$ and $y_{\text{half}}$. All $y$ coordinates are in wall units. All results are at $Ra = 6.4 \times 10^8$ using Sigma model.
vertical locations respectively. Here, $P_{ij}$ and $B_{ij}$ refer to the production and buoyant production terms respectively in the $\langle u'_i u'_j \rangle$ transport equation,

$$P_{ij} = -\langle u'_i u'_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} - \langle u'_j u'_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}, \quad B_{ij} = Pr \left( \delta_{i3} \langle u'_j T' \rangle + \delta_{j3} \langle u'_i T' \rangle \right).$$

(3.11)

It is seen that $P_{23}$ is negative near the wall at all three locations, while $B_{23}$ is negative only at $z = 0.8$. The total production $P_{23} + B_{23}$ is negative at all three locations, although its magnitude at $z = 0.2$ and $z = 0.5$ is very small. Thus, the sign of the shear stress $\langle v'w' \rangle$ follows the sign of the total production $P_{23} + B_{23}$ at $z = 0.8$, while the remaining term in the shear stress transport equation - the transport term - is responsible for the behaviour of the shear stress near the wall at $z = 0.2$ and $z = 0.5$.

Similar to the near-wall behaviour of $\langle v'w' \rangle$, the streamwise turbulent heat flux $\langle w'T' \rangle$ shows interesting characteristics. $\langle w'T' \rangle < 0$ has been observed in the transitional regions in the 5:1 aspect ratio cavity of Barhaghi and Davidson [6], but $\langle w'T' \rangle > 0$ has been observed in turbulent regions. In the present 4:1 aspect ratio cavity, we observe in Figure 3.22a that $\langle w'T' \rangle < 0$ at $z = 0.8$, but not at $z = 0.2$ and $z = 0.5$. Figures 3.22(b-d) depict profiles of production and buoyant production terms in the $\langle w'T' \rangle$ transport equation, with the definitions

$$P_{iT} = -\langle u'_i u'_k \rangle \frac{\partial \langle T \rangle}{\partial x_k} - \langle u'_k T' \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}, \quad B_{iT} = Pr \delta_{i3} \langle T'T' \rangle.$$

(3.12)

It can be seen that $P_{3T}$ is negative at all three locations, while $B_{3T}$ is constrained to be non-negative by definition. The combined $P_{3T} + B_{3T}$ remains positive at $z = 0.2$ and $z = 0.5$, but turns negative at $z = 0.8$.

It is interesting to note that the local Grashof numbers at $z = 0.5$ and $z = 0.8$ are $Gr_z = 5.6 \times 10^7$ and $Gr_z = 2.3 \times 10^8$ respectively, which are of similar order of magnitude as $Gr_z = 2.6 \times 10^7$ and $Gr_z = 5.5 \times 10^8$ at $z = 0.1$ and $z = 0.2$ respectively in the simulations of Barhaghi and Davidson [6]. The structure of the buoyant turbulent boundary layers at these corresponding locations with similar $Gr_z$ are not exactly similar. For example, $\langle w'T' \rangle$ is negative near the wall at both, $z = 0.8$
Figure 3.21. (a) Profiles of $\langle v'w' \rangle$, along the vertical hot wall at different vertical locations. Production, $P$, buoyant production, $B$, and total production, $P + B$ at (b) $z = 0.2$, (c) $z = 0.5$ and (d) $z = 0.8$. Solid vertical lines mark the locations $y_{\text{max}}$ and $y_{\text{half}}$. All $y$ coordinates are in wall units. All productions are scaled with $u^2/\tau_{\text{max}}$, where $u^2 = Pr/\sqrt{Ra}\left(\partial \langle W \rangle / \partial y\right)_{y=0}$ is the square of the friction velocity. All results are at $Ra = 6.4 \times 10^8$ using Sigma model.
Figure 3.22. (a) Profiles of $\langle w'T' \rangle$, along the vertical hot wall at different vertical locations. Production, $P_{3T}$, buoyant production, $B_{3T}$, and total production, $P_{3T} + B_{3T}$ at (b) $z = 0.2$, (c) $z = 0.5$ and (d) $z = 0.8$. Solid vertical lines mark the locations $y_{max}$ and $y_{half}$. All $y$ coordinates are in wall units. All productions are scaled with $u_\tau^2 T_\tau/y_{max}$, where $u_\tau^2 = Pr/\sqrt{Ra} \langle \partial \langle W \rangle / \partial y \rangle_{y=0}$ is the square of the friction velocity and the temperature scale $T_\tau = -1/\sqrt{Ra} \langle \partial \langle T \rangle / \partial y \rangle_{y=0}$. All results are at $Ra = 6.4 \times 10^8$ using Sigma model.
in our simulations, and at $z = 0.2$ in the simulations of Barhaghi and Davidson [6]. However, $\langle w'T' \rangle$ turns positive near the wall at $z = 0.5$ in our simulations, while it remains negative at $z = 0.1$ in the simulations of Barhaghi and Davidson [6]. A similar comparison of $\langle v'w' \rangle$ between our simulations and the simulations of Barhaghi and Davidson [6] would be interesting, however it is precluded by the lack of mention of profiles of $\langle v'w' \rangle$ at locations other than the cavity mid-height by Barhaghi and Davidson [6]. These observations suggest the rather intuitive result, that the structure of the vertical boundary layer in a thermal cavity is not solely dependent on the local Grashof number, but is possibly also dependent on the distance from the top and bottom walls, or equivalently, the cavity aspect ratio. Further studies in cavities of different aspect ratios and different values of $Ra$ are needed to explore this dependence.

To summarize the discussion in this section, the flow in the thermal driven cavity is characterized by high velocities in the thin boundary layers close to the vertical walls. The region of vertical extent roughly from $z = 0.3$ to $z = 0.7$ exhibits homogeneous, wave-like motion with turbulent fluctuations concentrated near the top-left and bottom-right corners. The dissipation is balanced by production and buoyant production terms. The velocity cross-correlation $\langle v'w' \rangle$ and the streamwise turbulent heat flux $\langle w'T' \rangle$, particularly, reveal interesting features, tied to their respective production and buoyant production terms.

### 3.5 Summary and Conclusions

The suitability of four different SGS models for incompressible Boussinesq LES of buoyant turbulent flows has been evaluated with the thermal driven cavity as a benchmark problem. The LES models have been tested in conjunction with a high-order numerical scheme, and include three eddy-viscosity models with the Smagorinsky, Vreman and Sigma kernels, and a non-eddy-viscosity model of the Stretched Vortex family. The model constants were fixed for the Sigma kernel, while they were deter-
mined using the Lilly [61] localized dynamic procedure for the Smagorinsky kernel and the You and Moin [126] global dynamic procedure for the Vreman kernel. Comparison of the LES results to previously published DNS data exhibited excellent agreement using dynamic Smagorinsky, Stretched Vortex and Sigma models. The results also indicated the need for higher resolution for simulation at higher $Ra$. The dynamic Vreman model was found to be inaccurate, and further tests are required to determine the suitability of the global dynamic procedure for simulating buoyant turbulent flows. Although it is known that the WENO scheme does not guarantee preservation of scalar bounds, no violation of scalar bounds was observed in the present simulations. Further, the results show that the present 5th order WENO scheme for scalars was not overly dissipative as compared to BQUICK scheme. Finally, based on the LES results, the flow structure in the thermal driven cavity has been investigated in detail. The thermal cavity shows regions of enhanced inhomogeneity near the top-left and bottom-right corners and interactions between wave and vortical motions near the top and bottom walls. The turbulent kinetic energy budget reveals interesting characteristics, particularly, regions of negative production associated with negative velocity cross-correlation and the streamwise turbulent heat flux.
4. A NEW MODEL FOR SUBGRID DIFFUSIVITY IN BUOYANT TURBULENT FLOWS

4.1 Introduction

Three existing eddy-viscosity models, with different kernels and different methods of determining the model coefficients, were evaluated in the previous chapter. It was found that the Vreman [114] model, coupled with a global dynamic procedure [125, 126] did not give accurate results. This chapter identifies deficiencies with the Vreman kernel, and with the global dynamic procedure, in the context of buoyant turbulent flows, and attempts to improve on these. A modification to the kernel is proposed, which results in a new model for the subgrid diffusivity. A modified global dynamic procedure, which reduces to the existing global dynamic procedure of You and Moin [126] for non-buoyant flows, is also outlined. The new model, termed $\Pi_T$ model, and the improved global dynamic procedure are evaluated, again, by carrying out LES of the three-dimensional thermal-driven cavity. The next two sections outline the need for a new model, and the model development, while the modified dynamic procedure is developed in Section 4.4. Large eddy simulations testing these modifications are described in Section 4.5. This chapter ends with conclusions, drawn in Section 4.6. In order to retain consistency with the thermal-driven cavity simulations described in the previous chapter, the discussion in this chapter is presented in terms of a temperature field, $T$, and the associated SGS thermal or heat flux, $\tau_jT$.

4.2 Motivation for a new model

Eddy-viscosity type models for the SGS terms in equations governing LES are made up of the kernel and the model constant. The role of the kernel is to provide
sensitivity to local flow conditions, and ensure that the model switches off in locally laminar regions, while the role of the constant is to provide adequate level of dissipation. Various subgrid scale models which are currently in use have been detailed in Chapter 2. The models use different kernels, and either static or dynamic procedures for determining the model constant and the SGS Prandtl number. As discussed earlier, the main drawback of these models is the assumption that the kernel for SGS viscosity is identical to the kernel for SGS diffusivity, as stated by equation (2.10). As a result of this assumption, the SGS diffusivity is a function only of the resolved velocity field, and does not depend explicitly on the resolved temperature field. The velocity field in a buoyant flow is determined by the temperature field, and the SGS diffusivity is indeed dependent on temperature via the velocity field. However, an explicit dependence on the temperature field can potentially lead to more accurate modeling of the subgrid scale heat flux.

The model of Vreman [114] has been shown to be superior at distinguishing between laminar and turbulent regions in non-buoyant flows. LES of a turbulent mixing layer and turbulent channel flow using the Vreman model showed better agreement to DNS data than the constant coefficient Smagorinsky model and was comparable in its accuracy to the dynamic Smagorinsky model [114]. The Vreman model, coupled with the global dynamic procedure of You and Moin [125] has also been shown to be good at predicting turbulent statistics in fully inhomogeneous situations, such as the flow in a lid-driven cavity [99]. The extension of the dynamic procedure by You and Moin [126] for passive scalar mixing has also shown better performance than the dynamic Smagorinsky model. The dynamic Vreman model applied to buoyant convection in the thermal driven cavity described in Chapter 3, however, did not yield good results. This indicates that modifications to the Vreman kernel may be necessary for accurate simulation of buoyant turbulent flows. A new model for the SGS diffusivity is developed, based on the procedure of Vreman [114].
4.3 Development of new model

The aim of SGS modeling of non-buoyant flows is to write an analytical expression for the SGS viscosity $\nu_{SGS}$ in terms of components of the resolved velocity $\bar{u}_i$, and its gradients $\partial \bar{u}_i / \partial x_j$. The model development by Vreman [114] involved the following steps:

1. Established that whenever all derivatives of the $i^{th}$ component of velocity are zero, i.e. $\partial \bar{u}_i / \partial x_j = 0$ for all $j$, all components of the $i^{th}$ row of the SGS stress tensor, $\tau_{ij}$, are zero.

2. Identified 320 cases depending on the number of components (from any 1 to all 9) of the velocity gradient tensor $\partial \bar{u}_i / \partial x_j$ that are zero. Showed that for all cases among these 320, the metric $B^g_{\beta}$ is zero if and only if the theoretical subgrid dissipation is zero.

3. Used realizability conditions to determine an appropriate function for the SGS viscosity $\nu_{SGS}$ in terms of the functional $B^g_{\beta}$.

4. Estimated the value of the model coefficient by analogy to Smagorinsky model in the case of homogeneous isotropic turbulence.

A similar procedure is applied here to determine an expression for the SGS diffusivity. For a fixed location $x$, and a linear filter $G$ with compact support in a region $\Omega$ around $x$, we have

$$\tau_{jT} = \bar{u}_j \bar{T}(x) - \bar{u}_j(x) \bar{T}(x)$$

$$= \bar{u}_j \bar{T}(x) - \bar{u}_j(x) \bar{T}(x) - \bar{T}(x) \bar{u}_j(x) + \bar{u}_j(x) \bar{T}(x)$$

$$= \int_{\Omega_x} G(y) [u_j(y) - \bar{u}_j(x)] [T(y) - \bar{T}(x)] \, dy. \quad (4.1)$$

The above equation indicates that $\tau_{jT}$ is zero whenever either the velocity or the temperature is locally constant over the region $\Omega_x$. Similar to the assumption in Vreman [114], we assume that a locally constant velocity implies $\partial \bar{u}_i / \partial x_j = 0$, and
a locally constant temperature implies \( \partial \bar{T} / \partial x_j = 0 \) at \( x \). Thus, \( \tau_{jT} \) at a location is zero whenever all derivatives of \( \bar{u}_j \) are zero, or all derivatives of \( \bar{T} \) are zero at that location. Let \( \Pi^T \) be a measure which is zero if all derivatives of \( T \) are zero. A SGS diffusivity proportional to the Vreman kernel \( \Pi^g \), and proportional to this measure \( \Pi^T \) would be zero whenever \( \tau_{jT} \) is zero. Thus,

\[
k_{SGS} \propto \Pi^g \Pi^T. \tag{4.2}
\]

Any of the algebraic norms of the temperature gradient could serve as the measure \( \Pi^T \). Choosing the \( L_2 \) norm,

\[
\Pi^T = \left[ \left( \frac{\bar{\Delta}}{\Delta T} \right) \left( \frac{\partial \bar{T}}{\partial x_j} \frac{\partial \bar{T}}{\partial x_j} \right)^{1/2} \right]^q, \tag{4.3}
\]

where \( \bar{\Delta} \) and \( \Delta T \) are typical length and temperature scales respectively, which have been used to ensure that the kernel is non-dimensional. Putting the model for the SGS diffusivity together and introducing a model constant, we have

\[
k_{SGS} = C_T \Pi^g \left[ \left( \frac{\bar{\Delta}}{\Delta T} \right) \left( \frac{\partial \bar{T}}{\partial x_j} \frac{\partial \bar{T}}{\partial x_j} \right)^{1/2} \right]^q. \tag{4.4}
\]

One difference between modeling buoyant and non-buoyant turbulent flows is the fact that unlike the SGS stress tensor \( \tau_{ij} \), the subgrid scale heat flux \( \tau_{jT} \) is not subjected to realizability constraints. This precludes determination of a unique value for the parameter \( q \) in the above model. It can be noted that \( q \geq 0 \) in order to avoid a singularity when \( \Pi^T = 0 \). The model reduces to the Vreman model for \( q = 0 \). Further, for \( q > 0 \), the parameter controls the relative importance of the contribution of the temperature field to the SGS diffusivity over that of the velocity field. We expect that for a larger value of \( q \), the SGS diffusivity would be dependent on the temperature field to a greater degree. The effect of \( q \) on the model performance needs to be evaluated in subsequent simulations.
The model constant $C_T$ can be determined using the dynamic procedure of You and Moin [126]. The formula for $C_T$ is

$$C_T = k_T \frac{\left\{ \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} - \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} \right\}}{\left\{ \Pi^t \Pi^t \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} - \Pi^T \Pi^g \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} \right\}}. \quad (4.5)$$

This formula for the model coefficient results in a SGS Prandtl number which is weakly dependent on time and independent on space. The effective SGS Prandtl number is

$$Pr_{SGS} = C_V \frac{\left\{ \Pi^t \Pi^t \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} - \Pi^T \Pi^g \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} \right\}}{\left\{ \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} - \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} \right\}}. \quad (4.6)$$

$\Pi^T$ is given by equation (4.3), and $\Pi^\hat{t}$ is given by the corresponding quantities at the test-filter level,

$$\Pi^\hat{t} = \left[ \left( \frac{\Delta}{\Delta T} \right) \left( \frac{\partial \hat{T}}{\partial x_j} \frac{\partial \hat{T}}{\partial x_j} \right)^{1/2} \right]^q. \quad (4.7)$$

The difference between $\Pi^t$ defined in equation (2.21) and the kernels $\Pi^T$ and $\Pi^\hat{t}$ defined above should be noted.

The model developed in this section is referred to as the $\Pi^T$ model. $\Pi^T$ model with two values of $q = 1$ and $q = 2$ will be evaluated in this chapter.

4.4 An improved Global Dynamic Procedure for Buoyant Turbulent Flows

The global dynamic procedure of You and Moin [125] gives a formula for the model coefficient $C_V$ of the Vreman model. This procedure is based on the assumption of global equilibrium between viscous dissipation and subgrid dissipation. The formal
derivation begins with a derivation of transport equation for \( L_{ii} = T_{ii} - \hat{\tau}_{ii} \), where \( T_{ii} \) is the test-filtered total kinetic energy, and \( \tau_{ij} \) is the SGS stress tensor,

\[
\frac{\partial L_{ii}}{\partial t} = \frac{\partial}{\partial x_j} \left\{ - (\hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j) - 2(\hat{u}_j \hat{p} - \hat{u}_j \hat{p}) + \nu \left( \frac{\partial \hat{u}_i}{\partial x_j} - \frac{\partial \hat{u}_i}{\partial x_j} \right) \right\} - 2(\tau_{ij} \hat{u}_i - T_{ij} \hat{u}_i) - 2\nu \left( \frac{\partial \hat{u}_i}{\partial x_j} - \frac{\partial \hat{u}_i}{\partial x_j} \right) + 2(\tau_{ij} \hat{S}_{ij} - T_{ij} \hat{S}_{ij}). \tag{4.8}
\]

Taking the global average, and assuming that the unsteady term and the transport term \( \frac{\partial \{} / \partial x_j \) drop out, we get the formula for \( C_V \) as given by equation (2.18). Following the same procedure, and accounting for the body force term in buoyant flows, results in a modified formula for the dynamic model coefficient

\[
C_V = -\frac{\nu}{2} \left\{ \hat{\alpha}_{ij} \hat{\alpha}_{ij} - \hat{\alpha}_{ij} \hat{\alpha}_{ij} \right\} + \frac{\hat{F}_i \hat{u}_i - \hat{F}_{ij} \hat{S}_{ij}}{2 \left\{ \Pi \hat{S}_{ij} \hat{S}_{ij} - \Pi' \hat{S}_{ij} \hat{S}_{ij} \right\}}, \tag{4.9}
\]

where \( F_i = g_i (\rho(\rho_*) - \rho_0) / \rho_0 \) is the buoyant body force term. This expression for the model coefficient reduces to equation (2.18) in non-buoyant situations, where the acceleration due to gravity \( g_i \), and consequently, the body force \( F_i \), are zero. The contribution of the second term in equation (4.9) may be non-trivial in buoyant flows.

The model with corrected formula for \( C_V \) is referred to as the ‘Corrected \( C_V \)’ model. In the next section, the performance of the Corrected \( C_V \) model along with \( \Pi^T \) models developed in the previous section is evaluated with the thermal-driven cavity described in Chapter 3 as a test problem.

### 4.5 Application to LES of Thermal-Driven Cavity

A summary of the new models developed in the previous two subsections can be found in Table 4.1. All models employ equation (2.16) to determine the SGS viscosity. In the baseline DVM model, over which we are seeking improvements, the model constants \( C_V \) and \( C_T \) are determined using equations (2.18) and (2.19) respectively. The \( \Pi^T \) model uses equation (2.18) to determine \( C_V \), equation (4.4) to determine the SGS diffusivity, and equation (4.5) for \( C_T \). \( \Pi^T \) models with \( q = 1 \)
Table 4.1. Summary of improvements to the dynamic Vreman model.

<table>
<thead>
<tr>
<th>Model</th>
<th>Label</th>
<th>Kernels</th>
<th>Model Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline Dynamic Vreman Model</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DVM</td>
<td>$\Pi^q$, eq. (2.16)</td>
<td>$C_V$, eq. (2.18)</td>
<td>and $C_T$, eq. (2.19)</td>
</tr>
<tr>
<td>$\Pi^T$ model with $q = 0$</td>
<td>$\Pi_0^T$</td>
<td>$\Pi^q$, eq. (2.16)</td>
<td>$C_V$, eq. (2.18)</td>
</tr>
<tr>
<td>$\Pi^T$ model with $q = 1$</td>
<td>$\Pi_1^T$</td>
<td>$\Pi^q$, eq. (2.16)</td>
<td>$C_V$, eq. (2.18)</td>
</tr>
<tr>
<td>DVM with Corrected coefficient</td>
<td>Corrected $\Pi^q$, eq. (2.16)</td>
<td>$C_V$, eq. (4.9)</td>
<td>and $C_T$, eq. (4.5)</td>
</tr>
</tbody>
</table>

and $q = 2$ are evaluated here. Finally, the corrected $C_V$ model utilizes the same expressions as $\Pi^T$, $q = 1$ model, except for $C_V$, which is given by the corrected formula, equation (4.9).

