FIELD EXPERIMENTAL STUDY OF
THE SMAGORINSKY MODEL AND
APPLICATION TO LARGE EDDY
SIMULATION

by

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Abstract

Large-eddy simulation (LES) has become an indispensable tool for prediction of turbulent atmospheric boundary layer (ABL) flow. In LES, a subgrid-scale (SGS) model accounts for the dynamics of the unresolved scales of motion. The most widely used SGS model is an eddy-viscosity closure, the Smagorinsky model, which includes a parameter that must be prescribed in some fashion, the Smagorinsky constant $c_s$. In this dissertation, $c_s$ is measured in a specifically designed field experiment. And, the ability of so-called dynamic SGS models to predict $c_s$ is studied based on the data obtained, as well as in numerical simulations.

In the field study, two vertically separated horizontal arrays of 3d-sonic anemometers are placed in the atmospheric surface layer. Results indicate that $c_s$ is reduced when the integral scale of turbulence is small compared to the grid or filter scale, such as near the ground and in stable atmospheric conditions. The field data are processed further to test whether dynamic SGS models can predict the correct coefficient values. In the scale-invariant dynamic model (Germano et al. 1991), the coefficient is derived from various data test-filtered at a larger scale assuming that $c_s$ is the same as at scale $\Delta$. The results show that $c_s$ is significantly underpredicted whenever $\Delta$ is larger than the large-scale limit of the inertial range. The scale-dependent dynamic model (Porté-Agel et al. 2000b) uses a second test-filter to deduce the dependence of $c_s$ on filtering scale. This model provides excellent predictions of $c_s$ and its dependence upon stability and height.

Large eddy simulations of flow over a homogeneous surface with a diurnal heat flux forcing are conducted to study the prediction of $c_s$ over a wide range of stabilities in a numerical framework. The scale-invariant and scale-dependent Lagrangian dynamic SGS model are tested and compared to the field data. Consistent with the field studies, the prediction of $c_s$ from the scale-invariant model is too small, whereas the scale-dependent coefficients are more realistic. The simulation also yields new results: $c_s$ exhibits hysteresis behavior in the mixed layer. It is found that in unstable conditions, neither a surface layer parameter (Obukhov length) nor other stability parameters (gradient Richardson number) could uniquely characterize $c_s$ there. Thus, we conclude
that the dynamic model, which does not require such ad-hoc characterizations, is an attractive parameterization strategy for LES of ABL.

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Chapter 1

Introduction

1.1 Atmospheric boundary layer turbulence

The earth’s atmosphere sustains most life on our planet. Its chemical composition protects us from excessive solar radiation, it enables life by absorbing infrared solar radiation (greenhouse effect), and it mixes aerosols and heat efficiently from the ground into larger altitudes. The lower part of the atmosphere can be subdivided into the troposphere and the stratosphere. The stratosphere contains gases with absorption peaks in the UV-spectrum, e.g. ozone and water vapor, which causes the potential temperature to increase with height. Below, the troposphere reaches up to 10 km above the earth’s surface. In the troposphere the potential temperature decreases with increasing altitude (see Wallace and Hobbs 1993 for a general review).

The atmospheric boundary layer (ABL) is defined as “that part of the troposphere that is directly influenced by the presence of the earth’s surface, and which responds to surface forcings with a timescale of about an hour or less” (Brutsaert 1982, Stull 1997). The diurnal cycle of the ABL is illustrated in Stull (1997, p. 11). The upper limit is defined by the inversion layer at ~ 1 km, where the positive potential temperature gradient and the corresponding stable stratification suppress vertical exchange. Above the inversion height the free atmosphere is driven by geostrophic winds induced by large scale pressure gradients. Below the inversion height the ABL is typically
broken into the mixed layer (above \(\sim 100 \text{ m}\)) and the surface layer (below \(\sim 100 \text{ m}\)). The surface layer (or “logarithmic layer”, or “inner layer”) is strongly influenced by the heterogeneous earth surface. Due to the strong mixing in the ABL, contributions of different heterogeneous surface areas tend to diffuse with height, such that the mixed layer is more horizontally homogeneous than the surface layer.

Of particular interest for this thesis are the length scales of turbulence in the ABL. The Reynolds number describes the turbulence properties of a flow. It is defined as \(Re = \frac{uh}{\nu}\), where \(u\) is a velocity scale, \(h\) is a length scale and \(\nu = 1.5 \times 10^{-5} \text{ m}^2\text{s}^{-1}\) is the viscosity of air. Taking the boundary layer height and the average horizontal velocity in the numerator, the Reynolds number in the ABL is on the order of \(10^8\), suggesting a highly turbulent flow field. We study flow over a rough surface, parameterized by the roughness length \(z_0\). The flow structures which are responsible for the transport of momentum and scalars are called eddies. The maximum size of the eddies typically scales with the height above ground \(z\), whereas the minimum size is given by the Kolmogorov scale \(\eta = (\nu^3/\epsilon)^{1/4}\), which is on the order of 1 mm in the ABL (\(\epsilon\) is the dissipation rate). The structure of atmospheric turbulence also depends strongly on the atmospheric stability. The most important parameter, relating buoyancy to shear production terms in the budget of turbulent kinetic energy (Stull 1997), is the Obukhov length \(L\).

\[
L = \frac{-u_*^3 \rho}{\kappa g \left[ \frac{H}{c_p \theta_0} + 0.61E \right]} \approx \frac{-u_*^3}{\kappa \frac{g}{\theta_0} \langle w' \theta'^1 \rangle}.
\]  

Here \(u_* = (-\langle u'w' \rangle)^{1/2}\) is the friction velocity, \(\rho = 1.225 \text{ kg m}^{-3}\) is the density of air, \(H = \rho c_p \langle w' \theta' \rangle\) is the sensible heat flux, \(\theta_0\) is the mean air temperature, \(E = \rho L_v \langle w' q' \rangle\) is the water vapor flux, \(g\) is the gravitational acceleration and \(\kappa = 0.4\) is the von Kármán constant, \(c_p = 1004.7\) J kg\(^{-1}\) K\(^{-1}\) is the specific heat capacity of dry air, and \(L_v = 2440\) J g\(^{-1}\) is the latent heat of vaporization. Henceforth, \((x, y, z) = (x_1, x_2, x_3)\) will be used interchangeably for the coordinate system and \((u, v, w) = (u_1, u_2, u_3)\) is the velocity vector defined in this coordinate system. The vertical coordinate is denoted by \(z\) or \(x_3\), and \(w\) is the vertical velocity component. The angular
bracket \( \langle \rangle \) implies time, spatial, or ensemble averaging, depending on the context. Primes denote fluctuations.

A positive \( L \) occurs in a stable boundary layer, i.e. the temperature gradient is larger than the dry adiabatic lapse rate \((-g/C_p = -0.0098 \text{ K/m}, \text{ where } C_p \text{ is the specific heat at constant pressure for air})\). If \(|L| \to \infty\), this indicates neutral conditions, i.e. the temperature gradient is equal to the dry adiabatic lapse rate. An unstable boundary layer is given by \( L < 0 \) and a temperature gradient smaller than the dry adiabatic lapse rate. In stable conditions \( L > 0 \), and represents an integral length scale of the surface layer flow.

### 1.2 Filtered Navier-Stokes equations and Large Eddy Simulation

Computational simulations of atmospheric flows have a wide range of applications. The most well-known application is weather prediction, which uses relatively coarse numerical resolutions and attempts to predict synoptic scale phenomena (> 100 km). In this dissertation the focus is on mesoscale and microscale meteorology, with a horizontal scale of < 20 km. Even in simulations of mesoscale flow we encounter the problem that the computational performance of supercomputers is not sufficient to capture all scales of motion.

The degrees of freedom which are necessary in a simulation to represent all scales of motion can be estimated as follows: The domain, in which the computation is performed must be large enough to accommodate the largest turbulent scales. In the vertical direction the size of eddies is limited by the height of the boundary layer. In the horizontal direction autocorrelation analysis can be used to determine the integral scale of turbulence. Each dimension of the simulation domain should be at least twice the integral scale \( L_I \). The grid spacing has to be smaller than the smallest scales of motion, the Kolmogorov scale, \( \eta \), which depends on the Reynolds number. An estimate for the order of magnitude of the number of grid points in each direction is then given by \( L_I/\eta \). In the atmospheric boundary layer \( L_I \sim 1000 \text{ m} \), while \( \eta \sim 1 \text{ mm} \). Thus \( 2 \times 10^6 \) grid points are required in each direction using this simple estimate. Using a more general approach Tennekes and Lumley
(1972) show that $L_I/\eta$ is proportional to $Re_L^{3/4}$:

$$L_I/\eta = \frac{L_I}{\nu^{3/4} L_I^{1/4}} = \frac{L_I u'^3}{\nu^{3/4} L_I^{1/4}} = \left( \frac{u'L_I}{\nu} \right)^{3/4} = Re_L^{3/4},$$

(1.2)

where the standard large-scale dissipation estimate $\epsilon = u'^3/L_I$ has been used (Tennekes and Lumley 1972). In other words, the memory requirement scales like $Re_L^{9/4}$ for a 3-dimensional simulation. $Re_L$ is the Reynolds number based on the magnitude of the velocity fluctuations and the integral scale. In the ABL this requirement with $u' \sim 1.5 \text{ m s}^{-1}$ and $L_I = 1000 \text{ m}$ necessitates $10^6$ grid points for each dimension. With current processing speed and memory of supercomputers we are only able to represent and simulate $\sim 10^3$ points in each direction for a 3d flow. This problem has been addressed in different ways.

The most widely used approach in practice is Reynolds averaging of the Navier-Stokes equations (RANS). This approach involves the solution of the Reynolds equations to solve for the mean velocity field (averaged over time or ensembles). Thus, in RANS simulations, there is no explicit information on turbulent structures in the flow.

In the last thirty years an improved, but more computationally intensive approach has become more popular. Today this is the preferred computational approach to ABL research. Unlike RANS, Large Eddy Simulation (see e.g. Deardorff 1970; Moeng 1984; Nieuwstadt et al. 1991; Mason 1994; Andren et al. 1994; Lesieur and Métai 1996; Albertson and Parlange 1999, 2000) does explicitly simulate the larger scales of motion while modeling only the small scales. Specifically, Large Eddy Simulation (LES) resolves the transport equations for all scales of motion larger than the grid size $\Delta$, while the effects of the subgrid-, or subfilter-scales (smaller than $\Delta$) on the resolved field are parameterized using subgrid-scale (SGS) models. For definitions of SGS and subfilter-scale (SFS) quantities and a discussion of their differences see Carati et al. (2001). This scale separation is carried out at the grid size $\Delta$, scales larger than $\Delta$ are retained while scales smaller than $\Delta$ are discarded for the simulation. This operation can be achieved analytically by filtering the Navier-Stokes equations. A filtering operation is defined as
\[ \tilde{u}(x) = \int u(x') F_\Delta(x - x') dx', \quad (1.3) \]

where \( \tilde{u} \) is the ‘resolved’ velocity vector and \( F_\Delta \) is the (homogeneous) filter function for a scale \( \Delta \).