Figures 4.1 and 4.2 compare the results obtained using the above four models with DNS results at off-center vertical locations in the thermal cavity. Results for $Ra = 6.4 \times 10^8$ at $z = 0.8$ are shown in Figure 4.1 and results for $Ra = 2.0 \times 10^9$ at $z = 0.9$ are shown in Figure 4.2. For both the Rayleigh numbers, the Corrected $C_V$ model yields results very similar to baseline DVM results. Results obtained using $\Pi^T$ models too are very close to those obtained using baseline DVM. Further, the $\Pi^T$ model results with $q = 1$ are not very different from the $\Pi^T$ model with $q = 2$. Thus, $\Pi^T$ model does not show much dependence on the parameter $q$. For the thermal cavity test case, the newly developed models do not show much improvement over, and are as good as, the dynamic Vreman model.
Figure 4.1. Second order turbulent statistics at off-center location $z = 0.8$ for $Ra = 6.4 \times 10^8$ using dynamic Vreman model, dynamic Vreman model with corrected $C_V$, $\Pi_T^T$ model with $q = 1$ and $\Pi_T^T$ model with $q = 2$. (a-d) RMS quantities (e-g) Correlations
Figure 4.2. Second order turbulent statistics at off-center location $z = 0.9$ for $Ra = 2.0 \times 10^9$ using dynamic Vreman model, dynamic Vreman model with corrected $C_V$, $\Pi^T$ model with $q = 1$ and $\Pi^T$ model with $q = 2$. (a-d) RMS quantities (e-g) Correlations
4.6 Summary and Conclusions

A new model for the SGS diffusivity has been developed in this chapter, following a process of reasoning similar to that used for developing the Vreman [114] model. This model, has been named the $\Pi T$ model, and builds an explicit dependence of the SGS diffusivity on the resolved temperature (or scalar) field, which was missing from the original Vreman model discussed in Section 2.3.4. This model has been tested in LES of thermal-driven cavity. Contrary to expectations, although there is no degradation of the results, the $\Pi T$ model did not lead to any significant improvement in the results over the baseline dynamic Vreman model in this test problem either. The model needs to be further evaluated in other test problems, in order to ascertain if the improved sensitivity of the model kernel offers any advantages over a kernel which determines the eddy-diffusivity exclusively based on the resolved velocity field.

The global dynamic procedure of You and Moin [126] has also been modified in this chapter, so as to include contributions from the buoyant body force term in the Navier-Stokes equations. This modified model neatly reduces to the formulation of You and Moin [126] in non-buoyant flows. This correction has also been tested in LES of thermal-driven cavity, with, again, insignificant changes over the baseline DVM. It should be noted that previous studies [78, 125, 126] on global dynamic procedures for determining the model coefficient suggest that the value of the global coefficient, determined by the global dynamic procedure, is highly dependent on the test problem considered, the numerical schemes used to discretize the equations, the test-filtering operation, and the flow conditions being simulated. It is anticipated that the body force term contribution to the determination of the global coefficient can be significant in buoyancy-dominated or strongly stratified problems, and should be included in future LES studies of such flows.
5. A PRIORI EVALUATION OF LARGE EDDY SIMULATION
SUBGRID-SCALE SCALAR FLUX MODELS IN ISOTROPIC PASSIVE-SCALAR
AND ANISOTROPIC BUOYANCY-DRIVEN HOMOGENEOUS TURBULENCE

5.1 Introduction

Evaluation and testing of subgrid scale (SGS) models for large eddy simulation (LES) follows from two broad philosophies. The first philosophy involves comparing results (first, second or higher order statistics, flow structures, etc.) obtained from LES computations, with benchmark Direct Numerical Simulation (DNS) or experimental results. This is termed a posteriori test, since it involves comparisons after an actual LES computation. An alternate methodology, termed a priori test, involves computing actual SGS terms and comparing them to different model terms, both extracted from high resolution data from a DNS or an experiment [86]. The previous two chapters focussed on a posteriori evaluation of different eddy-viscosity subgrid-scale models. This chapter turns to a priori evaluation of eddy-viscosity and non-eddy-viscosity models. A priori tests of different eddy-viscosity and non-eddy-viscosity subgrid scale models for the flux of a transported scalar are performed in this chapter.

A large number of models for SGS scalar flux have appeared in the literature over the years, and have been reviewed extensively in Chapter 2. The earliest, Smagorinsky model with a constant SGS Schmidt (or Prandtl) number approximation (e.g. [30]), belongs to the so-called eddy-viscosity type of models. Recent examples of eddy-viscosity models include the Vreman [114] and Sigma [72] models, both of which attempt to be more sensitive to the velocity flow field as compared to the Smagorinsky model. The SGS Schmidt number, coupling models for the SGS stress tensor to models for the SGS scalar flux, can also be computed dynamically in a number of
different ways [61, 78, 126]. Other families of models include Stretched Vortex [88], Similarity [63], Tensorial Eddy-Diffusivity [119], Dynamic Structure [19] and Gradient [65, 66] type models. Classes which model the non-linear terms directly instead of the SGS stress tensor or the SGS scalar flux include regularization [111], approximate deconvolution [105] and non-linear LES (nLES) [11, 13] methods. In addition, mixed models, employing a combination of more than one of the above methods, also exist in the literature [127, 63, 52, 115, 101].

Eddy-viscosity models are simple, inexpensive, and robust, since these models do not allow for backscatter, or transfer of energy from small scales to large scales. However, the principal disadvantage of eddy-viscosity models is that the models are inaccurate, on account of the modeled SGS terms being very poorly correlated with the actual SGS terms [63]. Dynamic Structure and Gradient models seek to improve the correlations with actual SGS terms, however, at an increased computational complexity and cost. The Dynamic Structure model, introduced and developed in Chumakov and Rutland [20, 21] and Chumakov [19], explicitly involves the SGS scalar variance, which requires the solution of an additional transport equation. Furthermore, this additional equation for the SGS scalar variance involves unclosed terms, which in turn, need to be modeled. The Gradient model for the SGS stress tensor was introduced and investigated in an a priori study by Lu et al. [67]. This model, termed GCDSM by Lu et al. [67], also involved the subgrid kinetic energy, for which, a transport equation was recommended. An algebraic (zero-equation) version of the Gradient model, termed the Modulated Gradient model, was developed and evaluated through a posteriori simulations of the Atmospheric Boundary Layer (ABL) by Lu and Porté-Agel [65]. The Gradient and Modulated Gradient models for the SGS stress tensor were extended to model SGS scalar fluxes by Lu and Porté-Agel [66]. The Modulated Gradient model was evaluated, again through a posteriori tests in neutral and stably stratified ABL, and was found to show significant improvement as compared with standard eddy-viscosity models. A priori investigations of the Gra-
dient and Modulated Gradient models for the SGS scalar flux have not been carried out so far, and are of interest so as to get more insight into these models.

Three eddy-viscosity type models (namely, Smagorinsky, Vreman and Sigma), a Dynamic Structure model and two variants of Gradient type (Gradient and Modulated Gradient) models are investigated here using a priori methods. The a priori tests are carried out based on data generated from DNS of homogeneous turbulence with a transported passive scalar (i.e. turbulence without buoyancy effects), as well as homogeneous turbulence with an active scalar (i.e. homogeneous buoyant turbulence). Owing to its high accuracy and parallel scalability, the pseudo-spectral method is a natural candidate for performing DNS of homogeneous flows. The governing equations, numerical method, time stepping and forcing schemes employed are described in Section 5.2. A description of the simulations and the DNS results are presented in Section 5.3. A priori studies are presented next, in Section 5.4. The aim is to examine two different aspects of the models, viz. their ability to predict the direction and the magnitude of the SGS scalar flux. Based on the observations, new models, which do not involve terms requiring additional transport equations, and which are expected to be more accurate than the Modulated Gradient model, are proposed. A brief a posteriori evaluation of the existing and proposed models in the homogeneous context is presented in Section 5.5. Section 5.6 summarizes the results and presents conclusions.

5.2 Pseudo-Spectral Method

Homogeneous non-buoyant and buoyant turbulence simulations are performed here using a standard pseudo-spectral algorithm. The numerical code was first developed by Chandy and Frankel [18] and has also been used in Shetty et al. [100]. A few modifications, pertaining to the time stepping, forcing, dealiasing and incorporation of buoyancy effects, have been subsequently incorporated. The governing
equations, numerical method, and time stepping and forcing schemes are described in the sub-sections below.

### 5.2.1 Governing Equations

The equations governing the evolution of a turbulent flow field without background shear or rotation effects, but including background stratification effects are given by

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{5.1}
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - g \beta \phi \delta_{i3} + f_i \tag{5.2}
\]

\[
\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} + u_j \alpha_j = k_\phi \frac{\partial^2 \phi}{\partial x_j \partial x_j} \tag{5.3}
\]

The velocities \( u_i \), with \( i = 1, 2, 3 \), and the pressure \( p \), may be thought of as perturbations over a background state, which is constant in time and space. Similarly, \( \phi \) denotes the fluctuations superimposed on a mean (background) scalar field denoted by \( \Phi \). \( \Phi \) is constrained to be constant in time, and vary linearly in space, i.e. \( \Phi = \Phi_0 + \alpha_i x_i \), with \( \alpha_i = \partial \Phi / \partial x_i \) denoting the gradient in the \( i \) direction.

The scalar field may represent either temperature, or a species concentration. The density is assumed to be related to the scalar field via the linear equation of state

\[
\rho = \rho_0 [1 + \beta \phi (\Phi + \phi)] ,
\]

where \( \rho_0 \) is the reference density, and \( \beta \phi \) is the expansion coefficient with respect to the scalar \( \phi \). The equations above assume that the density variations (background as well as fluctuations) are small, and that the Boussinesq approximation, restricting effects of density variations to the body force term, is valid.

It should be noted that the contribution of the background scalar profile \( \Phi \) to the body force term is balanced by the mean pressure, and does not appear in eqn. (5.2).

In addition, the background scalar profile does not appear in the viscous or the temporal derivative terms in eqn. (5.3) on account of its linearity in space and invariance in time. \( g, \nu \) and \( k_\phi \) denote the gravitational acceleration (with gravity acting in the negative \( x_3 \) direction), fluid viscosity and the scalar diffusivity, respectively. \( f_i \) denotes an artificial forcing term, which is described later in Section 5.2.4.
It may be noted that setting either \( g \) or \( \beta_\phi \) to zero decouples the momentum equations from the scalar equation, and the same form of equations as above can be used to describe the evolution of a non-buoyant turbulent flow field, with a transported passive scalar.

### 5.2.2 Numerical Methodology

The governing equations described above are solved on a rectangular domain, of size \([L_x, L_y, L_z]\) in the three directions. The constraints on the background state described above allow imposition of fully periodic boundary conditions on the domain. This in turn, renders the system of equations amenable to solution via a Fourier collocation pseudo-spectral method. The velocity and scalar fields are expanded in terms of Fourier basis functions as

\[
\begin{align*}
\mathbf{u}(\mathbf{x}, t) &= \sum_\kappa e^{i\kappa \cdot \mathbf{x}} \hat{\mathbf{u}}(\kappa, t), \\
\phi(\mathbf{x}, t) &= \sum_\kappa e^{i\kappa \cdot \mathbf{x}} \hat{\phi}(\kappa, t),
\end{align*}
\]

(5.4)

where \( i \) denotes the unit imaginary number, \( \kappa \) denotes the wavenumber vector \([\kappa_1, \kappa_2, \kappa_3]\), and \( \hat{\mathbf{u}} \) and \( \hat{\phi} \) denote the complex Fourier coefficients of the velocity and scalar fields respectively. It should be noted that \( \hat{\mathbf{u}} \) is a vector with three components, \([\hat{u}_1, \hat{u}_2, \hat{u}_3]\). The summation is over all wavenumber vectors \([l, m, n] = \left[ \frac{l2\pi}{L_x}, \frac{m2\pi}{L_y}, \frac{n2\pi}{L_z} \right] \), with \( l = 0, 1, 2, ...N_x-1 \), \( m = 0, 1, 2, ...N_y-1 \) and \( n = 0, 1, 2, ...N_z-1 \). If the domain is cubical with each side equal to \( 2\pi \), the wavenumbers components reduce to integers \([l, m, n]\). With the above representation of velocity and scalar fields, the governing equations (5.1)-(5.3) are transformed to [86]

\[
\begin{align*}
\left( \frac{d}{dt} + \nu \kappa^2 \right) \hat{u}_j(\kappa, t) &= -P_{jk}(\kappa) \left[ \hat{\mathbf{G}}_k + g\beta_\phi \hat{\phi} \delta k_3 - \hat{f}_k \right] \quad (5.5) \\
\left( \frac{d}{dt} + \nu \kappa^2 \right) \hat{\phi} &= -\hat{\mathbf{G}}_\phi - \hat{u}_j \alpha_j, \quad (5.6)
\end{align*}
\]

where \( \kappa = \sqrt{\kappa_1^2 + \kappa_2^2 + \kappa_3^2} \) is the magnitude of the wavenumber vector, and \( P_{jk} \) denotes the projection tensor

\[
P_{jk} = \delta_{jk} - \frac{\kappa_j \kappa_k}{\kappa^2}. \quad (5.7)
\]
Introduction of the projection tensor results in eliminating the pressure term in the transformed equation (5.5). This results in a huge simplification in the solution procedure, and is one of the attractive features of the pseudo-spectral method. \( \hat{G}_k \) and \( \hat{G}_\phi \) denote the convolutions arising out of the advective terms in the momentum and scalar transport equations respectively

\[
\hat{G}_j(\kappa, t) = i\kappa_k \sum_{\kappa'} \hat{u}_j(\kappa', t)\hat{u}_k(\kappa - \kappa', t) \tag{5.8}
\]

\[
\hat{G}_\phi(\kappa, t) = i\kappa_k \sum_{\kappa'} \hat{\phi}(\kappa', t)\hat{u}_k(\kappa - \kappa', t). \tag{5.9}
\]

Evaluating the terms \( \hat{G}_j \) and \( \hat{G}_\phi \) directly from their definitions (5.8) and (5.9) is prohibitively expensive, since they involve convolutions over the wavenumber vectors. This difficulty is overcome by computing the advective terms in the physical space following a three step procedure. The physical velocity and scalar fields are computed through inverse Fourier transforms of the respective Fourier coefficients, the advective terms are computed using simple multiplications instead of convolutions, and the advective terms are transformed back to the spectral space via forward Fourier transforms. This computation of advective terms in physical space is the reason why the method is termed pseudo-spectral, in lieu of spectral. It may be noted that all non-linear terms (including, e.g., terms arising out of SGS models in an LES) need to be computed in this pseudo-spectral manner in order to keep computational costs at a manageable level. The computation of advective terms in physical space gives rise to aliasing errors, which need to be removed. Three methods appear in the literature, namely padding, truncation and phase shifting. In the current implementation, dealiasing is achieved by truncating the number of useful modes to 2/3 times the actual number in each direction. Thus, a simulation referred to as having been carried out on \( N^3 \) physical grid points, actually utilizes \( 3N/2 \) grid points in each direction. Thus, the \( 32^3 \), \( 64^3 \) and \( 128^3 \) simulations referred to in Section 5.3 below, actually require \( 48^3 \), \( 96^3 \) and \( 192^3 \) grid points respectively.

The simulations are carried out on multiple processors, communicating with each other using Message Passing Interface (MPI) library subroutines. All Fourier trans-
forms are carried out using the P3DFFT library [79], which allows for fast computation of Fourier transforms with the data spread over processors arranged in a two dimensional grid. The P3DFFT library in turn utilizes FFTW [35] for computing Fourier transforms in individual directions. Output data is handled efficiently using the HDF5 library [46].

5.2.3 Time Steping Schemes

Equations (5.5) and (5.6) are integrated in time, starting from a specified initial condition. Two time stepping schemes have been implemented, based on combining a third-order accurate Runge-Kutta (RK3) scheme with the integration factor (IF) approach [15], and with the exponential time differencing (ETD) approach [22]. The basic idea behind the methods is illustrated by concentrating on equation (5.5) below. Equation (5.5) can be written as

$$\left( \frac{d}{dt} + \nu \kappa^2 \right) \hat{u}_j(\kappa, t) = -R_j(\hat{u}, \hat{\phi}, t). \quad (5.10)$$

The first step is to multiply both sides by the integration factor $e^{\nu \kappa^2 t}$. The left hand side can then be rearranged to give

$$\frac{d}{dt} \left( e^{\nu \kappa^2 t} \hat{u}_j \right) = -e^{\nu \kappa^2 t} R_j(\hat{u}, \hat{\phi}, t). \quad (5.11)$$

The IFRK3 approach discretizes the above equation using a 3 stage RK3 method. The precise equations can be found in Canuto et al. [15] and Shettty [97]. Under the ETD approach, the equations are integrated from time $t_n$ to time $t_{n+1} = t_n + h$, and rearranged to yield

$$\hat{u}_j(t_{n+1}) = \hat{u}_j(t_n) e^{-\nu \kappa^2 h} - e^{-\nu \kappa^2 h} \int_0^h e^{\nu \kappa^2 t'} R_j(\hat{u}, \hat{\phi}, t') dt'. \quad (5.12)$$

This equation is discretized in time using an RK3 method to give the ETDRK3 method. The formulation given in Cox and Matthews [22], needs to be modified slightly so as to ensure numerical stability, and to resolve singularities. The modifications provided by Kassam and Trefethen [55] are implemented here.
Both the above methods require three evaluations of the right hand side, some precomputation and additional memory to precompute and store the integration or exponential factors. However, compared to other explicit time integration methods, IF and ETD methods treat the linear terms in an exact and unconditionally stable manner [22]. Comparing among the two methods, ETD has been shown to treat the non-linear terms more accurately for some systems with stiff non-linear parts [22]. In our current implementation, the two methods were found to yield almost identical results for the Taylor-Green Vortex simulations described later in Section 5.3.1. As a result, all subsequent simulations have been carried out using only the IF approach.

5.2.4 Forcing Schemes

The final component of the algorithm involves the artificial forcing used to sustain turbulence in a homogenous flow. Two broad categories, of forcing schemes, deterministic [16, 75] and stochastic [33, 3], appear in the literature. A deterministic forcing scheme [16, 68, 88] has been implemented in this study. The Fourier coefficient of the artificial force applied at wavenumber $\kappa$ is given by

$$\hat{f}_\kappa = \frac{\epsilon_f}{N_f} \hat{u}_\kappa^* \hat{u}_\kappa, \quad |\kappa| \leq \kappa_0, \quad (5.13)$$

where the superscript $^*$ represents the complex conjugate, $\epsilon_f$ is a forcing parameter, and $\kappa_0 = 2$ is the radius of the shell in which forcing is applied. The forcing is zero for all wavenumbers with magnitudes larger than $\kappa_0$, and at the origin $\kappa = 0$. The integer $N_f$, represents the number of modes in the shell $0 \leq \kappa \leq \kappa_0$, with $N_f = 20$ for $\kappa_0 = 2$. This forcing scheme ensures that the energy injection rate is equal to $\epsilon_f$ at all time instants.

5.3 DNS Results

Direct Numerical Simulations under different flow configurations are performed and described in this section. The momentum solver, without scalar transport, is
first validated by performing DNS of decaying Taylor-Green vortex. This is followed by simulations of non-buoyant stationary (Section 5.3.2) and decaying turbulence (Section 5.3.3). Homogeneous buoyant turbulent simulations are reported in Section 5.3.4. In each case, the simulations are compared to results from previous DNS studies, in order to establish the accuracy of the current solver.

5.3.1 Validation of Momentum Solver

The evolution of a Taylor-Green vortex flow field, starting from an idealized state given by

\[ u_1(x, y, z, 0) = \sin(x) \cos(y) \cos(z) \]  
\[ u_2(x, y, z, 0) = -\cos(x) \sin(y) \cos(z) \]  
\[ u_3(x, y, z, 0) = 0, \]

is considered here. Simulations at three Reynolds numbers, \( Re = 800, 1600 \) and \( 3000 \) are carried out, on \( 128^3 \) physical grids, using both the time-stepping schemes described above. The rate of change of the total turbulent kinetic energy is shown in Figure 5.1, along with previous DNS results (denoted by square symbols) by Drikakis et al. [29]. It is seen that the turbulent kinetic energy decays monotonically, since \(-dK/dt\) is always positive. For all values of \( Re \), the rate of change of the turbulent kinetic energy increases at first, attains a peak at approximately \( t = 9 \) and then reduces. The present DNS results can be seen to be in good agreement with the previous DNS results of Drikakis et al. [29], especially at low times. At large times, the agreement continues to be good at \( Re = 800 \), while some discrepancies are observed at \( Re = 1600 \) and \( Re = 3000 \). Results using only IFRK3 scheme are shown in Figure 5.1, however, the ETDRK3 time stepping was found to yield identical results. The IFRK3 time stepping scheme has been used in all subsequent simulations.
Figure 5.1. Validation of momentum solver without a transported scalar. Decaying Taylor-Green vortex simulation results (lines) compared to previous DNS results (filled square symbols) [29].
5.3.2 Forced Passive Scalar Turbulence

Simulations of stationary turbulence with a passive scalar are described in this section. The simulations are started from randomly generated initial fields, obeying the spectrum

\[ E(k) = A_k k^4 e^{-2k^2/k_0^2}, \tag{5.17} \]

where \( k \) denotes the magnitude of the three-dimensional wavenumber vector, the constant \( A_k \) sets the initial turbulent kinetic energy (TKE), and \( k_0 \) determines the peak of the initial energy spectrum. We use values \( A_k = 0.01751 \) and \( k_0 = 3 \). The turbulence is driven to stationarity by applying deterministic forcing to the large scales, as described previously. Forcing is applied only to the momentum equations. The scalar fluctuations are initially set to zero, and a mean scalar gradient \( \alpha_2 = 1 \) is maintained in the \( y \) direction. The mean scalar gradient is zero in the other two directions, i.e. \( \alpha_1 = \alpha_3 = 0 \). The mean scalar gradient remains unchanged as the simulations progress, while the scalar variance and the scalar flux increase from zero to stationary values. The simulation setup mimics that reported in Overholt and Pope [74].