The velocity field \( U_i \) is represented as the sum of filtered (\( \tilde{u}_i \)) and sub-grid components (\( u_i \))

\[ U_i = \tilde{u}_i + u_i, \quad i = 1, 2, 3 \quad (1.4) \]

The filtering operation is applied to the Navier-Stokes equations

\[ \partial_t U_i = 0 \quad (1.5) \]
\[ \partial_t U_i + \partial_j U_i U_j = \nu \partial_j \partial_j U_i + \frac{1}{\rho} \partial_t p' - g \frac{\theta'}{\theta_0} \delta_{i3} + f_i \quad (1.6) \]

to yield

\[ \partial_t \tilde{u}_i = 0 \quad (1.7) \]
\[ \partial_t \tilde{u}_i + \partial_j \tilde{u}_i \tilde{u}_j = \nu \partial_j \partial_j \tilde{u}_i - \frac{1}{\rho} \partial_t \tilde{p}' - g \frac{\theta'}{\theta_0} \delta_{i3} + \tilde{f}_i - \partial_j \tau_{ij} \quad (1.8) \]

Here \( \tilde{\cdot} \) denotes a filtered variable, \( g \) is the gravitational acceleration, \( p \) is the pressure, \( j = 1, 2, 3, \) and the Einstein summation rules apply. External forcing is applied through \( f_i \), which is typically a streamwise pressure gradient. The Boussinesq approximation (see Stull, 1997, pp. 83-85) has been used such that a prime denotes fluctuations of temperature and pressure around the mean state (hydrostatic equilibrium). \( \tau_{ij} \) is the subgrid scale stress tensor,

\[ \tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j, \quad (1.9) \]

Further manipulations of these equations include the removal of the trace of \( \tau_{ij} \) to yield \( \tau_{ij}^d \) (the
deviatoric part of the subgrid-scale stress tensor),

\[ \tau_{ij}^d = \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} \]  

(1.10)

and the addition of this trace and the gradient of resolved kinetic energy \((\frac{1}{2} \partial_j \tilde{u}_j \tilde{u}_j)\) to the pressure term, yielding the modified pressure \(\tilde{p}^* = \tilde{p}/\rho + \frac{1}{3} \tau_{kk} + \frac{1}{2} \tilde{u}_j \tilde{u}_j\). This allows writing the convective term in the rotational form (Orszag and Pao 1974). Finally, the viscous term is neglected which can be justified in these high Reynolds number flows. Now Eq. 1.8 becomes

\[ \partial_t \tilde{u}_i + \tilde{u}_j (\partial_j \tilde{u}_i - \partial_i \tilde{u}_j) = -\partial_i \tilde{p}^* + \tilde{f}_i - g \frac{\tilde{\theta}'}{\theta_0} \delta_{i3} - \partial_j \tau_{ij}^d \]  

(1.11)

For more details on the derivation see Galperin and Orszag (1993). In LES, one must model the SGS stresses \(\tau_{ij}^d\), which are three-dimensional, time-dependent, turbulent fields with stochastic character and display a number of interesting statistical properties (for a review, see Meneveau and Katz 2000). Different models for \(\tau_{ij}\) will be discussed in the next chapter.

### 1.3 Eddy viscosity subgrid-scale models and energy dissipation

The realism of the SGS model is essential for the ability of LES to provide realistic turbulent fields in the ABL, especially in regions close to the lower boundary. There the local integral scale is on the order of the distance from the boundary, \(z\), and thus \(\Delta/z > 1\). Hence, the SGS model must represent the momentum fluxes carried by most of the eddies, even the large, energy-containing ones. The most commonly employed parameterization for the SGS stress is the Smagorinsky model (Smagorinsky 1963):

\[ \tau_{ij}^{\text{Smag}} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2 \nu_T \tilde{S}_{ij}, \quad \nu_T = (c_s \Delta)^2 \left| \tilde{S} \right|. \]  

(1.12)

\(\tilde{S}_{ij} = 0.5 (\partial \tilde{u}_i/\partial x_j + \partial \tilde{u}_j/\partial x_i)\) is the strain rate tensor and \(|\tilde{S}| = \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}}\) is its magnitude, \(\nu_T\) is the eddy viscosity, and \(c_s\) is the Smagorinsky coefficient, which in traditional LES is prescribed based on phenomenological theories of turbulence or adjusted empirically. The product of Smagorinsky
coefficient and filter scale is a mixing-length often denoted by \( l = \Delta c_s \). For a recent review of the Smagorinsky model and other SGS models see Meneveau and Katz (2000). As also discussed in this review, the magnitude of \( c_s \) determines the effectiveness with which kinetic energy is dissipated out of the resolved velocity field during LES. The mean rate of kinetic energy transfer from the resolved to the subgrid range of scales (the so-called SGS dissipation) is given by

\[
\langle \Pi^{\text{meas}} \rangle = -\langle \tau_{ij} \tilde{S}_{ij} \rangle,
\]

where \( \langle \rangle \) denotes ensemble or time averaging, depending on the context. The rate that results from replacing \( \tau_{ij} \) with the Smagorinsky model is given by

\[
\langle \Pi^{\text{Smag}} \rangle = 2 (c_s \Delta)^2 \langle |\tilde{S}_{ij} \tilde{S}_{ij}| \rangle.
\]

By requiring that \( \langle \Pi^{\text{meas}} \rangle = \epsilon = \langle \Pi^{\text{Smag}} \rangle \) (where \( \epsilon \) is the molecular dissipation rate), Lilly (1967) analytically derives a value of \( c_s \) of approximately 0.16 - 0.20 (the exact value depends on the filter shape and the Kolmogorov constant). His main assumption is the application of a filter operation at a scale \( \Delta \) that falls within an idealized inertial subrange of turbulence with energy spectrum

\[ E(k) = \alpha \varepsilon^{2/3} k^{-5/3} \]

to evaluate \( \langle |\tilde{S}_{ij} \tilde{S}_{ij}| \rangle \). This derived value of \( c_s \) exceeds significantly what LES calculations require to yield realistic results, especially close to the ground (Deardorff 1970; Moin and Kim 1982; Mason and Thomson 1992; Sullivan et al. 1994). As is widely recognized, near the ground \( \Delta \) approaches or exceeds energy containing scales and hence the basic assumption of Lilly (1967) breaks down.

Wall-blocking effects are known to cause a reduction in the coefficient when approaching the ground. Mason (1994) proposes to match the basic mixing length of the Smagorinsky model in the interior of the ABL, \( l_0 = c_0 \Delta \), with rough-surface expressions for the eddy viscosity \( \nu_T = \)
\( \kappa^2 (z + z_0)^2 \partial(u)/\partial z \) near the ground. Mason’s (1994) modified mixing length \( l \) reads:

\[
l = \left( \frac{1}{[\kappa(z+z_0)]^n} + \frac{1}{l_0^n} \right)^{-1/n}.
\] (1.15)

Thermal stratification also influences the SGS energy spectrum of turbulence, which in turn violates Lilly’s assumption of a long inertial subrange in deriving \( c_s \). In particular, the coefficient has to be decreased in stably stratified conditions. This trend is reflected in Deardorff’s (1980) empirical model, as well as in the model of Brown et al. (1994), who derive a stability-dependent model from the SGS energy equation assuming a state of local equilibrium. Canuto and Cheng (1997) employ a two-point closure to construct the SGS energy spectrum under the influence of shear and buoyancy. From the SGS energy spectrum they derive an analytical expression for the reduction of \( c_s \) under shear and buoyancy. Like stratification, the presence of mean shear also requires decreasing the Smagorinsky coefficient.

Similarly to the filtered momentum equations, the filtered scalar transport equations (e.g. heat equation) in LES include an additional term, the SGS scalar flux. The SGS heat flux is defined according to

\[
q_i = \tilde{\theta} \tilde{u}_i - \tilde{\theta} \tilde{u}_i,
\] (1.16)

where \( \theta \) is the temperature field. In the Smagorinsky, or eddy-diffusivity model, \( q_i \) is parameterized as

\[
q_i^{\text{Smag}} = -Pr_T^{-1} c_s^2 \Delta^2 \left[ S \frac{\partial \tilde{\theta}'}{\partial x_i} \right],
\] (1.17)

where \( Pr_T \) is the turbulent SGS Prandtl number, and \( \tilde{\theta} \) is the filtered temperature field. The prime indicates fluctuating quantities around the average \( \langle \tilde{\theta} \rangle = \langle \tilde{\theta} \rangle + \tilde{\theta}' \). The mean SGS dissipation of scalar variance \( \langle \chi^{\text{meas}} \rangle \) is usually defined as

\[
\langle \chi^{\text{meas}} \rangle = -\langle q \frac{\partial \tilde{\theta}'}{\partial x_i} \rangle.
\] (1.18)
Lilly’s analysis applied to a scalar variance spectrum in isotropic, neutral turbulence led to an estimate of the Prandtl number of about 0.5 for the Smagorinsky model (Mason 1994). Laboratory experimental investigations in the wake of a heated cylinder (Kang and Meneveau 2002) resulted in \( Pr_T \approx 0.3 \). As part of the present study we will also examine how \( Pr_T^{-1} c_s^2 \) (and \( Pr_T \)) depend on distance to the ground, flow stability, and averaging time-scale.

It is worthwhile to delineate that in this dissertation we restrict our attention to the basic structure of the eddy-viscosity Smagorinsky closure. This closure is based on the assumption that the SGS stresses and fluxes are aligned to the gradients of velocity and temperature. The drawbacks of this assumption have already been documented extensively in the literature: As reviewed in Meneveau and Katz (2000) and Tao et al. (2002) in the context of experimental studies in laboratory turbulence, the alignment hypothesis is not accurate. In the context of ABL turbulence, Higgins et al. (2003, 2004) confirm this limitation and show that addition of a so-called tensor eddy-diffusion model improves the alignment trends. Moreover, near the ground, Tong et al. (1999) show that the streamwise accelerations inherent in the eddy-viscosity closures cause unphysical couplings with the resolved velocity field. Moreover, Mason and Thomson (1992) argue that the SGS models must represent stochastic fluctuations of the unresolved stresses. Even with these limitations, the deterministic eddy-viscosity closure is still the most-often used in practical applications, providing continued interest in the dependence of \( c_s \) on physical flow parameters as studied here.

1.4 Experiments for the evaluation of subgrid-scale quantities

In order to determine subgrid-scale (SGS) quantities such as \( \tau_{ij}, \tilde{S}_{ij}, \) and \( c_s \) in field experiments, velocity fields need to be filtered in three dimensions in space (Eq. 1.3). Theoretical and computational analysis has shown that 2d filtering is a good approximation to 3d filtering. Tong et al. (1998) estimate that near the surface 2d filtering “removes wavenumber modes that contribute to more than 85% of variance of the SGS fluctuations”. They demonstrate from high resolution LES
data that 2d and 3d filtered fields are indistinguishable. From DNS data of turbulent channel flow, Murray et al. 1996 obtain a criterion of $y^+ > 10$ for the equivalence of 2d and 3d filtering. Specifically designed field experiments with horizontal arrays of high frequency sensors in the atmospheric boundary layer enable the SGS physics to be studied from variables filtered in 2d horizontal planes using Taylor’s hypothesis. In the vertical direction, typically only two heights are sampled. This resolution is not sufficient for filtering. As reviewed in Meneveau & Katz (2000), there also exist measurement techniques that do not require Taylor’s hypothesis. Particle Image Velocimetry (PIV) has been used in engineering flows. In atmospheric sciences radar and LIDAR (light detection and ranging) are being developed to get 3d information on the flow. These techniques still face many drawbacks and do not permit the necessary high resolution for turbulence measurements (ideally $\sim 3 \times 10^3 \text{ Hz} \sim U_c/\eta$, where $U_c$ is the turbulence convection velocity). In experiments analyzed in this thesis, 3d sonic anemometers are deployed, which are able to measure all three components of the velocity vector and the potential temperature. The sampling rate is up to 60 Hz, which is sufficient to resolve the energy containing scales and significant portions of the inertial range.