The Schmidt number is set to be equal to \( Sc = 1 \), of the same order of magnitude as \( Sc = 0.7 \) in Overholt and Pope [74]. The Reynolds number attained by the flow at stationary state can be controlled by varying the viscosity, \( \nu \), and the forcing parameter, \( \epsilon_f \). Furthermore, the number of grid points, \( N \), restricts the maximum Reynolds number that can be attained, while ensuring that all scales, including the smallest Kolmogorov scale in the flow remain fully resolved. In the present simulations, we choose to fix \( \epsilon_f = 0.5 \), and vary \( N \) and \( \nu \) in order to carry out DNS of homogeneous turbulence at different values of \( Re \). Time and volume averages of different quantities are extracted from the simulations. The computed quantities include a velocity scale,
\( u' \), the turbulent dissipation rate, \( \epsilon \), the Taylor microscale, \( \lambda \), the integral length scale, \( l \), and the Kolmogorov length scale, \( \eta \). These quantities are defined as

\[
\begin{align*}
    u'^2 &= \frac{2}{3} \int_0^{k_{max}} E(k) \, dk, \\
    \epsilon &= \langle 2\nu \tilde{S}_{ij} \tilde{S}_{ij} \rangle, \\
    \lambda &= \sqrt{\frac{15\nu u'^2}{\epsilon}}, \\
    l &= \frac{\pi}{2u'^2} \int_0^{k_{max}} \frac{E(k)}{k} \, dk, \\
    \eta &= \left( \frac{\nu^3}{\epsilon} \right)^{1/4},
\end{align*}
\]

where \( k_{max} \) denotes the largest wavenumber represented, and \( E(k) \) denotes the velocity spectrum.

Figure 5.2a shows the temporal evolution of the Taylor scale Reynolds number, \( Re_\lambda = u'\lambda/\nu \), from three different simulations. These three simulations are carried out on physical grids of \( N = 32^3, 64^3 \) and \( 128^3 \) collocation points, with viscosity values of \( \nu = 1/30, 1/80 \) and \( 1/210 \) respectively. It can be seen that for the \( \nu = 1/30 \) case, \( Re_\lambda \) starts from a low value at \( t = 0 \), increases with time, and attains a stationary value of around \( Re_\lambda \approx 25 \). Similarly, simulations with \( \nu = 1/80 \) and \( 1/210 \) attain Reynolds numbers of approximately \( Re_\lambda = 49 \) and \( 84 \) respectively. These values are very close to \( Re_\lambda = 28, 52 \) and \( 84 \) attained in the simulations reported by Overholt and Pope [74], using the same number of grid points. The slight differences are due to differences in the forcing schemes employed in our present study and by Overholt and Pope [74]. Figure 5.2b shows the evolution of \( k_{max}\eta \), where \( \eta \) denotes the Kolmogorov length scale. \( k_{max}\eta \) is consistently greater than 1 in the present simulations, indicating that the simulations are fully resolved at all times. Figure 5.3 shows the TKE spectra obtained from the three simulations. The imposed spectrum is seen at \( t = 0 \) in each case, while the spectra at later time instants lie on top of each other, confirming that the flow at these time instants is statistically stationary. The vertical dashed line denotes the forcing cut-off wavenumber (\( k_f = 2 \)). The spectra below \( k_f \) at all time instants beyond \( t = 0 \) are directly affected by the artificial forcing. Comparing the stationary spectra at different \( Re_\lambda \), it can be seen that the inertial sub-range, with a slope close to \(-5/3\), is virtually absent in the lowest \( Re_\lambda \) case, and its width increases with increasing \( Re_\lambda \).
Figure 5.2. Results of three forced passive scalar simulations. Time evolution of (a) Taylor scale Reynolds number, $Re_\lambda$, and (b) Kolmogorov scale, $k_{\text{max}}\eta$.

Figure 5.3. TKE spectra of forced passive scalar simulations at different time instants for (a) $Re_\lambda = 25$, (b) $Re_\lambda = 49$, and (c) $Re_\lambda = 84$. 
The behaviour of the passive scalar field, which is transported by the turbulence, in the presence of a mean scalar gradient, is now analyzed. Figure 5.4 shows the scalar flux in the direction of the mean scalar gradient, $\langle v' \phi' \rangle$, and variance, $\langle \phi'^2 \rangle$, at different $Re_\lambda$, under different normalizations. The present simulation results (denoted by hollow squares) are compared to the DNS results of Overholt and Pope [74] (denoted by filled circles). It is seen that under the first normalization, based on the length scale $L_c = u'^3/\epsilon$, the flux increases with $Re_\lambda$, while the variance decreases with $Re_\lambda$. On the other hand, under the second normalization, based on the integral length scale, $l$, the flux decreases, while the variance increases, with $Re_\lambda$. These trends seen in the present simulations are consistent with the trends seen in the previous DNS results [74]. Furthermore, the fluxes obtained from the present simulations compare very favorably with the fluxes obtained from the previous DNS. The scalar variances are under-predicted by the present DNS, and the under-prediction is more apparent under the second normalization. These discrepancies can be attributed to the differences in the forcing scheme employed in the present simulations and that employed by Overholt and Pope [74].
Figure 5.5. Time averaged PDFs of (a) \( u \), and (b) \( \phi \). Each variable normalized by its variance.

Time averaged probability density functions (PDFs) of the \( x \)–direction velocity component and the scalar field are shown in Figure 5.5. Each variable has been normalized by its respective standard deviation. Also shown in Figure 5.5 is the Gaussian curve, \( e^{-r^2} \). For all three values of \( Re_\lambda \), the PDFs of both \( u \) and \( \phi \) can largely be seen to be close to Gaussian. The tails of the PDFs ‘droop’, and are all contained inside the Gaussian curve. Turning to the PDFs of the scalar derivatives shown in Figure 5.6, it is seen that the PDFs of \( \partial \phi / \partial x \) and \( \partial \phi / \partial z \) are symmetric with respect to \( X = 0 \), and are almost identical to each other. As compared to these, the PDFs of \( \partial \phi / \partial y \) appear skewed in the \( X > 0 \) direction. This is because of the presence of the mean scalar gradient in the \( y \)–direction, \( \alpha_2 = 1.0 \). These observations are similar to those in Overholt and Pope [74], and other previous investigations of passive scalar turbulence with a mean scalar gradient, e.g. [11, 70, 120].

Finally, instantaneous snapshots of the scalar contours in the \( x = \pi \) plane have been extracted from the three simulation cases, and are shown in Figure 5.7. It is seen that the amount of small scale structure evident in the scalar contours increases with increasing \( Re_\lambda \). In these figures, regions marked red have relatively higher values of \( \phi \), while regions marked yellow or white have relatively lower values of \( \phi \). Regions of
Figure 5.6. Time averaged PDFs of the three components of the scalar gradient, $\partial \phi/\partial x_i$. (a) $Re_\lambda = 28$, (b) $Re_\lambda = 52$, and (c) $Re_\lambda = 84$. 
positive and negative values of $\phi$ can also be determined from the contour lines, with dashed lines indicating negative contour levels. It can be noted that the scalar field is marked by the presence of regions of positive scalar values adjacent to regions of negative scalar values. These are the so-called ramp-cliff structures, which have been observed in many previous studies. It is also seen that these ramp-cliff structures tend to align in the direction of the mean scalar gradient, i.e. in the $y$ direction, in the present simulations.

5.3.3 Decaying Passive Scalar Turbulence

The simulations described in the previous sub-section are sustained by artificial forcing imposed on the large scales of the velocity field. A different situation, in which forcing is applied initially to set up a desired flow, and then subsequently turned off, is described in this sub-section. Switching off the forcing, and the absence of any other mechanism of turbulence production, leads to a monotonic decay of turbulence. Decaying isotropic turbulence simulations have been carried out previously by many researchers, e.g. [19, 18].

The simulation described here is carried out on $N = 128^3$ collocation points, with viscosity $\nu = 1/210$, and the initial forcing parameter $\epsilon_f = 0.5$. A mean scalar
gradient $\alpha_2 = 1.0$ is maintained and the forcing is applied for the first 20 non-dimensional time units. At $t = 20$, the forcing is turned off, and the mean scalar gradient is set to $\alpha_2 = 0$. The mean scalar gradient in the other two directions is zero throughout. The molecular Schmidt number is again set equal to $Sc = 1$. The evolution of the instantaneous Taylor-scale Reynolds number with time is shown in Figure 5.8. It is seen that under the action of the imposed forcing, $Re_\lambda$ attains a stationary value of approximately 84 by about $t \approx 12$. Beyond $t = 20$, once the forcing is switched off, $Re_\lambda$ decays to approximately $Re_\lambda \approx 10$ by $t = 80$. It can also be seen that at $t = 60$, the flow attains a value of $Re_\lambda \approx 13$, which is very close to the final value at $t = 80$. Thus, most of the decay of turbulence has already occurred by $t = 60$. In the subsequent analysis, we focus on the decaying turbulence in the region between $t = 20$ and $t = 60$.

Figure 5.9a shows the evolution of $\delta/\eta$ with time, where $\delta$ denotes the grid size. The condition $k_{max} \eta \geq 1.0$ for all scales to be fully resolved, translates to $\delta/\eta \leq 2.1$, \begin{figure}[h] 
\centering
\includegraphics[width=0.5\textwidth]{fig5.8.png}
\caption{Time evolution of Taylor scale Reynolds number, $Re_\lambda$, in decaying passive scalar turbulence.}
\end{figure}
since δ = π/k_{max}. It is seen that this condition is always satisfied, indicating that the flow is fully resolved at all times. The evolution of the velocity derivative skewness,

\[ Su = -\frac{1}{3} \left[ \frac{\left\langle \left( \frac{\partial u_i}{\partial x_i} \right)^3 \right\rangle}{\left\langle \left( \frac{\partial u_i}{\partial x_i} \right)^2 \right\rangle^{3/2}} \right], \tag{5.20} \]

is shown in Figure 5.9. \( Su \) is a measure of the nonlinear cascade of energy from large scales to small scales [19], and thus, a measure of the extent of development of the flow [19], [17]. Typical values reported in the literature range from 0.44 to 0.52 [106, 23, 19, 17]. It is seen that for the entire time period considered, the present simulation yields values around 0.5, consistent with all these previous studies. The decay of turbulent kinetic energy is seen in Figure 5.10a, while Figure 5.10b shows the evolution of the exponent \( n \) in the expression \( TKE = TKE_0(t - 20)^{-n} \). The decay of TKE is known to be either inertia-dominated or viscous-dominated [86], with typical values of \( n \approx 1.3 \) and \( n = 2.5 \) respectively. Figure 5.10a shows that the rate of decay in the present simulations appears to be close to inertial for a short interval around \( t \approx 25 \). Figure 5.10b shows that the exponent continues to increase.
Figure 5.10. Results of decaying isotropic turbulence with a passive scalar. Time evolution of (a) turbulent kinetic energy and (b) exponent in the expression, \( TKE \sim (t - 20)^{-n} \).

Beyond this time, and tends to 2.5, as the flow approaches the viscous-dominated, so-called, ‘final period of decay’.

Visualizations of the passive scalar fields in decaying isotropic turbulence are seen in Figure 5.11. As expected, the small scale structure decreases as time progresses, and the turbulence is characterized by decreasing values of \( Re_\lambda \). The typical ramp-cliff structures are again observed in Figure 5.11. All these observations are similar to previous studies of decaying isotropic turbulence with a passive scalar field.

### 5.3.4 Decaying Active Scalar Turbulence

The final set of simulations reported in this section involves decaying homogeneous anisotropic turbulence, driven by the effects of buoyancy. The scalar field now affects the flow field through the body force term which acts as a source in the governing momentum equations. The simulations are set up to reproduce the results reported in Gerz and Yamazaki [37]. All simulations are carried out in a \( 4\pi^3 \) triply periodic
Figure 5.11. Instantaneous snapshots of the passive scalar contours in the plane $y = \pi$. Snapshots at (a) $Re_\lambda = 84.7$, (b) $Re_\lambda = 38.5$, (c) $Re_\lambda = 31.5$, and (d) $Re_\lambda = 26.2$. 
cubical domain, using \( N = 96^3 \) collocation points. A random initial scalar field, obeying the spectrum

\[
S(k) = \frac{16}{2\pi} \sqrt{\frac{2}{\pi}} \frac{k^4}{k_p^5} e^{-2k^2/k_p^2}
\]  

(5.21)

is generated, and is used to start the simulations, with all the velocity components initially set to zero. \( k_p \) is the wavenumber at which the spectrum peaks, and is set to be equal to \( 1/\sqrt{2\pi} \). The governing equations are non-dimensionalized using \( l_\phi^* \), \( 1/N^* \) and \( \phi^* \) as the length, time and scalar scales respectively. \( l_\phi^* \), \( \phi^* \) and \( N^* \) denote the length scale associated with the initial scalar spectrum, the initial scalar RMS value, and the Brunt-Vaisala frequency respectively, and are given by

\[
l_\phi^* = \frac{\pi}{2} \int_0^\infty \frac{1}{k} S(k) dk, \quad \phi^* = \sqrt{\langle \phi'\phi' \rangle_0}, \quad N^{*2} = g\beta \frac{d\Phi}{dz}.
\]

(5.22)

The parameters arising out of this non-dimensionalization are the integral-scale Reynolds number, the Schmidt number, and the Stratification number

\[
Re = \frac{N^*l_\phi^*}{\nu}, \quad Sc = \frac{\nu}{k_\phi^*}, \quad St = \frac{l_\phi^*}{\phi^*} \frac{d\Phi}{dz},
\]

(5.23)

where \( \Phi \) denotes the mean background scalar profile. Following Gerz and Yamazaki [37], we fix \( Sc = 1 \) and \( Re = 57.4 \), and consider three values of \( St \), equal to 1.0, 0.25 and 4.0. It should be noted that the effect of buoyancy increases with decreasing \( St \).

The results of decaying homogeneous anisotropic buoyancy-driven turbulence are displayed in Figures 5.12 and 5.13. Figure 5.12 shows the evolution of the volume averaged kinetic energy \( (KE = 1/2 \langle u'_i u'_i \rangle) \), potential energy \( (PE = 1/2St \langle \phi'\phi' \rangle) \), and total energy \( (TE = KE + PE) \) for the three cases. In each case, the results have been normalized by the initial total energy, \( TE_0 \). It is seen that \( KE \) is zero initially, while \( PE \) is non-zero. As the simulation begins from \( t = 0 \), \( PE \) reduces and \( KE \) increases, as the potential energy is converted to kinetic energy, due to the action of the buoyancy term in the momemntum equations. The situation is reversed around \( t/2\pi \sim 0.2 - 0.3 \), and kinetic energy starts being converted back into potential energy. These oscillations of the \( KE \) and \( PE \) curves continue till both are eventually damped.
out by the action of viscosity at large times. It should be noted that while $KE$ and $PE$ oscillate, the total energy decays monotonically with time. Thus, contrary to non-buoyant decaying turbulence, in which the kinetic energy decays monotonically, the kinetic energy in buoyant decaying turbulence oscillates, while the total energy decays monotonically. This observation is in accordance with previous investigations of buoyant homogeneous decaying turbulence \cite{37,113}.

The DNS results of Gerz and Yamazaki \cite{37} are depicted by the open symbols in Figure 5.12. It is seen that the present DNS results compare very well with the previous DNS results for $St = 1.0$ and $St = 4.0$. Both, the frequency of oscillations of $KE$ and $PE$, as well as their magnitudes, and the decay of $TE$ are well captured. For the $St = 0.25$ case, the frequency of oscillations of $KE$ and $PE$ obtained from the present simulations compares well with that obtained from the previous DNS results. While some discrepancies in the magnitudes of $KE$ and $PE$, especially at early times, are observed between the present DNS results and the results of Gerz and Yamazaki \cite{37}, there is a good overall agreement between these two data sets. Volume averaged variances of the scalar, and the $x$–direction and $z$–direction velocities for the three cases are displayed in Figure 5.13. The oscillations seen in kinetic and potential energies in Figure 5.12 are apparent in the individual variances as well. The anisotropy of the flow field is also seen in Figure 5.13, since the $z$–direction velocity differs significantly from the $x$–direction velocity. The $v$ velocity is very close to $u$ velocity, and has not been shown. This indicates the anisotropy of the flow field in buoyancy driven homogeneous turbulence. It is also seen that the anisotropy increases with decreasing $St$, as expected. Finally, similar to the kinetic, potential and total energies displayed in Figure 5.12, the variances of the individual velocity components and the scalar field too, are in good agreement with the DNS results of Gerz and Yamazaki \cite{37}. 
Figure 5.12. Time evolution of kinetic, potential and total energy in decaying turbulence with active scalar. (a) $St = 1.0$, (b) $St = 0.25$, and (c) $St = 4.0$. Results compared to the DNS results of [37].
Figure 5.13. Time evolution of variances of active scalar, $\phi'$, horizontal velocity, $u'$, and vertical velocity, $w'$ in decaying turbulence with active scalar. (a) $St = 1.0$, (b) $St = 0.25$, and (c) $St = 4.0$. Results compared to the DNS results of [37].
5.4  *A priori* tests of LES Models

The buoyant and non-buoyant simulations presented in the previous section have been very well validated, both qualitatively as well as quantitatively, with other existing DNS results. Thus, accurate flow and scalar field data at a variety of flow conditions have been generated. The purpose of this section is to employ these data sets to evaluate existing LES models, and build improved models for the SGS scalar flux. A brief review of the term to be modeled, existing LES models, and the general procedure for processing the available DNS data for the purpose of evaluation and development of LES models is given in sub-section 5.4.1. The SGS scalar flux is a vector with three components, and this vector can be separated into its orientation and its magnitude. Using the DNS data, orientation of the SGS scalar flux is considered in sub-section 5.4.2, while the magnitude is examined in sub-section 5.4.3. The focus is on evaluating components of the existing models, which contribute to the direction and magnitude respectively. The two parts are put together in sub-section 5.4.4, and comments highlighting the positive and negative aspects of the existing models are presented. Finally, drawing from the observations extracted from the DNS data, new models for the SGS scalar flux are proposed in sub-section 5.4.4.

5.4.1 Overview of Modeling Procedure

**LES SGS Models Evaluated**

The purpose of LES modeling is to write analytical expressions for the unclosed terms, $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ and $\tau_{i\phi} = \overline{u_i \phi} - \bar{u}_i \bar{\phi}$, occurring in the LES filtered Navier-Stokes equations. Here, we are concerned with modeling only the latter of these terms, namely, the SGS scalar flux, $\tau_{i\phi}$. An extensive review of many of the existing models for the SGS scalar flux has been given earlier, in Chapter 2, A short summary, mentioning all the models, has also been included in Section 5.1. In this section, we
revisit six of those models. The six models considered here may be categorized into three families.

Firstly, three eddy-viscosity type models are considered, namely Smagorinsky [103], Vreman [114] and Sigma [72] models. Only constant coefficient versions of these models are considered, with $C_S$, $C_V$ and $C_\sigma$ set to be equal to their respective, typical recommended values. Also, we fix $Pr_{SGS} = 1/3$ for all three eddy-viscosity type models. The fourth model considered is the Dynamic Structure model of Chumakov [19], given by

$$
\tau_{i\phi} = \frac{\theta}{\Theta} L_{i\phi} - \frac{\bar{\phi}\tilde{\phi} - \bar{\tilde{\phi}}\bar{\phi}}{\bar{\phi}\tilde{\phi} - \bar{\tilde{\phi}}\bar{\phi}} \left( \tilde{u}_i \tilde{\phi} - \bar{u}_i \phi \right). \tag{5.24}
$$

This model does not include any tunable coefficients. It should be noted that the term $\theta = \bar{\phi}\tilde{\phi} - \bar{\tilde{\phi}}\bar{\phi}$ cannot be determined purely from the resolved field in an actual LES computation, and DSM is usually accompanied by a transport equation for $\theta$ [20, 21, 19]. However, in the present a priori study, the value $\theta$ can be calculated directly from the DNS data. The computation of $\Theta$ presents no trouble, either in a priori testing from DNS data, or in an a posteriori LES computation.

The last two models examined belong to the so-called Gradient [73, 67, 66] family of models. These models also appear in the literature under other names, such as non-linear model [63] and Clark model [19]. The expression for the SGS scalar flux is

$$
\tau_{i\phi} = C_G \Delta^2 \sqrt{k_{SGS}} \sqrt{\theta} \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right), \tag{5.25}
$$

where $k_{SGS} = \frac{1}{2} \tau_{ii}$ is half the trace of the SGS stress tensor, $\theta$ is as defined above for DSM, and $G_{i\phi} = \Delta^2 \frac{\partial u_i}{\partial x_j} \frac{\partial \phi}{\partial x_j}$. Similar to the Dynamic Structure Model, the Gradient Model, denoted GM in Table 5.1, contains terms ($k_{SGS}$ and $\theta$) which cannot be determined from the resolved velocity and scalar fields in an actual LES simulation. The Modulated Gradient Model (MGM) introduced by Lu and Porté-Agel [66] approximates $k_{SGS}$ and $\theta$ in terms of $G_{ij} = \Delta^2 \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}$ and $G_{i\phi}$ respectively. A mechanism for backscatter control, via Heaviside functions $H(P)$ and $H(\theta)$ which switch off the
model when either velocity \((P = -\tau_{ij} \bar{S}_{ij})\) or scalar SGS production \((P_\theta = -\tau_{i\phi} \frac{\partial \bar{\phi}}{\partial x_i})\) is negative, is also incorporated in MGM. The final expression for MGM is
\[
\tau_{i\phi} = C_M \bar{\lambda}^2 \left( - \frac{G_{i\phi}}{|G_{k\phi}| \frac{\partial \bar{\phi}}{\partial x_i}} \right) \left( - \frac{G_{ij}}{|G_{kk}|} \bar{S}_{ij} \right) \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right) H(P_\theta) H(P). \tag{5.26}
\]

The various scaling factors have been incorporated into single coefficients, \(C_G\) and \(C_M\), in front of models GM and MGM respectively. Both these coefficients are set equal to \(2/3\) in the present \textit{a priori} studies. The precise value of the coefficients does not affect the conclusions drawn from the \textit{a priori} studies, as is explained in subsection 5.4.3. Table 5.1 summarizes the six models described above. The components accounting for the orientation in 3D space, and the magnitude of the SGS scalar flux have been written out separately in Table 5.1.

**DNS Data Sets**

The DNS data obtained from the simulations described previously in Section 5.3 are divided into 19 data sets. A description of the data sets is given in Table 5.2. Data sets 1-3 are from stationary turbulence simulations with a transported passive scalar, at \(Re_\lambda = 25, 49, 84\) respectively. Each of these data sets is composed of ten snapshots after the flow has reached a stationary state. Data sets 4-7 have been extracted from the decaying turbulence simulation with a passive scalar, at times corresponding to \(Re_\lambda = 26, 31, 38, 84\). It should be noted that the data sets have been arranged in reverse chronological order, since the actual simulation progresses from higher to lower values of \(Re_\lambda\). The last 12 data sets are composed of buoyant decaying turbulence simulations with an active scalar. Data at non-dimensional times \(t/2\pi = 0.16, 0.32, 0.56\) and 0.88 form the data sets 8-11 \((St = 1.0)\), 12-15 \((St = 0.25)\) and 16-19 \((St = 4.0)\).
Table 5.1. Summary of LES SGS models evaluated in homogeneous turbulence.

<table>
<thead>
<tr>
<th>Model</th>
<th>Orientation</th>
<th>Magnitude</th>
<th>Model Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smagorinsky (Smag)</td>
<td></td>
<td>( \frac{(C_S\Delta)^2}{Pr_{SGS}}</td>
<td>S</td>
</tr>
<tr>
<td>Vreman (Vrem)</td>
<td></td>
<td>( \frac{C_V}{Pr_{SGS}}\Pi^g</td>
<td>\partial \bar{\phi}/\partial x_i</td>
</tr>
<tr>
<td>Sigma (Sigm)</td>
<td></td>
<td>( \frac{(C_\sigma\Delta)^2}{Pr_{SGS}}D_\sigma</td>
<td>\partial \bar{\phi}/\partial x_i</td>
</tr>
<tr>
<td>Dynamic Structure (DSM)</td>
<td>( \frac{L_{i\phi}}{L_{k\phi}} )</td>
<td>( \frac{\theta}{\Theta}</td>
<td>L_{i\phi}</td>
</tr>
<tr>
<td>Gradient Model (GM)</td>
<td>( \frac{G_{i\phi}}{G_{k\phi}} )</td>
<td>( C_G \Delta^2 \sqrt{k_{SGS}} \sqrt{\theta} )</td>
<td>( C_G = 2/3 )</td>
</tr>
<tr>
<td>Modulated Gradient Model (MGM)</td>
<td>( \frac{G_{i\phi}}{G_{k\phi}} )</td>
<td>( C_M \Delta^2 \left(-\frac{G_{i\phi}}{G_{k\phi}}\frac{\partial \bar{\phi}}{\partial x_i}\right)\left(-\frac{G_{ij}}{G_{kk}}\bar{S}<em>{ij}\right)H(P</em>\theta)H(P) )</td>
<td>( C_M = 2/3 )</td>
</tr>
</tbody>
</table>
Table 5.2. Summary of the analyzed DNS data sets.

<table>
<thead>
<tr>
<th>Data Set No.</th>
<th>Description</th>
<th>Parameter Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-3</td>
<td>Forced Passive Scalar</td>
<td>$Re_\lambda = 25, 49, 84.$</td>
</tr>
<tr>
<td>4-7</td>
<td>Decaying Passive Scalar</td>
<td>$Re_\lambda = 26, 31, 38, 84.$</td>
</tr>
<tr>
<td>8-11</td>
<td>Decaying Active Scalar, $St = 1.0$</td>
<td>$t/2\pi = 0.16, 0.32, 0.56, 0.88.$</td>
</tr>
<tr>
<td>12-15</td>
<td>Decaying Active Scalar, $St = 0.25$</td>
<td>$t/2\pi = 0.16, 0.32, 0.56, 0.88.$</td>
</tr>
<tr>
<td>16-19</td>
<td>Decaying Active Scalar, $St = 4.0$</td>
<td>$t/2\pi = 0.16, 0.32, 0.56, 0.88.$</td>
</tr>
</tbody>
</table>
Grid and Test Filtering

A priori testing of LES models requires determination of various quantities based on filtering of the DNS data. Firstly, determination of the SGS scalar flux from its definition requires filtering of the products $u_i \phi$, the individual velocity fields $u_i$ and the scalar field $\phi$. Secondly, LES models themselves are nothing but expressions in terms of the filtered fields $\overline{u_i}$ and $\overline{\phi}$. Finally, LES model expressions might also involve quantities filtered at the test-filter level. Thus, the choice of the shape and size of filters is important in a priori testing of LES models. Furthermore, it is important that the filtering be performed in a consistent manner [63]. The pitfalls of drawing wrong conclusions based on a priori evaluation of LES models using inconsistent filtering have been very well pointed out by Liu et al. [63].

The a priori studies presented here are based on a consistent application of the ‘box’ filter. This shape for the filter is chosen since it is used most commonly in actual LES codes. Based on previous studies [63, 67, 66], changing the shape of the filter to any other filter which allows for enough localization in physical space (i.e. a filter such as Gaussian or linear; but not spectral cut-off), is not expected to change the conclusions drawn from these a priori studies. The grid-filter is primarily taken to be four times as large as the DNS grid size, $\Delta/\delta = 4$. The effect on the results of varying $\Delta$ from $2\delta$ to $16\delta$ is also examined. The test-filter is always taken to be twice as large as the grid-filter, i.e. $\hat{\Delta}/\Delta = 2$.

5.4.2 Orientation of SGS Scalar Flux

At any time instant, the term to be modeled, $\tau_{i\phi}$, is a vector field with three components. The purpose of this section is to investigate the alignment trends between $\tau_{i\phi}$, and different vectors obtained from the resolved velocity and scalar fields. In order to illustrate the idea, a portion of the $\tau_{i\phi}$ vector field, from an arbitrary slice in $X - Z$ plane extracted from one of the simulations described above, is shown by black arrows with hollow arrow heads, in Figure 5.14. The blue arrows with filled
arrow heads denote another vector field, composed of the resolved scalar gradient, \( \partial \bar{\phi} / \partial x_i \). It can be seen that the two vector fields are aligned with each other at some locations in the domain, but do not align with each other at others. For example, \( \tau_{i\phi} \) and \( \partial \bar{\phi} / \partial x_i \) point in exactly opposite directions towards the upper-right corner of Figure 5.14. On the other hand, the two vectors appear to be orthogonal to each other towards the center-left, and seem to be almost aligned with each other towards the center-right of Figure 5.14. A more rigorous method of quantifying the alignment trends between these two vector fields (or any other pair of vector fields) is to determine the PDF of the cosine of the angle between the two vectors. The cosine of the angle between two vectors \( V_i \) and \( W_i \) is given by simply

\[
\cos(\alpha) = \frac{V_i W_i}{|V_i||W_i|},
\]

(5.27)

where the magnitudes in the denominator equal the \( L^2 \)-norm of the vectors, i.e. \( |V_i| = \sqrt{V_i^2} \).

Alignment trends between \( \tau_{i\phi} \) and three other vectors are studied in Figures 5.15, 5.16 and 5.17. The three vectors examined are \( \partial \bar{\phi} / \partial x_i \), \( L_{i\phi} = \overline{u_i \phi} - \overline{u_i \bar{\phi}} \) and \( G_{i\phi} = \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{\phi}}{\partial x_j} \). These vectors have been chosen since all eddy-viscosity type models get their directions from \( \partial \bar{\phi} / \partial x_i \), while the Dynamic Structure and the Gradient Model derive their directions from \( L_{i\phi} \) and \( G_{i\phi} \) respectively. Figure 5.15 shows alignment trends extracted from the data generated by passive scalar turbulence simulations (Data Sets 1-7), while Figure 5.16 is extracted from homogeneous buoyant turbulence simulations (Data Sets 8-19).

Concentrating on Figure 5.15a, it is observed that, for all three values of \( Re_\lambda \), the PDFs marked EV peak close to \( \cos \alpha = 0 \). This indicates that most of the SGS scalar flux vectors tend to be orthogonal to the resolved scalar gradient vector. Further, the peaks are not very sharp, implying that there is a large spread in the angles between \( \tau_{i\phi} \) and \( \partial \bar{\phi} / \partial x_i \). Compared to these, the PDFs of the angles between \( \tau_{i\phi} \) and \( L_{i\phi} \), marked DSM, show much sharper peaks near \( \cos \alpha = 1 \). It can thus be concluded that \( \tau_{i\phi} \) and \( L_{i\phi} \) tend to be aligned in the same direction at a majority of locations in the flow field. The PDFs marked GM depict even stronger and sharper peaks at the
far right of Figure 5.15, near $\cos \alpha = 1$, indicating an even better alignment between $\tau_{i\phi}$ and $G_{i\phi}$. Similar conclusions can be drawn from the alignment trends extracted from passive scalar fields in decaying turbulence, shown in Figure 5.15b. At different time instants, when the flow is characterized by different values of $Re_\lambda$, the peaks of the alignment PDFs suggest that the SGS scalar flux continues to show a wide range of angles with the resolved scalar gradient, while being aligned with $L_{i\phi}$ and $G_{i\phi}$. Figures 5.16a-c show that the alignment between $\tau_{i\phi}$ and $\partial \bar{\phi}/\partial x_i$ in decaying active scalar turbulence is different from their alignment in passive scalar turbulence. The PDFs no longer peak near $\cos \alpha = 0$. Instead, the peaks tend to be dependent on the level of stratification ($St$), and also shift as the turbulence decays with time. However, the alignment of $\tau_{i\phi}$ with $L_{i\phi}$ as well as $G_{i\phi}$, continues to be good, with sharp peaks visible near $\cos \alpha = 1$ in the PDFs at all time instants, and for all values of $St$.

Figures 5.15 and 5.16 have been generated with the grid-filter size fixed at $\bar{\Delta}/\delta = 4$. The effect of changing the grid-filter size is seen in Figure 5.17, which shows alignment trends extracted from Data Set 3. It is seen that the PDFs corresponding to eddy-viscosity models remain diffuse for different grid-filter sizes. For $\bar{\Delta}/\delta = 2$, DSM and GM PDFs retain their sharp peaks near $\cos \alpha = 1$, with the GM PDF being slightly sharper than the DSM PDF. Increasing the grid-filter size to $\bar{\Delta}/\delta = 16$ reduces the sharpness of the peaks near $\cos \alpha = 1$. However, the fact that the peaks near $\cos \alpha = 1$ are maintained, indicates that $L_{i\phi}$ and $G_{i\phi}$ continue to be better indicators of the orientation of $\tau_{i\phi}$, as compared to $\partial \bar{\phi}/\partial x_i$.

The alignment trends presented here are qualitatively similar to those extracted from passive scalar turbulence DNS data by Chumakov [19]. Sharp peaks for the alignment between $\tau_{i\phi}$ and $L_{i\phi}$, and between $\tau_{i\phi}$ and $G_{i\phi}$, near $\cos \alpha = 1$ were observed in that study as well. Also, the PDFs of the angles between $\tau_{i\phi}$ and $\partial \bar{\phi}/\partial x_i$ were found to be diffuse, similar to the present results. Based on the present results, overall, the SGS scalar flux can be concluded to be in very good alignment with the Leonard vector, and the Gradient Model vector, than with the resolved scalar gradient vector.
Figure 5.14. Vector fields in an arbitrary portion of a 2D $X - Z$ slice of the cubical computational domain. Black arrows with hollow arrow heads denote the actual SGS scalar flux, $\tau_{i\phi}$. Blue arrows with filled arrow heads denote resolved scalar gradient, $\partial \bar{\phi} / \partial x_i$.

Consequently, a SGS model for $\tau_{i\phi}$, which derives its orientation based on either $L_{i\phi}$ or $G_{i\phi}$ is expected to be better than a model oriented based on $\partial \bar{\phi} / \partial x_i$. Finally, among the vectors $L_{i\phi}$ and $G_{i\phi}$, a model based on the latter would be expected to be slightly better than one based on the former.

5.4.3 Magnitude of SGS Scalar Flux

Magnitudes of the actual and modeled SGS scalar fluxes are examined in this sub-section. The precise expressions for the six model SGS scalar fluxes have been given in Table 5.1. The approach used is similar to that followed by Lu et al. [67] for evaluating models for the SGS stress tensor. The performance of different SGS models is analyzed with respect to two measures, namely correlation coefficients and regression coefficients. Joint PDFs of the actual and modeled SGS scalar fluxes are also examined to get a qualitative feel for the different models.
Figure 5.15. PDF of the cosine of the angle between the SGS scalar flux, $\tau_{i\phi}$, and the resolved scalar gradient, $\partial \bar{\phi} / \partial x_i$ (denoted by EV), the Leonard term, $L_{i\phi}$ (denoted by DSM), and the Gradient Model term, $G_{i\phi}$ (denoted by GM); using data from homogeneous (a) stationary turbulence (Data Sets 1-3), and (b) decaying turbulence (Data Sets 4-7) with a passive scalar. Grid filter size is $\Delta / \delta = 4$.

Figure 5.16. PDF of the cosine of the angle between the SGS scalar flux, $\tau_{i\phi}$, and the resolved scalar gradient, $\partial \bar{\phi} / \partial x_i$ (denoted by EV), the Leonard term, $L_{i\phi}$ (denoted by DSM), and the Gradient Model term, $G_{i\phi}$ (denoted by GM); using data from decaying homogeneous turbulence with active scalar with (a) $St = 1.0$ (Data Sets 8-11), (b) $St = 0.25$ (Data Sets 12-15), (c) $St = 4.0$ (Data Sets 16-19). Grid filter size is $\Delta / \delta = 4$. 
Figure 5.17. Effect of grid-filter sizes on the PDF of the cosine of the angle between the SGS scalar flux, $\tau_{i\phi}$, and the resolved scalar gradient, $\partial \bar{\phi} / \partial x_i$ (denoted by EV), the Leonard term, $L_{i\phi}$ (denoted by DSM), and the Gradient Model term, $G_{i\phi}$ (denoted by GM); using data from stationary homogeneous turbulence with passive scalar at $Re_\lambda = 84$ (Data Set 3).
Correlation Coefficients

The models are analyzed first by examining the correlation coefficients between the predicted magnitudes and the magnitude of $\tau_{\phi}$. The correlation coefficient between two variables $a$ and $b$ is given by

$$\rho(a, b) = \frac{\langle ab \rangle - \langle a \rangle \langle b \rangle}{\sqrt{(\langle a^2 \rangle - \langle a \rangle^2)(\langle b^2 \rangle - \langle b \rangle^2)}}, \quad (5.28)$$

where the angled brackets $\langle \rangle$ denote an ensemble average over different grid points. The correlation coefficient is bounded between $-1 \leq \rho \leq 1$, with $\rho = 0$ denoting no correlation, and $\rho = 1$ and $\rho = -1$ denoting perfect positive and perfect negative correlations respectively. The aim is to look for quantities in terms of resolved velocity and scalar fields, which correlate well with the magnitude of the actual SGS scalar flux. An ideal model would yield $\rho = 1$. In the absence of an ideal model, a model with a larger value of $\rho$ can be deemed to be better than a model that yields a lower value of $\rho$.

Before presenting correlation coefficients for the SGS scalar flux, correlation coefficients for three different components of the SGS stress tensor, $\tau_{ij}$ are presented. Correlation of $\tau_{11}$, $\tau_{13}$ and $\tau_{33}$ with the corresponding components predicted by four different models are shown in Figure 5.18. Data from all 19 data sets has been extracted, with a fixed grid-filter size of $\bar{\Delta}/\delta = 4$. Lines with filled circles denote correlations with the Gradient Model, while lines with hollow symbols denote correlations with the three eddy-viscosity type models. For all components and for all data sets, GM yields high values of correlation coefficients, consistently close to unity. All the eddy-viscosity models yield correlation coefficients centered around approximately 0.25. The effect of varying the grid-filter size is demonstrated in Figure 5.19, which shows the correlation coefficients extracted from a stationary passive scalar data set (Data Set 3) and from a decaying active scalar data set (Data Set 14). It is seen that although the correlation coefficients obtained from the Gradient Model decrease with increasing grid-filter size, they are always considerably higher than correlation coefficients obtained from the eddy-viscosity type models. These observations, regarding
low correlations with eddy-viscosity type models, and large correlations with Gradient
Model, are consistent with a number of previous a priori studies [63, 67]. Reproducing
these previously established results serves to validate our current methodology of
filtering and processing the DNS data.

Correlation coefficients between $|\tau_{i\phi}|$ and the six model SGS scalar flux magnitudes
tabulated in Table 5.1 are shown in Figure 5.20. As in Figure 5.18, results extracted
from the passive scalar data sets are presented in Figure 5.20a, while results extracted
from active scalar data sets are presented in Figure 5.20b. Firstly, DSM and GM
models yield very high correlation coefficients, almost always in excess of 0.9. Among
these two models, GM can be said to be slightly better, since it yields larger correlation
coefficients for all but three data sets. The modulated variant of the Gradient Model
yields correlation coefficients which are significantly lower than those obtained from
the Gradient Model. For passive scalar data sets, the correlation coefficients obtained
from MGM hover around approximately 0.45, while for active scalar data sets too,
the correlation coefficients are low, averaging approximately 0.3. The three eddy-
viscosity type models yield correlation coefficients which are larger than MGM, but
smaller than DSM and GM. Among these three models, Smagorinsky model gives high
correlations - averaging approximately 0.85 in passive scalar cases and approximately
0.8 in active scalar cases. Vreman model yields average correlation coefficients of 0.8
and 0.75, while Sigma model yields correlation coefficients averaging 0.65 and 0.55,
in passive and active scalar data sets respectively.

Figure 5.21 shows correlation coefficients extracted from 2 out of the 19 data sets,
but with differing grid-filter sizes. It is seen that the correlation coefficients consist-
tently decrease as the grid-filter size increases from $\bar{\Delta}/\delta = 2$ to $\bar{\Delta}/\delta = 16$ in the
case of Data Set 3, and to $\bar{\Delta}/\delta = 8$ in the case of Data Set 14. In addition, it is
seen that all the conclusions drawn from Figure 5.20 remain valid across all grid-filter
sizes. GM yields the largest correlations, followed closely by DSM. MGM yields much
lower correlation coefficients, while the three eddy-viscosity type models yield inter-
Figure 5.18. Correlation coefficients $\rho(\tau_{ij}, \tau_{ij}^{\text{mod}})$, where the subscripts $ij$ denote either 11-, 13- or 33- components, and the superscript $\text{mod}$ denotes any one among GM, Smagorinsky, Vreman and Sigma models. All 19 data sets, with fixed grid-filter size $\bar{\Delta}/\delta = 4$.

Figure 5.19. Correlation coefficients $\rho(\tau_{ij}, \tau_{ij}^{\text{mod}})$, where the subscripts $ij$ denote either 11-, 13- or 33- components, and the superscript $\text{mod}$ denotes any one among GM, Smagorinsky, Vreman and Sigma models. Varying grid-filter size $\bar{\Delta}/\delta$, and correlations extracted from (a) stationary passive scalar data set 3, and (b) decaying active scalar data set 14.

mediate correlation coefficient values. Among the three eddy-viscosity type models, Smagorinsky model yields the largest, while Sigma yields the least correlations.
Figure 5.20. Correlation coefficients $\rho(|\tau_{i\phi}|, |\tau_{i\phi}^{mod}|)$, where the superscript $mod$ denotes any one among the six models tabulated in Table 5.1. All 19 data sets, with fixed grid-filter size $\bar{\Delta}/\delta = 4$.

Figure 5.21. Correlation coefficients $\rho(|\tau_{i\phi}|, |\tau_{i\phi}^{mod}|)$, where the superscript $mod$ denotes any one among the six models tabulated in Table 5.1. Varying grid-filter size $\bar{\Delta}/\delta$, and correlations extracted from (a) stationary passive scalar data set 3, and (b) decaying active scalar data set 14.
Regression Coefficients

The regression coefficient between two variables $a$ and $b$ is defined by

$$\gamma(a, b) = \frac{\langle ab \rangle - \langle a \rangle \langle b \rangle}{\langle a^2 \rangle - \langle a \rangle^2}, \quad (5.29)$$

where, again, the angled brackets $\langle .. \rangle$ denote an ensemble average over different grid points. Unlike the correlation coefficient, the regression coefficient cannot be negative, but can take any positive real value, viz. $0 \leq \gamma < \infty$. The regression coefficient is a measure of the relative magnitudes of the variables $a$ and $b$. A value of $\gamma(a, b) = 1$ implies the two variables are of equal magnitude, while $\gamma(a, b) > 1$ ($< 1$) implies $a < b$ ($a > b$) in a least-squares sense. Furthermore, unlike the correlation coefficient, scaling either of the variables with a constant scaling factor results in a change in the value of $\gamma(a, b)$. This is an important property, which will be useful in evaluating the different SGS models, as well as in determining the optimal coefficients for the new models to be proposed in Section 5.4.4.