In the context of LES of the atmospheric boundary layer, a number of field studies have aimed at measuring $q_i$ and $\tau_{ij}$ from field data and at analyzing the results to improve SGS modelling. A study using data from a single 3d-sonic anemometer (Porté-Agel et al. 1998) restricted the analysis to 1d filtering (time-filtering and interpreting the results as spatial filtering in the $x_1 = x$ direction using Taylor’s hypothesis). Tong et al. (1998) proposed deploying a horizontal array of sensors and examined filtering issues using LES data. Their results showed that filtering in two horizontal directions was required for quantitatively more accurate results. Experimental results from one horizontal array of sensors using 2d filtering were reported in Tong et al. (1999), and Porté-Agel et al. (2000a). The latter paper showed that while filter dimensionality did not have a strong effect on the previously reported trends based on 1d filtering, atmospheric stability had strong effects on the results. Limiting the setup of Porté-Agel et al. (2000a) was the inability to compute vertical derivatives. This issue was addressed by using two vertically displaced horizontal arrays as proposed in Tong et al. (1999), and also in the Davis 1999 experiment (Porté-Agel et al. 2001a). As described
in chapter 2.2, a similar setup is used in the Horizontal Array Turbulence Study (HATS, Fig. 1-1) now including two more anemometers, and including more data under stable stratification, due to prevailing wind conditions at night.

In order to become familiar with measured physical quantities and scales of motion in these experiments it is instructive to look at the data in horizontal planes (Fig. 1-2 for the HATS experiment). In the $x$ direction there are nine data points (nine sonics) for the lower height ($z_d = 3.45$ m). The time series of all sonics are plotted in the $y$ direction. A correlation between $u_3$ and $\theta$ is observed. In this unstable situation (daytime) hot air from the ground is transported upwards, while colder air from above is mixed down to the ground. In addition there is an anti-correlation between $u_1$ and $u_3$, which follows from mass continuity. From this type of data the SGS stresses and their model predictions can be obtained experimentally by filtering the signals and by appropriate post-processing, in order to address the research questions outlined in the section below.
Figure 1-2: Horizontal contour plots of streamwise velocity, vertical velocity, and temperature at $z_d = 3.45$ m on September 6, 2000, 1603h PST in Kettlemen City, CA.

1.5 Research Questions

This dissertation addresses research questions related to SGS modeling in LES. In particular, the Smagorinsky coefficient is measured from atmospheric field data and $a$ priori and $a$ posteriori tests of dynamic SGS models are performed. An $a$ priori test “uses experimental or DNS data to measure directly the accuracy of a modeling assumption, for example, the relation for the residual-stress tensor (...) given by the Smagorinsky model” (Pope 2000, p. 601). In $a$ posteriori tests, “the model is used to perform a calculation for a turbulent flow, and the accuracy of calculated statistics (e.g. $\langle U \rangle$ (...) is assessed, again by reference to experimental or DNS data. It is natural and appropriate to perform $a$ priori tests to assess directly the validity and accuracy of approximations being made.
However, for the LES approach to be useful, it is success in *a posteriori* tests that is needed.” (Pope 2000, p.601). Through this research the following questions are addressed:

- Can SGS model coefficients be measured accurately from field measurements with horizontal arrays of sonic anemometers in the atmospheric surface layer?

- Which turbulence length scales does $c_s$ depend on? Investigators have proposed that $c_s$ decreases in stable conditions and near the surface (Deardorff 1980, Brown et al. 1994, Canuto and Cheng 1997). Can these trends be confirmed and quantified from the field data?

- Do dynamic SGS models predict the correct $c_s$ under different flow conditions when tested *a priori* in field experiments? It is known that the scale-invariance assumption in the classic dynamic SGS model (Germano et al. 1991) causes an underprediction of $c_s$ near the wall. Does the scale-dependent dynamic model (Porté-Agel et al. 2000b) improve the prediction?

- Is the prediction for $c_s$ of dynamic SGS models in LES similar to the results from the field experiment? Do these SGS models improve turbulence properties such as non-dimensional velocity gradients *a posteriori*?

- How does the coefficient of the eddy viscosity model for the SGS heat flux depend on turbulence length scales?

1.6 Outline of the thesis

This thesis is organized as follows: Chapter 2 is dedicated to measuring and characterizing $c_s$ from the field data. In chapter 2.2, the field experiment and the data set used in the present study are described. Chapters 2.3 - 2.7 describe the results on the magnitude of the measured $c_s$ as a function of atmospheric stability, distance to the ground, and local strain-rate magnitude. A similar analysis for the SGS heat flux is also presented. In chapter 3 it is determined whether the scale-invariant dynamic model and the scale-dependent dynamic model can predict the correct $c_s$ under different stability conditions and heights. Chapter 4 presents the application of these
dynamic models to Large Eddy Simulation of atmospheric flow forced by a diurnal cycle of surface heat flux. A summary and conclusions are presented in chapter 5.
Chapter 2

Magnitude and Variability of subgrid-scale eddy-diffusion coefficients in the atmospheric surface layer