In the present analysis, one of the variables is fixed to be the magnitude of the actual SGS scalar flux, $|\tau_{i\phi}|$, while magnitudes of different model vectors form the second variable. From the 19 data sets tabulated in Table 5.2, a total of 61 data sub-sets are formed, by taking different values of the grid-filter sizes. The precise combinations of data sets and grid-filter sizes chosen are as follows: two (corresponding to $\Delta/\delta = 2, 4$) from Data Set 1, three ($\Delta/\delta = 2, 4, 8$) from each of Data Sets 2 and 8 through 19; and four ($\Delta/\delta = 2, 4, 8, 16$) from each of Data Sets 3 through 7. Regression coefficients are determined based on each of these 61 data sub-sets, yielding 61 data points of $\gamma$, corresponding to each model. As an example, Figure 5.22 shows the regression coefficients obtained from these 61 data sub-sets, corresponding to models GM and MGM. For each of these models, Figure 5.22 also shows the mean ($\langle \gamma \rangle_{dp}$) and standard deviation ($\sigma_{dp}(\gamma)$), computed over these 61 data points. It is seen that GM yields $\langle \gamma \rangle_{dp} = 1.13$ and $\sigma_{dp}(\gamma) = 0.07$, while MGM yields $\langle \gamma \rangle_{dp} = 0.51$ and $\sigma_{dp}(\gamma) = 0.25$. In order to avoid clutter, other models are not depicted on Fig-
Figure 5.22. Regression coefficients $\gamma(|\tau_{i\phi}|, |\tau_{i\phi}^{mod}|)$, where the superscript $mod$ denotes either GM or MGM, extracted from 61 data sub-sets. Mean, $\langle \gamma \rangle_{dp}$, and standard deviation, $\sigma_{dp}(\gamma)$, over 61 data points for each model are also shown as $\langle \gamma \rangle_{dp} \pm \sigma_{dp}(\gamma)$.

Figure 5.22. The means and standard deviations obtained from these 61 data points, corresponding to all the models are instead tabulated in Table 5.3.

An ideal model would yield $\gamma$ exactly equal to 1 for all data sets and grid-filter sizes. That is, an ideal model would be one with $\langle \gamma \rangle_{dp} = 1$ and $\sigma_{dp}(\gamma) = 0$. However, since $\gamma$ can be changed by scaling the model vector (which can be easily achieved by changing the coefficient in front of a model), it is possible to achieve $\langle \gamma \rangle_{dp} = 1$ for every model. This indicates that the mean $\langle \gamma \rangle_{dp}$ is not an appropriate measure for evaluation of different SGS models. A more appropriate statistic would be the normalized standard deviation, $\sigma_{dp}(\gamma) / \langle \gamma \rangle_{dp}$. For a model with a small value of normalized standard deviation, a single model coefficient can be expected to be sufficient, to ensure that the actual and modeled SGS scalar fluxes are of similar magnitudes, under a wide variety of flow conditions. On the other hand, a model with a large value of normalized standard deviation may require different values of the model coefficient,
Table 5.3. Statistics of the regression coefficients of $\tau_{i\phi}$, based on 61 data sub-sets and different SGS models.

<table>
<thead>
<tr>
<th>SGS Model</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Normalized Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\langle \gamma \rangle_{dp}$</td>
<td>$\sigma_{dp}(\gamma)$</td>
<td>$\sigma_{dp}(\gamma) / \langle \gamma \rangle_{dp}$</td>
</tr>
<tr>
<td>DSM</td>
<td>0.99</td>
<td>0.20</td>
<td>0.20</td>
</tr>
<tr>
<td>GM</td>
<td>1.13</td>
<td>0.07</td>
<td>0.06</td>
</tr>
<tr>
<td>MGM</td>
<td>0.51</td>
<td>0.25</td>
<td>0.49</td>
</tr>
<tr>
<td>Smag</td>
<td>1.03</td>
<td>0.25</td>
<td>0.24</td>
</tr>
<tr>
<td>Vrem</td>
<td>0.88</td>
<td>0.22</td>
<td>0.24</td>
</tr>
<tr>
<td>Sigm</td>
<td>0.86</td>
<td>0.24</td>
<td>0.28</td>
</tr>
</tbody>
</table>
under different flow conditions, in order to ensure that the modeled and SGS scalar fluxes are of similar magnitudes. In other words, a constant coefficient version of a model with smaller normalized standard deviation can be expected to be more accurate than a constant coefficient version of a model with a larger normalized standard deviation. In this sense, a model with a smaller normalized standard deviation can be deemed to be better than a model with a larger normalized standard deviation.

Table 5.3 reveals that the Gradient Model has the least normalized standard deviation, followed by the Dynamic Structure Model. MGM has the largest normalized standard deviation, while the three eddy-viscosity type models yield intermediate values. Again, Smagorinsky model has the lowest normalized standard deviation among these three, followed by Vreman and Sigma models.

Joint PDFs

A qualitative picture of the performance of different models can be gained by examining joint PDFs of the actual and modeled SGS scalar fluxes. Six joint PDFs, corresponding to the six models have been extracted from Data Set 3, and are shown in Figure 5.23. The grid-filter size is fixed to be $\bar{\Delta}/\delta = 4$. In each figure, the actual scalar flux appears on the $y$ axis, while the respective model scalar flux appears on the $x$ axis. The joint PDFs have been evaluated by dividing each variable into 100 equally spaced bins. For each bin of $\tau_{i\phi}$, and for each SGS model, the value of $\tau_{i\phi}^{mod}$ at which the peak of the joint PDF lies, is determined. These PDF peaks have also been marked in each sub-figure, by the dashed blue lines. Each PDF has been normalized by its maximum value. Two features can be discerned from each joint PDF. Firstly, the slope of the line joining the PDF peaks is related to the corresponding regression coefficient. Secondly, the ‘spread’ or the ‘width’ of the PDF around the line joining the peaks is related to the corresponding correlation coefficient.

The joint PDFs obtained from GM, DSM, Smagorinsky and Vreman models, have been shown in Figures 5.23a-d with exactly equal extents in the $x$ and $y$ directions.
Visually comparing these four figures, it is apparent that the Gradient Model yields the narrowest joint PDF. This is consistent with the fact that GM yields the maximum correlation coefficient among all models. Further, it can be seen that the joint PDFs given by the other three models too, are reasonably narrow, reflecting the relatively high correlation coefficients. For each bin of $\tau_{i\phi}$, the joint PDF given by each of these four models has only a single peak, marked by the dashed blue line. This is in contrast to the behaviour of MGM and Sigma models, which show additional peaks towards the far left of Figures 5.23e-f respectively. It should be noted that these peaks of PDFs occur at very small values (smaller than machine precision) of model scalar fluxes. Further, it should be recalled that the backscatter control mechanism incorporated in the Modulated Gradient model sets $\tau_{i\phi}^{MGM}$ equal to zero whenever the local SGS production turns negative. Similarly, it may be recalled, that the Sigma kernel, $D_\sigma$ is very sensitive to the flow field, and is designed to switch off under a number of local flow conditions [72]. In our computation, $\tau_{i\phi}^{mod}$ is actually set to be equal to a number less than machine precision, and these data points show up as second peaks in Figures 5.23e-f. These zeroed out values also reduce the correlation coefficients corresponding to these models, and render them less desirable than the other four models, in the a priori sense.

5.4.4 SGS Scalar Flux Models

The observations on alignment trends and correlations of magnitudes presented in the previous sub-sections can be utilized to comment on some existing models, and propose new models for the SGS scalar flux. Comments on the three eddy-viscosity models, viz. Smagorinsky, Vreman and Sigma, are presented first, followed by comments on the Dynamic Structure model. Finally, based on the above observations, new models are proposed.

Eddy-viscosity type models assume alignment of the SGS scalar flux, $\tau_{i\phi}$, with the negative of the resolved scalar gradient, $-\partial \tilde{\phi}/\partial x_i$. The results of sub-section 5.4.2
Figure 5.23. Joint PDF contours of $\log|\tau_{i\phi}|$ and different models: (a) $\log|\tau_{i\phi}^{GM}|$, (b) $\log|\tau_{i\phi}^{DSM}|$, (c) $\log|\tau_{i\phi}^{SMag}|$, (d) $\log|\tau_{i\phi}^{Vrem}|$, (e) $\log|\tau_{i\phi}^{MGM}|$, and (f) $\log|\tau_{i\phi}^{Sigm}|$. Joint PDFs evaluated by dividing each variable into 100 bins, from Data Set 3, with $\bar{\Delta}/\delta = 4$. Peaks of PDFs are denoted by dashed blue lines.
show the alignment between these two vectors to be very poor. Thus, alignment between the model and actual SGS scalar fluxes is a weakness of all three eddy-viscosity type models. On the other hand, the results of sub-section 5.4.3 show that the correlations between the magnitudes of the model and actual SGS scalar fluxes are very good. The Smagorinsky model in particular, has correlation coefficients very close to those given by DSM and GM. Among the eddy-viscosity type models, the least correlations are shown by Sigma model. Thus, the increased sensitivity of the Sigma kernel, which is a desirable feature in modeling the SGS stress tensor, actually makes the model less desirable for modeling the SGS scalar flux. Overall, eddy-viscosity models, especially, Smagorinsky and Vreman models, are good at predicting the magnitude of the SGS scalar flux.

Under the Dynamic Structure model of Chumakov [19], the SGS scalar flux takes its direction from the Leonard term, \( L_{i\phi} \). In terms of alignment between model and actual SGS scalar fluxes, the DS model is clearly superior to eddy-viscosity models. However, the DS model also involves the term \( \theta/\Theta \), where \( \theta = \overline{\phi \phi} - \overline{\phi} \overline{\phi} \) is the grid-filter scale scalar variance, and \( \Theta = \overline{\hat{\phi} \hat{\phi}} - \overline{\hat{\phi}} \overline{\hat{\phi}} \) is the test-filter scale scalar variance. While \( \Theta \) can be evaluated from the filtered scalar field, the evaluation of \( \theta \) requires either a model or solving an additional transport equation [19]. The first option, of writing a model for \( \theta \) brings in its own uncertainties and inaccuracies. The second, solving a transport equation for \( \theta \) increases the computational effort, while also requiring modeling of additional terms, such as the triple correlation, and the scalar dissipation, \( \chi \).

The Gradient Model is by far the best, in terms of orientation as well as magnitude. However, similar to DSM, GM involves terms which cannot be evaluated directly in an actual LES computation. The Modulated Gradient model, which seeks to address this issue by providing expressions for \( k_{SGS} \) and \( \theta \) in terms of \( G_{ij} \) and \( G_{i\phi} \), however, is characterized by much lower correlation coefficients. Furthermore, MGM also shows a large variability of regression coefficients, which indicates that a single coefficient may
be unsuitable for ensuring that the model SGS scalar flux has the same magnitude as the actual SGS scalar flux.

In view of the above difficulties associated with the Dynamic Structure and the Gradient models, simpler models are proposed here. The idea is to combine orientation derived from one among DSM and GM, with magnitude derived from one among Smagorinsky and Vreman eddy-viscosity models. In order to ensure that the actual and modeled SGS scalar fluxes are of similar magnitudes, the magnitude for each model can be divided by its respective $\langle \gamma \rangle_d$. Writing out two of the proposed models, based on the orientation from GM, we have

$$
\tau_{i\phi}^{SGM} = C_{SG} \Delta^2 |\vec{S}| \left| \frac{\partial \vec{\phi}}{\partial x_i} \right| \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right), \quad C_{SG} = \frac{C_S^2}{Pr_{SGS} \langle \gamma \rangle_d} \approx 0.075 \quad (5.30)
$$

$$
\tau_{i\phi}^{VGM} = C_{VG} \Delta^2 \Pi^g \left| \frac{\partial \vec{\phi}}{\partial x_i} \right| \left( \frac{G_{i\phi}}{|G_{k\phi}|} \right), \quad C_{VG} = \frac{C_V}{Pr_{SGS} \langle \gamma \rangle_d} \approx 0.239 \quad (5.31)
$$

These models have been named as Smagorinsky-Gradient (SGM) and Vreman-Gradient (VGM) models respectively. These models have very good alignment and magnitude correlation properties, while at the same time, are easy to compute in an a posteriori LES run, since all terms involved can be computed directly from the resolved velocity and scalar fields. As mentioned above, two more models (Smagorinsk-Structure and Vreman-Structure), with the orientation term replaced by $L_{i\phi}/|L_{k\phi}|$ can be built, in the exact same manner as the above two models. The coefficients based of these models would again be equal to $C_{SG}$ and $C_{VG}$, since the orientation component of the models does not contribute to its magnitude.

It may be pointed out that the models proposed here are similar in a sense to ‘mixed models’, wherein an eddy-viscosity term is added to a term (or multiple terms) which has good correlation properties, e.g. [127, 63, 115, 101]. However, the big difference between the models proposed here and the mixed models is that, in the present models, Smagorinsky and Vreman terms are multiplied, not added, to terms which improve the correlation of the model and actual flux. Finally, the models proposed here may be further modified to include backscatter control and dynamic computation of coefficients. It is mentioned without details, that incorporating backscatter control
reduces the correlation coefficients between magnitudes of $\tau_{i\phi}$ and $\tau_{i\phi}^{Smag}$ and $\tau_{i\phi}^{Vrem}$ somewhat; however, these models still yield larger correlation coefficients, as compared to MGM. The need for these modifications, and improvements brought about by them, if any, must be evaluated through exhaustive \textit{a posteriori} LES simulations using these proposed models.

5.5 \textit{A posteriori} Evaluation

A brief \textit{a posteriori} analysis of some of the SGS models is presented in this section. The pseudo-spectral code described previously is modified to perform LES of stationary homogeneous turbulence with a transported passive scalar. LES simulations are carried out on $N = 32^3$ collocation grid points. As previously, the forcing parameter is fixed equal to $\epsilon_f = 0.5$, while the attained Reynolds number is controlled by varying the viscosity, $\nu$. The turbulent velocity, dissipation and length scales computed now include contributions from the subgrid scales. The expressions for turbulent dissipation, and velocity scales, including the subgrid contributions are

$$u'^2 = \frac{2}{3} \int_0^{k_{max}} E(k) \, dk + \frac{1}{3} \langle \tau_{ii} \rangle, \quad \epsilon = \langle 2\nu \bar{S}_{ij} \bar{S}_{ij} \rangle - \langle \tau_{ij} \bar{S}_{ij} \rangle (5.32)$$

It may be noted that the subgrid contribution $\langle \tau_{ii} \rangle$ is non-zero only for non eddy-viscosity models. The scalar flux $\langle u'\phi' \rangle$ is also supplemented by the subgrid contribution, $\langle \tau_{2\phi} \rangle$. However, it should be noted that an estimate for the subgrid contribution to the scalar variance, $\langle \phi'\phi' \rangle$, is not available from a SGS scalar flux model.

Among the six models outlined in Table 5.1, DSM and MGM cannot be applied in \textit{a posteriori} LES without additional transport equations, as mentioned previously. The three eddy-viscosity models are expected to be inaccurate on account of the poor alignment between the SGS scalar flux and the resolved scalar gradient vectors. Hence, only MGM is evaluated among these six models. Out of the four proposed models, we expect models oriented along the Gradient term to be more accurate than models based on the Leonard term. Furthermore, Smagorinsky-Gradient and Vreman-Gradient models are expected to be almost similar to each other, since the
Vreman kernel, $\Pi^g$, reduces to the Smagorinsky kernel, $|\vec{S}|$, in a homogeneous setting. Hence, only SGM is evaluated \textit{a posteriori} in the current study. Finally, the term $H(P_0)$ is multiplied to Smagorinsky-Gradient model so as to avoid backscatter in the scalar equation in the current simulations.

Results of LES of homogenous passive scalar turbulence over a range of Taylor microscale Reynolds numbers, using MGM and SGM for the SGS scalar flux, are shown in Figure 5.24. Results without a SGS model for the scalar flux (i.e. SGS scalar flux identically set to zero) are also included, along with DNS results of Overholt and Pope \cite{74}. In all LES runs, the SGS stress tensor is modeled by the Gradient Model \cite{67}. The variances and fluxes are normalized based on the dissipation length scale, $L_\epsilon$. It is seen that the simulations without any SGS scalar flux model significantly over-predict the scalar variance at high values of $Re_\lambda$. The results improve drastically with the introduction of SGS scalar flux models. Comparing the performance of MGM and SGM, MGM is accurate till approximately $Re_\lambda \approx 66$, and over-predicts the scalar variance beyond this $Re_\lambda$, while the agreement between SGM and DNS results is good till approximately $Re_\lambda \approx 150$. Both SGM and MGM over-predict the scalar variance at $Re_\lambda \approx 210$ using the present pseudo-spectral method on $N = 32^3$ grid points. Similar conclusions can be drawn with regard to the normalized scalar flux, shown in Figure 5.5. It may be concluded that SGM offers an improvement over MGM, in \textit{a posteriori} evaluation of homogenenous passive scalar turbulence. It is reiterated that further exhaustive evaluation of these models in non-homogeneous situations may be carried out.

5.6 Summary and Conclusions

Direct Numerical Simulations (DNS) of homogeneous isotropic and anisoptropic turbulence have been carried out in this chapter using the pseudo-spectral method. The domain is a fully periodic cube, and Fourier expansions are used to discretize the Navier-Stokes equations. Three flow situations are considered, namely stationary
Figure 5.24. *A posteriori* evaluation of MGM and SGM models in homogeneous passive scalar turbulence. Variation of scalar flux and variance with $Re_\lambda$. No model simulation results and DNS [74] results also shown.
turbulence with a transported passive scalar, and decaying turbulence with passive and active scalars. In this context, a passive scalar is one which does not contribute to the density of the fluid, while an active scalar affects the density of the fluid field through a Boussinesq equation of state. In the stationary turbulence simulations, the flow is driven to statistical stationarity by a deterministic forcing applied to the large scales. Two time stepping methods have been implemented, viz. Integration Factor (IF) and Exponential Time Differencing (ETD) approach, with identical results. Thus, most of the simulations reported have been carried out using the IF approach.

Stationary passive scalar simulations in the presence of a mean scalar gradient in one direction, similar to those reported by Overholt and Pope [74], have been carried out for three Taylor microscale-based Reynolds numbers of $Re_\lambda = 25, 49$ and 84, on $32^3$, $64^3$ and $128^3$ physical grids, respectively. The simulations are fully resolved, and reproduce features such as Gaussian PDFs of the fields with drooping tails, typical ramp-cliff structures, symmetric nature of the scalar derivative PDFs in two directions, and skewed nature of the PDF of the derivative in the direction of the mean scalar gradient. The scalar fluxes and variances obtained from the present simulations, agree reasonably well with previous DNS results [74]. A $128^3$ grid simulation of decaying passive scalar turbulence has been carried out by first forcing the fluid and scalar fields to a steady state at $Re_\lambda = 84$, and subsequently turning off the forcing and the mean scalar gradient. This results in a monotonic decay of turbulent kinetic energy and increase of the turbulence length scales, in accordance with previous decaying turbulence simulations [19]. The last set of simulations, involving decaying active scalar turbulence, have been initialized with fluctuations of only the scalar field. These scalar fluctuations, along with an imposed mean background scalar gradient, drive the flow field initially, through the buoyant source term in the momentum equations. In active scalar simulations, the total energy decreases monotonically, while potential and kinetic energies oscillate with a frequency determined by the governing parameters. Simulations have been carried out for three levels of mean background scalar gradient, and are in very good agreement with the DNS results of
Gerz and Yamazaki [37]. The anisotropy displayed by active scalar turbulence is also well captured by the present simulations.

From the rigorously validated simulations, 19 data sets, spanning a variety of flow conditions, have been extracted. These 19 data sets have been employed to study six different subgrid scale (SGS) models for the SGS scalar flux. The SGS scalar flux is a vector, which can be thought to be composed of a magnitude and an orientation. *A priori* studies have been conducted to evaluate these two parts (magnitude and orientation) separately. In general, it is observed that eddy-viscosity type models are good at predicting the magnitude, but poor at predicting the orientation of the SGS scalar flux. The Dynamic Structure and Gradient models are better than eddy-viscosity models, with respect to both, magnitude as well as direction. However, these models are not easily realized in an actual LES, since they involve terms which cannot be computed directly from the resolved velocity and scalar fields. A variant of the Gradient model, the Modulated Gradient model, which can be easily applied in an *a posteriori* LES, however, is found to be inaccurate with respect to magnitude of the SGS scalar flux. Based on these observations, four new models, combining directions from Dynamic Structure and Gradient models, and magnitudes from Smagorinsky and Vreman eddy-viscosity type models, have been proposed. Typical values for the coefficients of these models have also been proposed.

By construction, these models are expected to perform better than eddy-viscosity and modulated Gradient models. Preliminary *a posteriori* tests have been performed, and the Smagorinsky-Gradient model has been shown to offer some improvement over the Modulated Gradient model. thorough *a posteriori* tests need to be carried out to ascertain this statement, as well as clarify the need for, and the effect of, further enhancements such as backscatter control and dynamic determination of model coefficients.
6. LARGE EDDY SIMULATION OF TURBULENT HORIZONTAL BUOYANT JETS

6.1 Introduction

A horizontal discharge of fluid, heavier or lighter as compared to the ambient, sets up what may be termed as a horizontal buoyant jet. This flow configuration occurs in many natural and engineering applications. Examples of horizontal buoyant jets include oceanic outfalls, waste water discharges, and leakage of a gas, such as hydrogen or nitrogen, from a gas cylinder. Most of these flows are turbulent, and accurate prediction of the flow in such a configuration is important. Laminar and turbulent jets, both with and without density differences, have been studied extensively using experimental, theoretical and numerical approaches. Most of the investigations of jets with density differences have, however, considered vertically released jets, in which the direction of injection is same or exactly opposed to the direction of buoyancy. The horizontal buoyant jet configuration has been studied to a lesser extent previously.

Theoretical studies on horizontal buoyant jets \[27, 77, 53, 121\] make use of integral methods, and are of limited validity and applicability. Integral models are based on assumptions about the radial profiles of velocity and scalar, and are useful for determining some quantities, such as the jet trajectory, and momentum and buoyancy fluxes. However, a detailed description of the radial structure of the jets is missing. On the contrary, the radial structure of the jet is an input to integral models, upon which all other predictions are based. Thus, a detailed investigation of the radial profiles using experimental or numerical techniques is essential for building better models and furthering our understanding of horizontal buoyant jets.

Many experimental studies of horizontal buoyant jets have been carried out, e.g. \[93, 4, 89, 26, 123\]. Satyanarayana and Jaluria \[93\] focussed on determining the
jet trajectories for a variety of jet discharge angles, including the horizontal. A secondary, plume-like motion is observed close to the discharge plane in a horizontal buoyant jet. This was first pointed out by Arakeri et al. [4], and has subsequently been studied by Querzoli and Cenedese [89] and by Deri et al. [26]. All the above studies considered laminar discharges, with a possible transition to turbulence at downstream locations. Furthermore, all these studies were carried out for jets with large density differences (> 5% of the mean), for which the Boussinesq approximation, restricting the changes in density to only the body force term in the Navier-Stokes equations, is invalid. The interaction between buoyancy and turbulence, in horizontal weakly (Boussinesq) buoyant jets with an initially turbulent discharge, was studied in recent experiments by Xu and Chen [123]. Using simultaneous Particle Image Velocimetry (PIV) and Particle Laser Induced Fluorescence (PLIF) measurements, the decay of centerline velocity, radial spread of the jet, and turbulent kinetic energy budgets were examined. A limited number of combinations of injection momentum (characterized by the Reynolds number) and density differences (characterized by the Richardson number) were considered in this study. The effect of a systematic variation of parameters on mixing and turbulence in horizontal buoyant jets has not been studied so far.

While a large number of numerical simulations of vertical buoyant jets have been carried out, e.g. [128, 34], very few simulations of horizontal buoyant jets appear in the literature. Horizontal jets issuing into a stably stratified ambient have been studied ([82], [83]), as also, horizontal buoyant jets in the vicinity of a wall [48]. Numerical simulation of horizontal buoyant turbulent jets with small density differences, and without confinement or background stratification effects, has not been carried out so far.

In this chapter, buoyancy and turbulence interaction in horizontal turbulent buoyant jets is studied using LES. Jets with small density differences are considered here. The governing equations, numerical methodology and sub-grid scale (SGS) model used are described in the next section. The numerical methodology is validated by
conducting non-buoyant turbulent jet simulations and comparing to experimental data. The classical experimental results of Hussein et al. [49] are used for this validation. Buoyant turbulent jet simulations are performed next, corresponding to the recent experiments of Xu and Chen [123]. Unlike non-buoyant and vertically buoyant jets, horizontally buoyant jets are marked by the simultaneous presence of a region of stable stratification on one side, and a region of unstable stratification on the other side of the jet centerline. The ability of the simulations to correctly capture this asymmetry between stable and unstable stratification regions is pointed out. The effect of varying the governing Reynolds and Richardson numbers on the horizontal buoyant jet is examined in detail. Finally, instantaneous snapshots of the flow and scalar fields are analyzed, and a dynamic mode decomposition is performed in order to identify the flow patterns, coherent structures, and instability mechanisms in a horizontal buoyant jet.

6.2 Problem Formulation

6.2.1 Governing Equations

LES of turbulent fluid flow with small density differences (< 5% of the mean) is governed by the filtered incompressible Boussinesq Navier-Stokes equations

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

\[
\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial \bar{\rho}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + Ri \bar{S} \delta_{ij} - \frac{\partial \tau_{ij}}{\partial x_j}
\]

\[
\frac{\partial \bar{S}}{\partial t} + \bar{u}_j \frac{\partial \bar{S}}{\partial x_j} = \frac{1}{ReSc} \frac{\partial^2 \bar{S}}{\partial x_j \partial x_j} - \frac{\partial \tau_{jS}}{\partial x_j}.
\]

Due to the small density differences, density variations have been neglected in all terms except the body force term in the above equations. \( S \) denotes the scalar field which determines the density, according to the linear equation of state \( \rho(S) = \rho_0(1 + \beta_S S) \). \( \rho_0 \) and \( \beta_S \) denote the density of the ambient fluid, and the scalar expansion coefficient respectively. The above equations have been non-dimensionalized with
the jet inlet nozzle diameter, $D$, as the length scale, the jet inlet velocity, $U_0$ as the velocity scale, and the difference in scalar value between the injected jet and the ambient domain, $\Delta S$, as the scalar scale. This non-dimensionalization leads to three non-dimensional parameters - Reynolds number, $Re$, Richardson number, $Ri$, and Schmidt number, $Sc$. The non-dimensional parameters governing the flow are defined as

$$Re = \frac{U_0 D}{\nu}, \quad Ri = \frac{g \beta S \Delta S D}{U_0^2}, \quad Sc = \frac{\nu}{k_S},$$

(6.4)

where $\nu$ denotes the fluid viscosity, $g$ denotes the gravitational acceleration, and $k_S$ denotes the diffusivity of $S$ in the fluid. Different values of $Ri$ and $Re$ are considered in this study, while the value of $Sc$ is fixed to be equal to 0.7 for reasons explained later.

$\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$ denotes the SGS stress tensor, while $\tau_{jS} = \bar{u}_j \bar{S} - \bar{u}_j \bar{S}$ denotes the SGS scalar flux. The SGS model used in this study is the constant coefficient Sigma model developed by Nicoud et al. [72]. This model is, by construction, superior at adjusting to local flow conditions by distinguishing between regions of zero and non-zero SGS dissipation, as compared to other traditional eddy-viscosity models [72]. The model has been shown to yield excellent results for non-buoyant decaying isotropic turbulence and for non-buoyant channel flow simulations [72]. The Sigma model, coupled with a constant SGS Prandtl (or Schmidt) number approximation to close the SGS thermal (or scalar) flux, has been applied to study a buoyancy-driven flow in a thermal cavity in Chapter 3), with very good results. Furthermore, the constant coefficient version of the Sigma model was found to be either better than or comparable to other dynamic models evaluated in Chapter 3. Specifically, the SGS stress tensor and SGS scalar flux are given by

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2 \nu_{SGS} \bar{S}_{ij}, \quad \tau_{jS} = -k_{SGS} \frac{\partial \bar{S}}{\partial x_j},$$

(6.5)
where \( \bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \) is the filtered strain-rate tensor. The SGS viscosity, \( \nu_{SGS} \), and the SGS scalar diffusivity, \( k_{SGS} \), are given by

\[
\nu_{SGS} = \left( C_\sigma \bar{\Delta} \right)^2 \frac{\sigma_3 (\sigma_1 - \sigma_2) (\sigma_2 - \sigma_3)}{\sigma_1^2}, \quad k_{SGS} = \frac{\nu_{SGS}}{\bar{S}_{CSGS}}. \tag{6.6}
\]

\( \bar{\Delta} \) denotes the filter width, and is equal to the numerical grid size [99]. \( \sigma_1 > \sigma_2 > \sigma_3 \) are the three singular values of the local velocity gradient tensor. A value of \( C_\sigma = 1.35 \) has been used, as recommended in [72], and used previously in [41], while a value of \( \bar{S}_{CSGS} = 0.7 \), equal to the molecular Schmidt number, has been used in the present study.

### 6.2.2 Numerical Methodology

A high-order LES framework, developed previously by Shetty et al. [99] for fully inhomogeneous non-buoyant turbulent flows, and extended for buoyant turbulent flows by Ghaisas et al. [41] is used here. The code, with modifications to the time-stepping method, has also been previously applied to other LES studies [25]. The numerical method is briefly described here. More details can be found in [99] and [41], and references therein.

The spatial discretization of the convective terms is carried out using a 5th-order Weighted Essentially Non-Oscillatory (WENO) scheme (Jiang and Shu [51]), while the viscous and SGS terms are discretized using the standard 4th-order central difference scheme. Boundary conditions, consistent with the high-order discretization, are applied by using three layers of ghost nodes. The values at the ghost nodes are updated using a Stokes flow boundary condition (Morinishi et al. [69]). A fractional time step method with a projection algorithm is used in order to achieve pressure-velocity decoupling. The velocity and scalar fields are first predicted using an explicit third-order accurate backward finite difference (BDF) method, detailed in Shetty et al. [100]. The velocity field is then made divergence-free, by correcting based on an updated pressure field. The pressure field is obtained by solving a Poisson problem.
using the multi-grid solver MUDPACK (Adams [1]). Computations are carried out on multiple processors using the shared-memory OpenMP paradigm.

### 6.2.3 Domain and Boundary Conditions

The rectangular domain and the conditions imposed at each boundary are depicted in Figure 6.1. We consider a round jet with inlet diameter $D$ injected at the origin $(0,0,0)$, issuing in the positive $x$ direction. The incoming fluid is heavier than the ambient fluid, and gravity acts vertically downward, as shown in Figure 6.1. The domain size is $32D$ in the $x$ direction, and $12D$ in the $y$ direction. Previous jet and plume simulations ([98], [43], [84], [124]) have shown that these axial and radial extents are sufficient to ensure that the boundaries do not have an effect on the region of interest. In the $z$ direction, the domain size is variable depending on whether the jet being simulated is buoyant or non-buoyant. Non-buoyant jets are simulated with a domain height of $12D$, equal to the domain extent in the $y$ direction, while buoyant jets are simulated in a larger domain, of extent $16D$, so as to allow for vertical deflection of the jet due to buoyancy.

Appropriate boundary conditions, especially at the outflow boundary, are critical to ensure stability and accuracy of numerical calculations of fluid flows. The boundary conditions imposed on the different boundaries are now described. $y$ and $z$ direction walls are considered to be zero-gradient, free-slip and impermeable, i.e. the normal derivatives of the scalar and all tangential velocity components, and the normal component of velocity are set to zero. At the inlet plane, the tangential components of velocity are set to zero. The axial velocity $U$ imposed has the same radial profile as that generated in the experiments of Xu and Chen [123] (reported in their Figure 1). In order to aid entrainment of fluid to the jet, a small co-flow of $U_{co} = 0.05$ is imposed at the inlet plane. Preliminary computations revealed that reducing the co-flow to a value below $U_{co} = 0.05$ leads to an instability at the outflow plane, since the computed jet tries to draw in fluid, needed for entrainment to the jet, from outside the domain,
Figure 6.1. Computational domain and boundary conditions for simulation of non-buoyant and buoyant turbulent jets.
leading to negative axial velocities at the outflow plane. Small values of coflow have been used in previous jet and plume simulations, e.g. [98], [43], [8] and [12]. Finally, in order to trigger early transition to turbulence, Gaussian random fluctuations of 5% of the mean are superimposed on the mean velocity profile. A top-hat scalar profile, equal to 1 in the circular inlet region, and 0 outside, is imposed at the inlet plane. No random fluctuations are imposed on the scalar profile at the inlet plane.

Imposing correct conditions to simulate open boundaries is challenging, and a topic of research in itself. The simplest, homogeneous Neumann, condition works well for laminar flows, but is found to be unstable for turbulent flows [9]. Various sophisticated outflow boundary treatments have been proposed, including convective boundary condition [2], and conditions on higher derivatives of velocity based on linearizing the incompressible Navier-Stokes equations [54]. Another class of conditions is based on artificial modifications in a small region near the outflow boundary, called the ‘buffer’ or the ‘sponge layer’. Examples of this approach include use of penalty terms driving the solution at the outflow to a pre-determined solution [7], and damping through an artificial increase of viscosity [62], [32], [31].

The outflow boundary condition used here is a combination of the buffer zone approach and a simple homogeneous Neumann condition. Beyond $x/D = 28$, the viscosity of the fluid is artificially increased according to the formula

$$\mu(x) = \mu_{\text{max}} \left[ \frac{1 + \exp\{15(\xi - 0.2)\}}{\mu_{\text{max}} + \exp\{15(\xi - 0.2)\}} \right], \quad (6.7)$$

where $\xi = 0.25(x/D - 28)$, varies linearly from 0 to 1 as $x/D$ goes from 28 to 32. $\mu_{\text{min}}$ is the unmodified viscosity of the fluid, and $\mu_{\text{max}} = 100\mu_{\text{min}}$. The function above is chosen so as to ensure a smooth and gradual increase of the viscosity by two orders of magnitude over the last 4 diameters of the domain. In the buffer zone, the viscous terms of the non-dimensionalized filtered Navier-Stokes equations, (6.1)-(6.3), above are replaced by

$$Visc_i = \frac{1}{Re} \left[ \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} \frac{\mu(x)}{\mu_{\text{min}}} + \frac{d}{dx} \left( \frac{\mu(x)}{\mu_{\text{min}}} \right) \frac{\partial \tilde{u}_i}{\partial x} \right], \quad (6.8)$$
with $Re$ defined based on the unmodified viscosity throughout the domain. At the last grid point, homogenous Neumann boundary conditions are applied, i.e. normal as well as tangential derivatives of all quantities are set to zero. Preliminary computations showed that the artificial outflow boundary treatment did not affect the flow upstream of $x/D = 28$. Furthermore, the region beyond $x/D = 28$ has been excluded from the analysis of results presented in Section 6.3.

### 6.2.4 Description of Simulations

This study is motivated by the horizontal buoyant jet experiments of Xu and Chen [123]. Four combinations of $Re$ and $Ri$ were examined in that study - two non-buoyant jets ($Re = 3200$ and $Re = 24000$; $Ri = 0$), and two buoyant jets ($Re = 24000$, $Ri = 2 \times 10^{-4}$; $Re = 3200$, $Ri = 0.01$). In this study, we cover a wider range of parameters, with two values of $Re = 3200$ and $Re = 24000$; and $Ri$ varying systematically over $Ri = 2 \times 10^{-4}$ to $Ri = 0.01$. The physical and numerical parameters used in this study are listed in Table 6.1.

A salt-water solution was used as the dense fluid, while an ethanol-water solution was used as the light fluid in the experiments of Xu and Chen [123]. Since the precise diffusivity of the dense fluid in the light fluid is unknown, the Schmidt number cannot be determined exactly. However, $Sc$ is expected to be of the order of unity, since both, the dense and the light fluids, make use of the same fluid (water) as the base. As a reasonable estimate, we fix $Sc = 0.7$ in this study.

The non-buoyant and buoyant jet simulations are carried out on uniform grids comprised of $192 \times 96 \times 96$ and $192 \times 96 \times 128$ discretization points respectively. For buoyant simulations, a larger number of grid points in the $z$ direction is required since the domain is longer in that direction. Simulations are also carried out on coarser grids, comprised of $160 \times 80 \times 80$ and $160 \times 80 \times 96$ points, for the non-buoyant and buoyant cases respectively. All simulations use a fixed time step, such that the maximum CFL number at each time step is always less than 0.4. No qualitative
Table 6.1. Physical and numerical parameters for horizontal buoyant jet simulations.

<table>
<thead>
<tr>
<th>( Ri )</th>
<th>( Re )</th>
<th>Domain ( (L_x \times L_y \times L_z) )</th>
<th>Grid ( (N_x \times N_y \times N_z) )</th>
<th>Reference Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3200</td>
<td>( 32D \times 12D \times 12D )</td>
<td>( 192 \times 96 \times 96 )</td>
<td>Hussein et al. [49], Xu and Chen [123]</td>
</tr>
<tr>
<td>0</td>
<td>24000</td>
<td>( 32D \times 12D \times 16D )</td>
<td>( 192 \times 96 \times 128 )</td>
<td>-</td>
</tr>
<tr>
<td>( 2 \times 10^{-4} )</td>
<td>3200</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.001</td>
<td>3200</td>
<td>( 32D \times 12D \times 16D )</td>
<td>( 192 \times 96 \times 128 )</td>
<td></td>
</tr>
<tr>
<td>0.005</td>
<td>3200</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>3200</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.005</td>
<td>24000</td>
<td>( 32D \times 12D \times 16D )</td>
<td>( 192 \times 96 \times 128 )</td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>24000</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
differences were observed between the results using the coarse and fine grids, and hence the results using only fine grids are reported here. The simulations are started at time $t = 0$ from a quiescent state, and are allowed to reach a statistically stationary state by simulating for 500 non-dimensional time units. Simulations are carried out for a further 1500 non-dimensional time units, over which time averaged statistics are collected. All the first and second order statistics reported in Section 6.3 converge over this time period.

6.3 Results

Results of LES of round turbulent jets with and without buoyancy are discussed in this section. Instantaneous flow visualizations are presented first in sub-section 6.3.1. Turbulent jets without buoyancy effects are considered in sub-section 6.3.2, followed by results of buoyant turbulent jets in sub-section 6.3.3. The LES results presented in these two sub-sections are compared to available experimental results, to validate the current numerical methodology. The effect of systematically varying $Ri$ and $Re$ is considered next in sub-section 6.3.4, followed by a discussion on the structure of horizontal buoyant jets in 6.3.5 and 6.3.6.

6.3.1 Instantaneous Visualizations

Before presenting converged, time averaged statistics of the turbulent flow field in buoyant and non-buoyant jets, some instantaneous flow visualizations are presented. Figure 6.2 shows contours of the scalar field in the mid-vertical ($y = 0$) plane, at an arbitrary time instant after the flow has achieved a statistically stationary state. Scalar contours for a non-buoyant jet at $Re = 3200$, and a buoyant jet at the same $Re$ and $Ri = 0.01$ are shown. The scalar $S$ simply acts as a passive scalar in the case of a non-buoyant jet, depicted in Figure 6.2a. Features typical of a turbulent jet - such as the jet core, large scale vortices due to entrainment and fine scale turbulence - can be seen in Figure 6.2a. On the other hand, in a buoyant jet, the scalar affects
Figure 6.2. Instantaneous visualizations of the scalar field in the mid-vertical ($y = 0$) plane in (a) non-buoyant jet, $Re = 3200$, and (b) buoyant jet, $Re = 3200$ and $Ri = 0.01$.

the velocity field, via density, which modifies the behaviour of the jet, as seen in Figure 6.2b. Gravity acts to deflect the jet vertically downward, and this results in a bent trajectory. The heavier jet injected horizontally into the lighter ambient results in a region of stable stratification (light fluid on top of heavy fluid) on the upper side, and a region of unstable stratification (heavy fluid on top of light fluid) on the lower side. This dichotomy leads to markedly different rates of entrainment, radial spread, mixing of momentum and scalar, and turbulence characteristics, as is studied throughout this chapter.

6.3.2 Non-buoyant Turbulent Jets

The centerline axial velocity of a round turbulent jet decays as the jet moves downstream, away from the nozzle. This decay of centerline velocity is accompanied by a radial spread of the jet, which is due to entrainment of fluid across the cylindrical shear layer. Simple mass and momentum balances imply that the decay of the centerline velocity and the radial spread (characterized by the half-width, $r_{1/2}$) should be $U_c \sim x^{-1}$ and $r_{1/2} \sim x$.

The decay of the centerline axial velocity for two non-buoyant jets at $Re = 3200$ and $Re = 24000$ is shown in Figure 6.3. It is seen that the decay of the centerline
velocity in the $Re = 24000$ jet starts slightly (approximately 2 diameters) earlier, as compared to the $Re = 3200$ non-buoyant jet. The centerline velocity decay is quantified by the decay rate $B$ given by

$$\frac{U_0}{U_c(x)} = \frac{1}{B} \frac{(x - x_0)}{D},$$

(6.9)

where $U_0$ and $x_0$ denote the centerline axial velocity at the inlet, and a virtual origin, respectively. The classical value of the decay rate is $B \approx 5.8$, while comparable values of $B = 5.25$ and $B = 5.08$ have been obtained in the present LES.

Figure 6.4 shows the evolution of the velocity half-widths for the two non-buoyant jets. The jet half-width is the radial distance from the jet centerline at which the velocity has decayed to half its value at the centerline. Two half-widths are shown for each jet: $r_{u+1/2}$, computed in the upper half of the $y = 0$ plane, and $r_{u-1/2}$, computed in the lower half of the $y = 0$ plane. For non-buoyant jets, the jets are expected to spread equally in all directions, and thus, $r_{u+1/2} \approx r_{u-1/2}$. This is seen in Figure 6.4 for both non-buoyant jets at $Re = 3200$ and $Re = 24000$. The rate of spread of the jets is also seen to compare well to experimental results of Xu and Chen [123].

Turbulent jets are known to lose their dependence on the inlet conditions, and exhibit self-similarity some distance downstream of the inlet plane. Figure 6.5 shows the self-similar nature of the present simulated jets. For both Reynolds numbers, profiles of the mean axial velocity scaled by its local centerline velocity are identical at different axial locations, with the radial distance scaled by the local half-width. The classical self-similar velocity profile obtained from experiments by Hussein et al. [49] is also shown in Figure 6.5, and is seen to be in close agreement with the present computations. Finally, radial profiles of second-order turbulent statistics from the $Re = 24000$ simulation are compared to experimental results of Hussein et al. [49] in Figure 6.6. It can be seen that $\langle u'u' \rangle$ and $\langle u'w' \rangle$ attain self-similarity by the axial location $x/D = 12$, while $\langle v'v' \rangle$ and $\langle w'w' \rangle$ attain self-similarity at further downstream locations. The self-similar turbulent statistics are in good agreement with the classical experimental results, as seen in Figure 6.6.
Figure 6.3. Decay of centerline axial velocity for non-buoyant turbulent jets.

Figure 6.4. Axial evolution of jet velocity half-width compared with experimental results [123] for (a) \( Re = 3200 \) and (b) \( Re = 24000 \).