2.1 Introduction

In this chapter we process data from field experiments using the horizontal array technique presented briefly in chapter 1.4 to measure $c_s$ under flow conditions prevalent in the atmospheric surface layer. In order to measure $c_s$ under flow conditions that are more general than the isotropic conditions of Lilly’s (1967) original derivation, his theoretical approach can be applied to analysis of experimental data by setting the dissipation from the Smagorinsky model equal to the real measured SGS dissipation, i.e. by setting $\langle \Pi^{\text{meas}} \rangle = \langle \Pi^{\text{Smag}} \rangle$. An empirically measurable SGS dissipation-based Smagorinsky coefficient can thus be defined as follows:

$$c_s^2 = -\frac{\langle \tau_{ij} \tilde{S}_{ij} \rangle}{\langle 2\Delta^2 \tilde{S}^2 \tilde{S}_{ij} \tilde{S}_{ij} \rangle}.$$  

(2.1)

This approach was pioneered by Clark et al. (1979) for the analysis of data from Direct Numerical Simulations (DNS). As reviewed in Meneveau and Katz (2000), since then many studies have used
this criterion to compute $c_s$.

In this chapter we aim at deriving, from the field data, empirical relationships for $c_s$ as a function of relevant parameters such as distance to the ground, strength of thermal stratification, and strain-rate magnitude. The distance to the ground, $z$, can be normalized with the filter scale, $\Delta$, yielding the parameter $\Delta/z$. Stratification can be characterized using the Obukhov length $L$, defined in Eq. 1.1. The dimensionless parameter comparing the filter scale to $L$ is $\Delta/L$. The local strain-rate will be quantified by $|\tilde{\mathbf{S}}|$, the magnitude of the strain-rate tensor already defined in Eq. 1.12. It can be normalized with a velocity scale and a length scale. The proper choice of velocity and length scales depends on whether $\Delta$ falls inside or outside the inertial range.

In addition to the dependence of $c_s$ on these parameters, the great variability of turbulence dynamics in general, and of atmospheric dynamics in particular, raises the issue of how the averaging procedures needed in evaluating terms in Eq. 2.1 should be performed, and how meaningful the results are. Variability in $c_s$ is caused by the inherent intermittency of turbulence, and of ABL flow patterns in particular. It is well known that the SGS dissipation $\Pi^{\text{meas}}$ in turbulence is highly intermittent. This was already shown for isotropic turbulence using DNS by Cerutti and Meneveau (1998) and for the ABL in the context of the SGS dissipation of scalar variance by previous experiments described in Porté-Agel et al. (2000a, 2001a, 2001b). To examine the effects of intermittency upon eddy-viscosity coefficients, the averages in the numerator and denominator of Eq. 2.1 can be computed over different time scales $T_c$. Then $c_s$ is no longer a single value but fluctuates from one time-period (of length $T_c$) to another. We wish to examine how this variability is affected by varying $T_c$ under different flow conditions. Moreover, in LES using the Lagrangian dynamic model (Meneveau et al. 1996), one needs to prescribe a time scale. This time scale is used in that model to set the duration of averaging over the history of turbulence following fluid trajectories.

The scalar eddy-diffusion coefficient can be determined from experimental data using the criterion that the mean modelled SGS dissipation of scalar variance $\langle \chi^{\text{mod}} \rangle = -\langle \bar{q}_i \partial \tilde{\theta} / \partial x_i \rangle$ matches
the mean measured SGS dissipation of scalar variance \( \langle \chi^{\text{meas}} \rangle \):

\[
P r_T^{-1} c_s^2 = \frac{\langle \partial_t \tilde{\theta}' \partial_x \tilde{\theta}' \rangle}{\langle \Delta^2 \tilde{S} \rangle}.
\] (2.2)

The Prandtl number can be obtained by dividing the result for \( c_s^2 \) from Eq. 2.1 by \( P r_T^{-1} c_s^2 \).

It is important to note that in this work the coefficient is measured based on the condition of SGS energy and scalar variance dissipation equivalence (Eqs. 2.1 and 2.2). While it is often argued that this is the most important condition (Meneveau and Katz 2000), we recall that accurate prediction of SGS dissipation is only one of many possible conditions with which an SGS model should comply.

As enumerated in Meneveau (1994) and Pope (2000, p. 603) several other statistics are of interest, such as dissipation of enstrophy, or wave-number dependent spectral transfer leading to spectral eddy-viscosity (Cerutti et al. 2000). In fact, in the context of near-surface ABL flows where the SGS stress carries a significant fraction of the total vertical fluxes of momentum, an additional condition could be that the modelled SGS shear-stress equals the real one. An alternative definition of the Smagorinsky coefficient, named \( c_s^{\text{mom}} \), which satisfies the condition of equivalence of vertical fluxes of momentum would read

\[
(c_s^{\text{mom}})^2 = -\frac{\langle \tau_{13} \rangle}{\langle 2\Delta^2 \tilde{S} \tilde{S}_{13} \rangle},
\] (2.3)

where \( x_1 = x \) and \( x_3 = z \) are streamwise and vertical directions, respectively. How to combine this condition with the energy-based condition of Eq. 2.1, and how to address the problem that Eq. 2.3 becomes ill-posed when \( \Delta/z \ll 1 \) (there the numerator and denominator of Eq. 2.3 become negligible), are questions that require significant attention beyond the scope of the present study.