Overall, the non-buoyant turbulent jet LES results are qualitatively and quantitatively similar to experimental non-buoyant turbulent jet results, which serves as a validation for our numerical methodology and SGS model.
Figure 6.5. Mean axial velocity of non-buoyant turbulent jets at (a) $Re = 3200$ and (b) $Re = 24000$, compared to the experimental self-similar profile of [49].
Figure 6.6. Second-order turbulent statistics in non-buoyant turbulent jets at $Re = 24000$, compared to the experimental results of [49]. (a) $\langle u' u' \rangle$, (b) $\langle u' w' \rangle$, (c) $\langle v' v' \rangle$ and (d) $\langle w' w' \rangle$, normalized by $U_c^2(x)$. 
6.3.3 Buoyant Turbulent Jets

In a non-buoyant jet, the mean axial velocity is always maximum at the centerline, which in the vertical plane has the coordinate $z = 0$. Contrary to this, a buoyant turbulent jet injected horizontally is deflected vertically as it propagates downstream. Xu and Chen [123] quantified this deflection by defining the centerline of a buoyant jet as the $z$ location at which the mean axial velocity $\langle U \rangle$ is maximum. The location of the centerline, $z_c^u$, and the centerline velocity, $U_c$, are then related by

$$U_c(x) = \langle U \rangle (x, 0, z_c^u).$$  \hspace{1cm} (6.10)

Half-widths above and below the jet centerline in the $y = 0$ plane can then be defined as usual, based on these definitions of the centerline and the centerline velocity. Half-widths of the mean scalar field can also be defined similarly. Although the jet centerline does not divide the vertical plane in exactly half, we call the portions above and below the jet centerline, the upper half plane and the lower half plane respectively.

The decay of the centerline velocity of non-buoyant and $Ri = 0.01$ buoyant turbulent jets at $Re = 3200$ is shown in Figure 6.7a. It can be seen that the buoyant jet decays faster, with a decay rate $B = 3.91$, as compared to the non-buoyant jet with a decay rate $B = 5.25$. Figure 6.7b shows that the $Re = 24000$ buoyant jet also decays faster than the $Re = 24000$ non-buoyant jet. Thus, the decay rate is dependent on $Ri$. This is in contradiction to that reported in Xu and Chen [123], who noted that $B$ is independent of $Ri$. This discrepancy is likely caused due to the conditions imposed at the inlet plane, especially, the imposed small co-flow. It should be noted that the decay rate was over-predicted by the present LES in the non-buoyant case, described in the previous section, as well. Other numerical simulations which have predicted a faster decay of centerline velocity include [43].

In addition to the rate of decay, Figure 6.7a shows that the decay of the centerline velocity, and consequently, its radial spread, starts at the downstream location $x/D \approx 8$. The buoyant jet in the experiments of Xu and Chen [123] on the other hand, starts spreading at around $x/D \approx 5$ (see Figure 11 in Xu and Chen [123]). In order to
account for this difference between the experiments and the present simulations in the axial location at which turbulence is triggered, the experimental results have been translated by 3 diameters in the axial direction, while comparing to the simulation results.

The evolution of velocity and temperature half-widths in the upper and lower half planes for the $Re = 3200$, $Ri = 0.01$ buoyant jet are shown in Figure 6.8. Half-widths obtained experimentally by Xu and Chen [123] are also shown in Figure 6.8. It can be seen that similar to the experimental results, the half-widths in the lower half plane, $r_{-1/2}$, are always larger than the half-widths in the upper half plane, $r_{+1/2}$. This is true of velocity as well as scalar half widths. The configuration of a jet issuing horizontally into a lighter ambient causes the upper half plane to be a region of stable stratification, while the lower half plane becomes unstably stratified. This indicates that the mixing of momentum and scalar, and the radial spread of the jet, is larger in the unstable stratification than in the stable stratification region. Figure 6.8 shows that the half-widths are predicted reasonably accurately by the present LES, as compared to the experiments. The rate of increase of the velocity half-widths in both unstable and stable stratification is reasonably accurate. The evolution of scalar half-width in stable stratification, $r_{+1/2}^S$ is also accurately captured, while some discrepancies are observed in the evolution of the scalar half-width in unstable stratification, $r_{-1/2}^S$, especially farther downstream.

Figure 6.9a compares the jet center location and the mean vertical velocity at the centerline obtained from the current LES to those obtained from experiments [123]. For the current LES results, both the time averaged results and curve fit to the raw data are presented. It is seen that there is close agreement between the LES and experimental trajectories till about 12 diameters, while the trajectories diverge somewhat beyond $x/D = 12$. The mean vertical velocity along the centerline shows a similar behaviour, as compared to the experimental results. This discrepancy is caused due to the small co-flow ($U_{co} = 0.05$) present at the inlet plane in our computations.
Self-similarity of the mean axial velocity in the buoyant jet is examined in Figure 6.10. It is seen that radial profiles of the mean axial velocity scaled by the local centerline axial velocity, \( \langle U \rangle / U_c \), at different axial locations collapse to one curve, with the radial coordinate adjusted for the jet deflection, \( z - z_u \), and scaled by the corresponding half-width. The half-width used to scale the radial coordinate is \( r_{u+1/2} \) in the upper half plane, and \( r_{u-1/2} \) in the lower half plane. This novel scaling, making use of different half-widths in different regions of the jet, was introduced by Xu and Chen [123], and is confirmed by our present LES. Also shown in Figure 6.10 is the experimental self-similar profile obtained for a non-buoyant jet. As compared to the non-buoyant self-similar profile, the computed self-similar profile can be seen to be more narrow, and flatter beyond \( (z - z_u/r_{1/2}) > 1.2 \) in both half planes. This is caused by the over-prediction of the velocity half-widths, seen in Figure 6.8a.

The evolution of turbulent kinetic energy (TKE) in buoyant turbulent flows is governed by

\[
\frac{\partial k}{\partial t} = T + P - \epsilon - B, \tag{6.11}
\]

where \( T \) is the turbulent transport term, and \( P, \epsilon \) and \( B \) denote the turbulent production, dissipation and buoyant production respectively, defined [86] as

\[
P = -\langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j}, \quad \epsilon = \frac{2}{Re} \langle s'_{ij} s'_{ij} \rangle, \quad B = Ri \langle u'_3 S' \rangle, \tag{6.12}
\]

with \( s'_{ij} \) denoting the fluctuating strain-rate tensor. The notation for buoyant production is the same as that for the decay rate, but the two should not be confused, since they are always discussed in appropriate context. Profiles of \( P, \epsilon \) and \( B \) at four different axial locations of \( x/D = 5, 9, 13 \) and 17 have been extracted for the \( Re = 3200, Ri = 0.01 \) buoyant jet, and are plotted in Figure 6.11. The computationally obtained profiles are compared to experimental results of Xu and Chen [123], extracted at axial locations 2, 6, 10 and 13 diameters. This is in keeping with the fact that experimental results need to be translated by about 3 diameters to compare with LES results, as explained above.
Production, which is usually positive and acts as a source in the TKE equation, has a double-peak shape at all axial locations. The two humps are caused by the two shear layers, one in stable stratification and one in unstable stratification. Dissipation, which acts as a sink of TKE, also has a double-peak shape close to the nozzle, but acquires a single peak shape farther downstream. This is well captured by the present LES. The magnitude of production is under-predicted by the LES close to the nozzle, at \( x/D = 5 \), while the prediction of magnitudes is better further downstream. The production profile can also be seen to be skewed downward at \( x/D = 9 \), due to a slight mismatch between the locations of the jet center. Similar to production, the magnitude of dissipation is under-predicted at \( x/D = 5 \), but the LES profiles compare well with experimentally obtained dissipation profiles at further downstream locations. The under-prediction close to the nozzle can be attributed to the artificially imposed turbulent inlet conditions, which may be different from the inlet conditions in the experiments.

Buoyant production is positive in stable stratification and negative in unstable stratification regions, as seen in Figure 6.11c. Thus, it acts as a sink of TKE in the stable stratification region, and a source of TKE in the unstable stratification region. The LES results are qualitatively similar to the experimental profiles of \( B \), although the magnitudes are over-predicted by the present LES.

To summarize the results in this sub-section, the current computational framework has been validated by conducting LES of buoyant jet at \( Re = 3200 \) and \( Ri = 0.01 \), and comparing to the experimental results reported in Xu and Chen [123]. The jet half-widths, vertical deflection of the jet centerline and the mean vertical velocity along the centerline are predicted accurately, especially close to the nozzle. The buoyant jet is found to be self-similar with the same scaling as reported in the experiments, although the computed self-similar profile is narrower than the experimental profile far away from the jet centerline. Contrary to experiments, the decay of the centerline velocity is found to depend on \( Ri \). Turbulent production and dissipation are under-predicted close to the nozzle, while the prediction is better away from the nozzle. Thus, the LES
Figure 6.7. Decay of mean centerline axial velocity in buoyant turbulent jets. (a) $Re = 3200$ and (b) $Re = 24000$.

Figure 6.8. Axial evolution of buoyant jet half-widths in upper half plane (stable stratification) and lower half plane (unstable stratification), compared with experimental results of [123]. (a) Velocity half-widths and (b) scalar half-widths.

results are qualitatively and in some cases, quantitatively accurate. The quantitative discrepancies may be attributed to the differences between the actual experimental and numerically imposed inlet turbulence conditions.
Figure 6.9. Axial evolution of (a) location of jet center and (b) center-line mean vertical velocity in buoyant jet, compared with experimental results of [123].

Figure 6.10. Self-similarity of mean axial velocity of buoyant turbulent jet at $Re = 3200$ and $Ri = 0.01$. Experimental self-similar profile in a non-buoyant jet ([49]) is shown for comparison.
Figure 6.11. Turbulent statistics of buoyant jet at $Re = 3200$ and $Ri = 0.01$ (solid lines), compared to experimental results (solid circles) of [123]. (a) Production, (b) dissipation and (c) buoyant production.
6.3.4 Effect of $R\dot{i}$ and $Re$

The experiments of Xu and Chen [123] reported results of buoyant jets at only four combinations of $Re$ and $Ri$. Thus, only a limited range in the $Re - Ri$ parameter space has been covered previously by the experiments. The experimental results are supplemented in this sub-section by systematically varying $Ri$ over two orders of magnitude, while keeping a fixed $Re = 3200$. Additionally, results at $Ri = 0.005$ and $Ri = 0.01$, with $Re = 24000$, are also reported in this sub-section, thus showing the effect of varying $Re$.

The radial growth of a non-buoyant turbulent jet is equal in all directions, i.e. $r_{+1/2} \approx r_{-1/2}$, while the radial growth of a buoyant turbulent jet in unstable stratification region has been shown to be larger than in the stable stratification region, i.e. $r_{-1/2} > r_{-1/2}$. We define two additional measures of the radial growth, viz. spread, $b = r_{-1/2} + r_{-1/2}$, and anisotropy, $a = r_{-1/2} - r_{-1/2}$. $b$ is a measure of the total radial width of the jet in both directions, while $a$ measures the extent to which the jet grows preferentially in the unstable stratification region over the stable stratification region.

Similar to the half-widths, spread and anisotropy can be defined based on the velocity field and the scalar field, viz. $b^u$, $b^S$ and $a^u$, $a^S$ respectively.

Figures 6.12 and 6.13 show the jet spreads and the anisotropies respectively, for jets with a fixed $Re = 3200$, and four different values of $Ri = 2 \times 10^{-4}$, $Ri = 0.001$, $Ri = 0.005$ and $Ri = 0.01$. The arrow in each figure shows the direction of increasing $Ri$. It is apparent that both $b^u$ and $b^S$ increase monotonically with increasing $Ri$. In other words, increasing $Ri$ increases the radial spread of the jet. This indicates that a heavier horizontal jet leads to greater entrainment and larger extent of radial mixing, of momentum and scalar, than a lighter horizontal jet. Figure 6.13 shows that, over most of the domain, the anisotropies $a^u$ and $a^S$ also increase with increasing $Ri$. Concentrating on Figure 6.13b, in the region $x/D = 5$ to $x/D = 15$, the anisotropy is almost zero for $Ri = 2 \times 10^{-4}$ and increases with $Ri$ for the other three cases. This indicates that $r^S_{+1/2}$ and $r^S_{-1/2}$ are almost equal, and the radial spread is almost
axisymmetric for the lowest $Ri$ jet. For progressively heavier jets, $r_{-1/2}^S > r_{+1/2}^S$, with the spread in the unstable stratification region being larger and larger as compared to the spread in the stable stratification region. Velocity anisotropy, $a^u$, follows similar trends as $a^S$, and the same conclusions as above, regarding enhancement of mixing in unstable stratification over that in stable stratification, can be drawn based on $a^u$.

The effect of $Re$ on jet spreads and anisotropies can be seen in Figures 6.14 and 6.15. Figure 6.14 shows that for $Ri = 0.005$ increasing $Re$ from 3200 to 24000 increases $b^u$ and $b^S$ slightly. At $Ri = 0.01$, $b^u$ and $b^S$ increase slightly over a portion of the domain and decrease slightly over the rest of the domain. Thus, it can be concluded that $Re$ has a weak effect on the total radial spread and mixing of momentum and scalar. Figure 6.15 shows that for both values of $Ri$, increasing the Reynolds number leads to significant reductions in both $a^u$ and $a^S$. Thus, a jet with larger $Re$ spreads more equally in stable and unstable stratification regions, and is closer to a non-buoyant axisymmetric jet in this respect.

The effect of $Ri$ and $Re$ on jet trajectories is seen in Figures 6.16a and 6.16b respectively. Time averaged results along with polynomial fitting lines are shown in Figure 6.16a, while only the fitting lines are shown in Figure 6.16b in order to avoid clutter. Firstly, Figure 6.16a shows the location of the jet center, $z^u_c$, for four different $Ri$ at a fixed $Re = 3200$. The location of the jet center does not decrease with axial
Figure 6.13. Effect of $Ri$ on anisotropy of buoyant turbulent jets. (a) Velocity anisotropy, $a^u$, and (b) scalar anisotropy, $a^S$. Arrow shows the direction of increasing $Ri$.

Figure 6.14. Effect of $Re$ on spread of buoyant turbulent jets. (a) Velocity spread, $b^u$, and (b) scalar spread, $b^S$.

Figure 6.15. Effect of $Re$ on anisotropy of buoyant turbulent jets. (a) Velocity anisotropy, $a^u$, and (b) scalar anisotropy, $a^S$. 
location for the lowest $Ri$ jet, indicating that at this $Ri$, the jet follows an almost flat trajectory, similar to a non-buoyant jet. The downward deflection of the jet trajectory increases with increasing $Ri$, as seen in Figure 6.16a. Figure 6.16b shows the location of the jet center for the two Reynolds numbers, at the two highest $Ri$ values. For both $Ri = 0.005$ and $Ri = 0.01$, the low Re and the high Re jets follow essentially the same trajectory. Thus, the trajectory of a horizontal buoyant jet can be concluded to depend only on $Ri$, and independent of $Re$.

TKE production, dissipation and buoyant production have been extracted at $x/D = 9$, and are plotted in the similarity scaling, in Figure 6.17, for jets at different $Ri$ and fixed $Re = 3200$. At this axial location, both production and dissipation have a double-peaked shape, as already seen in the previous sub-section. For the non-buoyant and weakly buoyant ($Ri = 2 \times 10^{-4}$ and $Ri = 0.001$) jets, the two peaks in the stable and unstable stratification regions are almost symmetric. With increasing $Ri$, production in the stable stratification region (Figure 6.17a) increases. The magnitude of production in unstable stratification region at higher values of $Ri$ is slightly reduced as compared to non-buoyant and weakly buoyant jets, although no clear monotonic trend is seen. The increase in production in the stable strati-
fication region is caused by the reduced half-width $r_{+1/2}$, which leads to increased radial gradient of the streamwise velocity, $\partial \langle U \rangle / \partial y$. Figure 6.17b shows that the dissipation increases monotonically with increasing $\text{Ri}$. Similar to $P$, the two peaks of the $\epsilon$ profile are symmetric for non-buoyant and weakly buoyant jets. For higher $\text{Ri}$ jets, the dissipation is larger in the unstable stratification region, as compared to that in the stable stratification region. Buoyant production is zero by definition for non-buoyant jets, and increases with increasing $\text{Ri}$. As mentioned earlier, it contributes as a source of TKE in the unstable stratification region, and a sink of TKE in the stable stratification region. The strength of $B$ can be seen to be almost equal in the two regions, and about one order of magnitude smaller than $P$ and $\epsilon$ for the two highest $\text{Ri}$ jets.

Figure 6.18 shows the effect of increasing $\text{Ri}$ at fixed $Re = 3200$ on some second order turbulent statistics. Profiles of $\langle u'u' \rangle$ and $\langle u'w' \rangle$ at $x/D = 9$, and $\langle v'v' \rangle$ and $\langle w'w' \rangle$ at $x/D = 17$ have been extracted and plotted, along with non-buoyant experimental results of Hussein et al. [49]. In order to compare results at different values of $\text{Ri}$, all turbulent quantities have been presented in the similarity scaling. It should be noted that the profiles presented are not self-similar, and have been chosen only as representative of other axial locations.

Buoyancy has different effects on different turbulent quantities in different regions of the jet. The streamwise fluctuating velocity, $\langle u'u' \rangle$ (Figure 6.18a), increases in stable stratification. In unstable stratification region, $\langle u'u' \rangle$ increases over a small region close to the centerline, but reduces away from the centerline. Horizontal velocity fluctuation, $\langle v'v' \rangle$ (Figure 6.18c), increases in both regions, but is unaffected towards the edge of the jet, beyond $|z - z^u_c/r^u_{1/2}| > 1.5$ on either side of the centerline. Vertical velocity fluctuation, $\langle w'w' \rangle$ (Figure 6.18c), shows a large increase throughout the unstable stratification region, and is also increased over a small region close to the centerline in stable stratification, while remaining unaffected over the rest of the stable stratification region. The cross-correlation $\langle u'w' \rangle$, depicted in Figure 6.18b, can be said to be largely unaffected by increasing $\text{Ri}$. 
Finally, the effect of $Re$ on turbulent statistics can be seen in Figure 6.19, which plots the four second order turbulent statistics as above, for jets with a fixed $Ri = 0.005$, and two different $Re = 3200$ and $Re = 24000$. Results of non-buoyant jet experiments of Hussein et al. [49] are also shown in Figure 6.19 as reference. From profiles of all four quantities, it may be concluded that $Re$ has a weak effect on turbulent quantities in horizontal buoyant jets.

In summary, $Ri$ has a drastic effect on the radial spread of the jet, the anisotropy of radial growth in stable and unstable stratification regions, the jet trajectory, and turbulent fluctuations. $Re$ on the other hand, has a weak effect on the jet spread, the trajectory and turbulent fluctuations. Increasing $Re$ significantly reduces the anisotropy of radial growth in stable and unstable stratification regions.

6.3.5 Structure of Horizontal Buoyant Jets

Although seemingly simple, the horizontal buoyant jet configuration presents a number of interesting phenomena, caused by the interaction between the horizontal momentum flux and the vertical buoyant force. In order to study these, an additional simulation of a buoyant jet at $Re = 3200$ and $Ri = 0.01$ has been carried out, utilizing a computational grid which is stretched in the radial direction. The stretching concentrates points near the origin $(0, 0)$ in the $y – z$ plane, which leads to better resolution of the shear layer close to the nozzle. The number of grid points and the CFL criterion are same as those for the uniform grid simulations.

The experiments of Arakeri et al. [4] demonstrated that for some combinations of $Re$ and $Ri$, laminar horizontal buoyant jets bifurcate into two clearly separated streams. They also hypothesized that turbulent jets with Schmidt numbers of the order of unity, which are conditions relevant to our present simulations, would not bifurcate [4]. This is consistent with our present simulation results, where two separate streams are not observed. Based on a dimensional analysis, the horizontal buoyant jet can be divided into three regions - the jet core, the shear layer, and the developed jet
Figure 6.17. Effect of $\text{Ri}$ on energetics of turbulent buoyant jet. (a) Production, (b) dissipation and (c) buoyant production.
Figure 6.18. Effect of $Ri$ on turbulent statistics in buoyant jets. (a) $\langle u'u' \rangle$, (b) $\langle u'w' \rangle$, (c) $\langle v'v' \rangle$ and (d) $\langle w'w' \rangle$, normalized by $U_c^2(x)$. 
Figure 6.19. Effect of $Re$ on turbulent statistics in buoyant jets. (a) $\langle u'u' \rangle$, (b) $\langle u'w' \rangle$, (c) $\langle v'v' \rangle$ and (d) $\langle w'w' \rangle$, normalized by $U_c^2(x)$. 

(a) 

(b) 

(c) 

(d)
The effect of buoyancy on the fully developed turbulent part of the jet (beyond, say, $x/D = 8$) has been elucidated in the previous sub-sections. Here, we focus on the part close to the nozzle.

Figure 6.20 shows three snapshots of the buoyant jet in the $x/D = 5$ plane, where vectors tangent to this plane have been overlaid on instantaneous contours of $S$. The jet core region (comprising of regions with high values of $S$) can be clearly distinguished from the mixed shear layer region (comprising of intermediate values of $S$), and the ambient fluid (low values of $S$). Concentrating on Figure 6.20a, the motion at this time instant is primarily directed vertically downward, due to the effect of buoyancy, and the jet core is almost circular. At the second time instant, Figure 6.20b, two stagnation points can be seen just above and below the jet core. The vertical downward velocities are largest at the edge of the jet core, and are smaller in the core and the mixed layer region. This indicates that the jet core acts similar to a cooled cylinder placed in warmer surrounding, as the entrained fluid curves around the core. This also gives rise to the characteristic veil-shaped scalar contour plot, similar to that observed in the experiments of Deri et al. [26]. Figure 6.20c shows a vortex being shed from the bottom edge of the jet core, towards the left of the figure. A weak vortex is also being formed towards the right of the jet core. A downward plume emerging from the jet core is seen in all three snapshots. All these observations are qualitatively similar to those in Deri et al. [26].