### 2.2 The HATS (Horizontal Array Turbulence Study) data set

The Horizontal Array Turbulence Study (HATS) was conducted in the San Joaquin Valley from 31 August 2000 until 1 October 2000. The field site was selected because of its homogeneous surface conditions with predictable wind directions. It was located 5.6 km ENE of Kettleman City at the
Table 2.1: Array properties for the HATS experiment. “d”: double filtered array, “s”: single filtered array, \( d_0 \): displacement height, \( \Delta \): filter size, \( z_s \): height AGL of “s” array, \( z_d \): height AGL of “d” array (see Fig. 1-1). The last three columns specify the type of filter used in \( x \)- and \( y \)-direction (trapezoidal is abbreviated by trapez.). The number following the filter type specifies the number of instruments over which the spatial average is computed. Note that for the remainder of the thesis the data for arrays 3 and 4 are merged, since their \( z/\Delta \) values are similar.

<table>
<thead>
<tr>
<th>#</th>
<th>Data</th>
<th>( z_d - d_0 )</th>
<th>( z_s - d_0 )</th>
<th>( \Delta )</th>
<th>( \Delta_{z_d-d_0} )</th>
<th>( \langle u_d \rangle )</th>
<th>x-filter</th>
<th>y-filter(_d)</th>
<th>y-filter(_s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>46.0</td>
<td>6.58</td>
<td>13.4</td>
<td>4.28</td>
<td>2.46</td>
<td>gaussian</td>
<td>trapez., 5</td>
<td>trapez., 3</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>38.7</td>
<td>4.01</td>
<td>8.34</td>
<td>8.68</td>
<td>2.16</td>
<td>gaussian</td>
<td>trapez., 5</td>
<td>trapez., 3</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>37.9</td>
<td>8.34</td>
<td>4.01</td>
<td>4.34</td>
<td>0.52</td>
<td>gaussian</td>
<td>trapez., 3</td>
<td>trapez., 5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>34.5</td>
<td>3.83</td>
<td>4.83</td>
<td>2.50</td>
<td>0.65</td>
<td>gaussian</td>
<td>top-hat, 4</td>
<td>trapez., 5</td>
<td></td>
</tr>
</tbody>
</table>

south-east corner of an area of unplanted farmland. Homogeneous surface conditions ranged at least 2 km in the upwind (northwest) direction. Vegetation consisted of crop stubble and weeds for which the aerodynamic displacement height \( d_0 = 32 \text{ cm} \) and roughness length \( z_0 = 2 \text{ cm} \) were calculated from near-neutral wind profiles. As outlined in the introduction the goal of the experiment was the examination of SGS quantities for a wide range of stabilities \( \Delta/L \) and array geometries \( \Delta/z \). The requirement of computing derivatives in all directions necessitated a setup of 3d sonic anemometers in two parallel horizontal arrays, which are separated in the vertical direction and centered in the lateral direction (see Fig. 1-1). Variation in \( \Delta/z \) was achieved by selecting four arrays with different geometrical arrangements (see table 2.1), each of which was in the field for 6-9 days with continuous sampling in order to record data for a wide range of stabilities \( \Delta/L \).

A total of 14 Campbell Scientific three-component sonic anemometer-thermometers (CSAT3) was partitioned into one array with 9 sonics and another array with 5 instruments. The former allows for computation of double filtered quantities and is named the subscript “d”-array, while the latter is referred to as subscript “s”-array as in single-filtered. An additional 2 sonics were mounted on a reference tower to examine flow obstruction. For additional information see Horst et al. (2004).
All 16 sonics were calibrated before and after the experiment in the NCAR wind tunnel and differences in the slope of regressions for the 16 sonics were in a range on the order of two percent (Horst et al. 2004). The standard deviation of the slope of the regressions was less than 0.5%. All sonics met the specification of the manufacturer of an intercept of less than 4 cm s\(^{-1}\), only one had an offset of 6 cm s\(^{-1}\) after the experiment. Other errors stem from the alignment of the sonic anemometers. Errors in the alignment of the \(x\)-\(y\)-plane of the sonic anemometers parallel to the surface can be corrected for in post-processing assuming that the mean wind vector is parallel to the local surface. This tilt was found to be less than 2°. The \(x\)-axis of all sonics should be parallel to each other and perpendicular to the \(x\)-\(z\)-array-plane. The error in this alignment was measured on-site with a theodolite. After correcting the data with the theodolite measurements intercomparisons of horizontal wind-components of the instruments still showed offsets of up to 6 cm s\(^{-1}\) and residual wind direction biases of up to 2°. This paragraph summarizes the descriptions in Horst et al. (2004), where a more detailed data quality analysis is presented.

The temperature measurements were uncalibrated. However, the present analysis does not involve any vertical gradients of mean temperature, but only gradients of temperature fluctuations. By subtracting the mean temperature \(\langle \theta \rangle_l, \ l = 1, \ldots, 16\) of a particular time segment from each instrument’s measurement \(\theta(t), \ l = 1, \ldots, 16\) any offset in the signals is eliminated. The remaining error is the “noise equivalent temperature”, defined as the standard deviation of instantaneous measurements made of a constant signal. The noise equivalent temperature is specified by the manufacturer as 0.026 K.

The arrays were oriented in a way that southeastward winds (315°) were perpendicular to the arrays and caused the least inter-instrumental flow obstruction. For our analysis all time periods with an angle of the downstream pointing array-normal and 6.8-min-averaged wind vector of \(-30^\circ < \alpha < 30^\circ\) are considered. Excluding all data violating this criterion leaves us with the amount of data specified in the second column of table 2.1. During data processing, the array is rotated to a position perpendicular to the prevailing wind using Taylor’s hypothesis. The center of rotation is for both arrays the center sonic (same \(y\) coordinate). The new (rotated) velocity for a
sonic with distance $\delta_y$ from the center sonic for given mean horizontal velocity vector $\langle u \rangle$ and angle of average wind vector with the array normal $\alpha$ is $u_i^{\text{new}}(x, y, z, t) = u_i(x, y, z, t - \delta_y \sin \alpha/\langle u \rangle)$. This rotation results in a decrease of the effective filter size to $\Delta_{\text{eff}} = \Delta \cos \alpha$. For the remainder of the thesis all statements involving filter size refer to the effective filter size. Sonic anemometer signals were sampled at a data acquisition frequency of 20 Hz.