Figure 6.21 shows two instantaneous snapshots of the iso-surface $\lambda_2 = -0.1$, where $\lambda_2$ denotes the intermediate eigenvalue of the tensor $S^2 + \Omega^2$ [50]. $S$ and $\Omega$ denote the filtered strain-rate and rotation-rate tensors respectively. The $\lambda_2$ iso-surfaces have been colored by the instantaneous axial velocity. Also shown, are gray scale contours of the instantaneous scalar field at the mid-$y$ plane, projected on to the far $y$ plane. At the inlet plane, $x/D = 0$, a circular ring of small-scale structures can be seen. This is due to the random forcing, applied so as to trigger transition to turbulence. Relatively far away from the nozzle, beyond $x/D = 8$, the developed jet, with small scale turbulence, is seen. In the region around $x/D = 5$, Figure 6.21a shows
Figure 6.20. Instantaneous contours of scalar in plane located at $x/D = 5$, with tangential vectors overlaid. The snapshots are at three arbitrary time instants, and are not correlated with each other.
well-formed, coherent, vortex rings. These vortex rings are susceptible to Kelvin-Helmholtz instability, evidence for which is seen in the projected scalar contours. Contrary to this, at the time instant shown in Figure 6.21b, a coherent vortex ring-like structure is seen only on the upper side of the jet, while small scale, non-coherent, structures are seen on the bottom side. Consistent with this, the projected $S$ contours show Kelvin-Helmholtz rollers only on the upper side of the jet, while the rollers are absent from the lower side. Instead, the motions described in the previous paragraph give rise to an intermittent vertically downward plume on the lower side, which breaks the coherent rings into small scale structure.

Putting the above observations together, the picture of the structures and instabilities in horizontal buoyant jet that emerges, is as follows. The upper side of the jet, which is in stable stratification, consistently forms coherent vortex rings, which undergo Kelvin-Helmholtz instabilities to transition to turbulence. The lower side of the jet being unstably stratified, forms coherent vortex rings intermittently, and undergoes a combination of Kelvin-Helmholtz and plume instabilities to transition to turbulence. Querzoli and Cenedese [89] provided a somewhat similar picture of the horizontal buoyant jet. However, the intermittent nature on the lower side, with an interaction between coherent rings and small scale structure caused by the plume, was not observed. This may be because the jets considered in [89] had larger density differences, with $Ri$ values at least five times larger than that considered in our present study.

6.3.6 Dynamic Mode Decomposition of Horizontal Buoyant Jet

The structure of a horizontal buoyant jet at $Re = 3200$ and $Ri = 0.01$ is further quantitatively analyzed here using the dynamic mode decomposition (DMD) technique introduced by Schmid [94]. A sequence of 800 snapshots over a time interval of 40 non-dimensional time units is used for the analysis. The DMD is performed on the instantaneous axial velocity sampled in a window $[3.83, 16.5] \times [-3.3, 2.9]$ in
Figure 6.21. Instantaneous iso-surfaces of $\lambda_2 = -0.1$, colored by axial velocity. Instantaneous (grayscale) contours of scalar field at the mid-$y$ plane, projected on to the far $y$ plane. Snapshots are at two arbitrary, uncorrelated time instants.
the $x$ and $z$ directions, in the $y = 0$ plane. This domain extent is chosen so as to include portions of the jet core, the surrounding cylindrical shear layer, and the fully developed jet.

The DMD algorithm has been described in detail in many previous studies ([94], [95], [58], etc.), and is briefly reviewed here. The algorithm involves composing a data matrix $V_{t}^{N-1}$, with each column containing the entire flow field at one time instant. A singular value decomposition, $V_{t}^{N-1} = U \Sigma W^{H}$, is carried out on the data matrix, and the resulting matrices are used to compute the so-called companion matrix, $\tilde{S}$. The eigenvalues, $\mu_{i}$, and eigenvectors, $y_{i}$, of $\tilde{S}$ are computed. $\mu_{i}$ are projected onto the complex plane via the transformation $\lambda_{i} = \log(\mu_{i}) / \Delta t$, while the DMD modes are obtained from the eigenvectors using the expression $\phi_{i} = U y_{i}$. Associated with each DMD mode, is an amplitude and a measure of coherence. The amplitude is given by $a_{i} = 1 / |A(:, i)|$, where the matrix $A = W \Sigma^{-1} Y$. The coherence is given by $\chi_{i} = y_{i}^{H} \Sigma y_{i}$, [58].

Results of the DMD analysis are displayed in Figures 6.22 and 6.23. Figure 6.22a plots the dynamic modes in the complex plane. The modes have been colored by their coherence, where the color gradation goes from blue to red with increasing coherence. Figure 6.22b shows the amplitudes corresponding to the individual modes. Since the initial data matrix is real, $\tilde{S}$ is symmetric, and the eigenvalues of $\tilde{S}$ occur in complex conjugate pairs. As a result, the spectrum and amplitudes are seen in Figure 6.22 to be symmetric with respect to $\lambda_{i}$, which is as expected [94]. Most of the modes seen in Figure 6.22a have negative real parts, which indicates that the modes are stable. The presence of a few unstable modes indicates that the processed signal contains some degree of transience, and that all the transient phenomena have not been averaged out completely over the time period considered. The amplitudes denote the energy content of the dynamic modes. It should be noted that the amplitude does not decay monotonically with $\lambda_{i}$. Thus, the most coherent modes do not necessarily have the largest amplitudes, and there is no direct correlation between coherence and
amplitude. This indicates that the smaller, less coherent modes can also contribute significantly to the energy of the flow.

Five representative modes have been extracted from the DMD, and are displayed in Figure 6.23. These five modes have also been marked in Figures 6.22a and b. As a reference, the location of the centerline is also shown in each sub-figure of Figure 6.23. The first mode has the largest amplitude as well as coherence, and can be seen to represent the mean flow in Figure 6.23a. This mode lies very close to the origin, and represents an absence of growth, decay as well as oscillations. Mode 2 represents large coherent vortices, which occur in both the stable stratification and unstable stratification regions (Figure 6.23b). Modes 3 through 5 have successively lesser coherence (Figures 6.22a), and, as seen in Figures 6.23c-e, the structures associated with these modes become progressively smaller. Closer to the nozzle, the structures lie in the cylindrical shear layer region, on either side of the centerline. Farther away from the nozzle, the structures occur closer to the centerline, which indicates a merging of the two shear layers into a fully developed turbulent jet.

One advantage of the DMD technique is that it can be applied to any arbitrarily shaped sub-domain of a flow field. In order to examine the differences between the structure of the stable and unstable stratification regions, the portions above and below the jet centerline have been extracted and fed to the DMD algorithm separately. The results of these two dynamic mode decompositions are shown in Figures 6.24 and 6.25. In each case, the sub-figures on the left show results of the analysis of the stable stratification region, while sub-figures on the right show results of the analysis of the unstable stratification region. This enables a direct comparison of the dynamics of the unstable and stable stratification regions.

Figures 6.24a and b show that a larger number of dynamic modes in unstable stratification are unstable (i.e. have $\lambda_r > 0$), as compared to stable stratification. This indicates that a greater degree of transience is associated with the flow field in unstable stratification. This is consistent with the picture presented previously in Section 6.3.5, comprising of coherent vortex rings in stable stratification and intermittent vortex
Figure 6.22. DMD analysis of horizontal buoyant jet at $Re = 3200$, $Ri = 0.01$. (a) spectrum with modes colored by their coherence, and (b) amplitudes of different modes. 5 representative modes are marked.
Figure 6.23. Representative dynamic modes of horizontal buoyant jet at $Re = 3200$ and $Ri = 0.01$. (a) $\lambda = (0.004, 0.00)$, (b) $\lambda = (-0.03, 1.11)$, (c) $\lambda = (0.03, 1.99)$, (d) $\lambda = (-0.002, 2.18)$ and (e) $\lambda = (-0.09, 3.54)$. The solid line denotes the jet centerline.
rings and small scale structure in unstable stratification. Comparing Figures 6.24c and d, the dynamic modes in unstable stratification have generally larger amplitudes, compared to the dynamic modes in stable stratification. The energy content of the jet can thus be seen to be split unevenly between the upper and lower parts. The lower part of the buoyant jet, in the unstable stratification region, has larger energy than the upper part of the jet, in stable stratification.

Four representative modes, with roughly the same values of $\lambda_i$, have been marked in Figure 6.24. These modes have been extracted from the flow field, and are plotted in Figure 6.25. Since it is not considered in the analysis, the unstable stratification region has been blanked out in all figures on the left. Similarly, the stable stratification region has been blanked out in all figures on the right. The conclusions drawn from this figure are similar to those drawn from Figure 6.23. It can be seen that the visualization formed by coalescing Figures 6.25a and b together would yield a dynamic mode very similar to that seen in Figure 6.23a. Similarly, Figures 6.25c-d, e-f and g-h can be put together to yield Figures 6.23b, c and e respectively. This gives a qualitative indication that the DMD can indeed be carried out on separate parts of the jet, without significantly altering the structures identified by the decomposition.

6.4 Summary and Conclusions

This chapter is concerned with LES of horizontally injected buoyant (heavier than the ambient) turbulent jets. This configuration has been studied less extensively, as compared to the non-buoyant and vertically buoyant jet configurations, and is marked by the simultaneous presence of stable stratification on one side and unstable stratification on the other side of the jet centerline. A previously validated high-order numerical method and Sigma SGS model [41] have been used. The numerical methodology has been further validated by performing simulations of non-buoyant and horizontally buoyant turbulent jets, and comparing to published experimental results.
Figure 6.24. DMD analysis of horizontal buoyant jet at $Re = 3200$, $Ri = 0.01$. (a) spectrum in stable stratification, (b) spectrum in unstable stratification, (c) amplitudes in stable stratification, and (d) amplitudes in unstable stratification. 4 representative modes are marked in all plots.
Figure 6.25. Representative dynamic modes of horizontal buoyant jet at $Re = 3200$ and $Ri = 0.01$. Stable stratification on the left and unstable stratification on the right. (a) $\lambda = (0.006, 0.000)$, (b) $\lambda = (0.00, 0.00)$, (c) $\lambda = (0.01, 1.11)$, (d) $\lambda = (-0.005, 1.13)$, (e) $\lambda = (0.03, 1.89)$, (f) $\lambda = (0.015, 1.83)$, (g) $\lambda = (-0.04, 3.58)$, and (h) $\lambda = (0.002, 3.71)$. 
In the non-buoyant case, the present results on the jet centerline velocity decay, radial spread, and self-similarity of mean velocities and turbulent fluctuations agree well with previous experimental results. In the buoyant jet case, although qualitatively similar, some discrepancies are observed between experimental results and results from the present LES study. Specifically, the velocity decay rate has been found to be dependent on the Richardson number, $R_i$, in contrast to the experiments. The velocity and scalar radial half-widths in stable and unstable stratification are predicted reasonably accurately, with the half-widths in unstable stratification being larger than in stable stratification. The jet trajectory, the axial evolution of the vertical velocity, the self-similar behaviour of the mean axial velocity profile, and predictions of turbulent production and dissipation agree well with the experiments, while the prediction of buoyant production in the TKE equation is qualitatively correct. All the discrepancies may be attributed to the artificial boundary conditions imposed at the inlet plane, in particular, the small co-flow and the random forcing applied in order to trigger an early transition to turbulence.

The Richardson number has a significant effect on the jet trajectory, with the vertical deflection increasing with increasing $R_i$. The total spread of the jet, as well as the anisotropy in the radial growths in stable and unstable stratification regions, increase with increasing $R_i$. Turbulent fluctuations are sensitive to $R_i$ as well, with $\langle u' u' \rangle$ and $\langle v' v' \rangle$ increasing mainly in the stable stratification region, while $\langle w' w' \rangle$ increases mainly in the unstable stratification region. The Reynolds number, $Re$, has no effect on the total radial spread, the jet trajectory, and the turbulent fluctuations, while it significantly affects the anisotropy between radial growths in stable and unstable stratification regions.

Closer to the inlet nozzle, too, horizontal buoyant jets reveal differing phenomena in stable and unstable stratification regions. Coherent vortex rings are consistently observed on the upper, stably stratified, side of the jet, while intermittent coherent vortices and small scale structures are observed on the lower, unstably stratified, part of the jet. The jet core acts similar to a cold cylinder placed in warmer environ-
ment, occasionally shedding vortices from the lower side, which feed a plume directed vertically downward. Finally, a dynamic mode decomposition on the whole jet, and considering the stably stratified and unstably stratified regions individually, reveals that the unstably stratified region has a larger energy content along with larger number of unstable modes.

These simulation results reveal the physical mechanisms which lead to suppressed and enhanced levels of mixing, brought about by the addition of buoyancy force, to a relatively simple flow configuration, thus furthering our understanding of the interactions between buoyancy and turbulence.
7. SUMMARY AND FURTHER WORK

7.1 Summary

This thesis has been concerned with issues related to large eddy simulation (LES) of buoyancy-driven or stratified turbulent flows. Only small differences in density have been considered, since this situation is widely encountered in atmospheric, oceanic, and turbulent flows of engineering interest. Fluid flows occurring under the effect of small density differences are governed by the so-called incompressible Boussinesq Navier-Stokes equations. These equations are the standard Navier-Stokes equations with a body force term, which depends linearly on a transported scalar. The scalar, which may be the concentration of a particular species, or the temperature of the fluid, is, in turn, governed by its own transport equation. LES of these flows are then governed by the filtered version of the incompressible Boussinesq Navier-Stokes equations, involving subgrid-scale (SGS) stress tensor and SGS scalar flux. The term ‘scalar’ has been used interchangeably, with a ‘species concentration’ (or simply, species), or ‘temperature’ throughout the thesis.

The issue of modeling the SGS scalar flux term has been studied chiefly in this thesis. Extensive LES have been carried out to study the behaviour of different SGS models in a posteriori evaluation. Direct numerical simulations (DNS) have also been carried out, and employed in a priori studies of SGS models. Improvements to various aspects of existing SGS models have been proposed and evaluated. This thesis has also delved into application of the LES technique for studying novel physical aspects of some buoyant turbulent flows. The problems studied include wall-bounded (thermal-driven cavity), as well as free-shear (horizontal jet), buoyant turbulent flows.

In the first part of this thesis, eddy-viscosity SGS models based on the Smagorinsky [103], Vreman [114] and Sigma [72] kernels have been studied in addition to
one non-eddy-viscosity type, Stretched Vortex [88], model. The model coefficients have been determined using appropriate local or global dynamic procedures with the Smagorinsky and Vreman kernels respectively, while the constant coefficient form of the Sigma model has been used. The kernels for SGS diffusivity in all these eddy-viscosity type models are identical to the velocity kernels. The model coefficient for SGS diffusivity is related through dynamically determined SGS Prandtl numbers for the Smagorinsky and Vreman models, and a constant SGS Prandtl number for the Sigma model.

The properties of these existing models have been tested in Chapter 3 by performing LES of the flow in a thermal-driven cavity, and comparing to results obtained using DNS. The constant coefficient Smagorinsky model was found to be too diffusive, while the constant coefficient Vreman model was found to be unstable due to inadequate dissipation. Excellent predictions were obtained with the dynamic Smagorinsky and constant coefficient Sigma models, while the dynamic Vreman model could not match predictions to DNS data. This study indicates that the Sigma kernel is superior to both Smagorinsky and Vreman kernels, since it yields excellent results without dynamic procedures, either for the model coefficient, or for the SGS Prandtl number. The results obtained using dynamic Vreman model, despite the superior theoretical formulation of the Vreman kernel, indicate that the global dynamic procedure may not be appropriate for modeling buoyant turbulent flows. The results also suggest that an improved kernel for the SGS diffusivity could possibly lead to improvements in the model performance.

Based on the results obtained in Chapter 3, an improved model for the SGS diffusivity has been proposed, which introduces an explicit dependence of the SGS diffusivity on the active scalar field. The Vreman kernel, $\Pi^g$, has been supplemented by the kernel $\Pi^T$, which theoretically makes the SGS diffusivity more sensitive to the resolved temperature or scalar field. An improvement has also been suggested to the global dynamic procedure for determining the model coefficient for the SGS viscosity, $C_V$. This improvement ensures that the contribution of the buoyant force
in evaluating $C_V$ is not neglected. These improved models have been tested for the thermal-driven cavity test case in Chapter 4. However, no significant improvement in results over the baseline dynamic Vreman model was obtained. Nevertheless, these modified forms of Vreman model, and especially the modified global dynamic procedure, should be utilized in simulations of buoyant turbulent flows. Further evaluation of these models, in other test problems, can also be carried out.

In direct continuation on the theme of subgrid scale modeling of the SGS scalar flux in buoyant turbulent flows, the second part of the thesis deals with evaluation of non-eddy-viscosity SGS models, in addition to the three eddy-viscosity models studied in the previous two chapters. In Chapter 5, the non-eddy-viscosity Dynamic Structure model [20, 21], and two variants of the Gradient model [67, 66], have been considered. The standard pseudo-spectral method, which offers high accuracy and efficiency, has been used to carry out DNS of homogeneous turbulent flows. A database encompassing three different flow situations - stationary and decaying isotropic turbulence with a passive scalar, and decaying anisotropic buoyant turbulence with an active scalar - has been generated. This database has been well validated with previous similar simulation results. A priori investigations reveal that the primary disadvantage of eddy-viscosity models is the non-alignment, in 3D space, between the modeled and actual SGS scalar fluxes. Eddy-viscosity model magnitude predictions have been shown to be pretty accurate. A similar evaluation of the Dynamic Structure and the Gradient models reveals that these are good at predicting the orientation, as well as the magnitudes, of the SGS scalar fluxes. However, it has been pointed out that these models are not realizable in an actual a posteriori LES run without additional transport equations. The Modulated Gradient model has been shown to be less accurate at predicting the SGS scalar flux magnitude, as compared to the eddy-viscosity models. Based on these observations, four new models, (termed Smagorinsky-Gradient (SGM), Vreman-Gradient (VGM), Smagorinsky-Structure (SSM) and Vreman-Structure (VSM) models) have been proposed, which are realizable in actual LES without requiring additional models or transport equa-
tions. A preliminary \textit{a posteriori} study has been carried out to confirm that the SGM model is more accurate than the realizable Modulated Gradient model.

Finally, Chapter 6, which comprises the last part of this thesis, is devoted to studying the physics of a novel horizontally injected buoyant jet configuration. This study has been motivated by the recent experiments by Xu and Chen [123]. Previous non-buoyant [49] and buoyant [123] jet experimental results have been accurately reproduced, using a constant coefficient Sigma model. The experimental results have been subsequently supplemented with LES results at different flow configurations. In agreement with previous studies, it is shown that the horizontal buoyant jet is characterized by regions of stable stratification on one side of the jet centerline, and unstable stratification on the other. A systematic variation of the governing non-dimensional parameters reveals that the Richardson number controls most of the jet properties such as vertical deflection, radial spread and turbulent energetics, all of which, are largeley independent of the Reynolds number. The horizontal buoyant jet is also marked by an asymmetry in radial spread and mixing between the stable and unstable stratification regions, and the Reynolds number has been shown to drastically affect this asymmetry. This asymmetry has also been pointed out via a dynamic mode decomposition of the horizontal buoyant jet. This asymmetry may be attributed to the intermittent breakdown of coherent vortex rings in unstable stratification into small-scale structures, and the jet core behaving like a cold cylinder placed in warmer surroundings.

The first two parts of this thesis have dealt with evaluation and development of different approaches for modeling the subgrid scale scalar flux. It may be concluded that the Sigma model is the best eddy-viscosity type model, and that Smagorinsky-Gradient and the other three newly proposed non-eddy-viscosity models also yield accurate simulations. In the third part of this thesis, the constant coefficient Sigma model has been employed to study the asymmetric structure of the horizontal buoyant jet flow configuration. The principal contributions of this work are:
• Evaluation of three eddy-viscosity SGS models and one non-eddy-viscosity model in large eddy simulation of three-dimensional thermal-driven cavity, with respect to DNS data, along with an extensive study of the physics of the three-dimensional thermal-driven cavity, Ghaisas et al. [41].

• Proposed modifications to the global dynamic procedure for determining the model coefficient in LES of buoyant turbulent flows, and a modified form of the kernel for SGS diffusivity.

• A priori evaluation of different sophisticated models for SGS scalar flux, based on data generated from DNS of different homogeneous turbulent flows; Proposed four new models combining magnitudes from Smagorinsky and Vreman eddy-viscosity models, and orientations from Dynamic Structure and Gradient models, Ghaisas and Frankel [39].

• LES study of novel horizontal buoyant jet, validation with experimental results, and identification of physical mechanisms responsible for asymmetry between the stably and unstably stratified regions, Ghaisas et al. [40].

7.2 Future work

The individual studies undertaken as part of this thesis can be pursued further in the following directions:

• Study of the physics of thermal-driven cavity of different aspect ratios, and at larger values of Rayleigh numbers, using LES.

• Evaluation of the $\Pi^T$ model and the modified global dynamic procedure in different test cases. Further development of the idea that the kernel for SGS diffusivity be explicitly dependent on the resolved scalar field, in addition to the resolved velocity field.
• Exhaustive *a posteriori* evaluation of the four new proposed models in homogeneous and inhomogeneous (e.g. neutrally, stably and unstably stratified channel flow) situations, and *a priori* investigations based on inhomogeneous turbulent flow data.

• Further investigations into the near-nozzle flow structure in horizontal buoyant jets, and studies such as LES of horizontal jets issuing into a stably stratified ambient.
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