Filtered quantities which were defined as a continuum in Eq. 1.3 have to be computed using discrete filters as specified in table 2.1. Many LES codes use a 2d-spectral cutoff filter in horizontal planes. However, this filter is not suited for our analysis, because its slow $x^{-1}$ decay in physical space aggravates its approximation with $O(5)$ sensors. Moreover the spatial cutoff filter produces a spatially non-local impact when filtering spatially localized phenomena (“ringing”). Thus we choose to use spatially localized filters, which can be well represented by the experimental arrangement. In the lateral ($y$) direction trapezoidal filter functions are used with the exception of array 4, for which a top-hat filter is used for the “d” array in order to match the filter sizes of “s” and “d” arrays. For increased smoothness Gaussian filter functions are applied in the streamwise ($x$) direction where a higher resolution is available due to the 20 Hz sampling that corresponds to a sampling distance of about 0.12 m, using Taylor’s hypothesis. Filtering is done in wave space using the Fourier transform of the Gaussian filter function $\hat{G}_\Delta = \exp \left[-\left(\frac{k_1^2 \Delta^2}{24}\right)\right]$, where $k_1$ is the wavenumber. Cerutti and Meneveau (2000) confirmed the feasibility of a box filter for spatially averaging a finite number of sensors; Porté-Agel et al. (2001a) concluded that their results for $c_s$ were not strongly affected by the choice of streamwise filter function.

Gradients are calculated in all directions using finite differences (FD). For gradients in the vertical direction ($x_3 = z$) a first order one-sided FD over a distance $(z_s - z_d)$ is imposed by the geometry $(\partial \tilde{u}_i/\partial z)_{z_d} = (z_s - z_d)^{-1} (\tilde{u}(z_s) - \tilde{u}(z_d)))$. In the horizontal directions a 4th-order centered FD scheme is applied, i.e.

$$
\left. \frac{\partial \tilde{u}_i}{\partial y} \right|_{y_0} = \frac{1}{12 \delta_y} \left[ \tilde{u}_i(y_0 + 2 \delta_y) + 8 \tilde{u}_i(y_0 + \delta_y) - 8 \tilde{u}_i(y_0 - \delta_y) - \tilde{u}_i(y_0 - 2 \delta_y) \right]
$$

(2.4)
for the $y$-direction. $\delta_y$ is the lateral spacing of the sonic anemometers. Eq. 2.4 with $\delta_x = \delta_y$ is used in the streamwise direction for computing spatial derivatives from time derivatives using Taylor’s hypothesis. Since the accuracy of spatial gradients is important for the analysis of modelled quantities and coefficients (e.g. Eqs. 2.1 and 2.2), they are examined in more detail in the Appendix A. The error associated with the use of Taylor’s hypothesis in this specific context is quantified in Appendix C.

2.3 Dependence of $c_s$ on stability and height

In order to study the effect of stability and height on the Smagorinsky coefficient, the HATS data are divided into segments of length $T_L$ (we mostly use $T_L = 6.8$ min long segments containing $2^{13}$ points), that are classified in terms of Obukhov length $L$ (Eq. 1.1), and height $\Delta/z$. To illustrate the total amount of data, the cumulative duration of all segments in each $\Delta/L$ bin and $\Delta/z$ bin is shown in Fig. 2-1. As can be seen, more data are available in the near-neutral bins while less data are available in the more stable bins. There are $\sim 40$ hours of useful data for each array, which implies that there is more data available for the $\Delta/z < 0.7$ case, because data from arrays 3 and 4 are combined in this bin. As outlined in chapter 2.1, in this thesis various averaging time scales $T_c$ will be used to compute $c_s$ from Eq. 2.1.

We begin by analyzing data from array 2, with $\Delta/z \sim 2.1$ (i.e. $\Delta \sim 8.6$ m) and divide the data into short subsegments of length $T_c = 3.2$ s. With a representative mean velocity of $\langle u \rangle \sim 2.72$ m s$^{-1}$ this time-scale corresponds to a length-scale $T_c\langle u \rangle \sim 8.7$ m, i.e. on the order of the filter-scale $\Delta \sim 8.6$ m. We consider data with $\Delta/L$ ranging between -3.0 and 11.5. We then proceed to compute the Smagorinsky model coefficient according to Eq. 2.1 by evaluating the averages over time $T_c$ and classifying the result according to the value of $\Delta/L$. Due to the smaller averaging time scale ($T_c = 3.2$ s) compared to Fig. 2-1, more values of $c_s$ are available and a finer bin-resolution for $\Delta/L$ is chosen (18 bins). Even for a fixed $\Delta/L$ the resulting $c_s$ displays considerable variability from one sample to another. Thus, we compute the conditional pdf of $c_s^2$, defined in terms of the
Figure 2-1: Cumulative time of available data in each data bin. All 6.8 min data segments whose average horizontal wind vector is less than 30° off the array-normal are binned according to their ∆/L and ∆/z value. The height range (∆/z) is partitioned into 3 bins: array 1 (∆/z ∼ 4.3), array 2 (∆/z ∼ 2.1) and arrays 3 and 4, which are combined (∆/z < 0.7). The stability range (∆/L) is partitioned into 8 bins, whose end-points are given by the list [−2.0, −0.5, 0, 0.5, 1.0, 2.0, 4.0, 7.0, 10.0].

Joint pdf $P(c^2_s, \Delta/L)$ according to

$$P\left(c^2_s, \frac{\Delta}{L}\right) = \frac{P\left(c^2_s, \frac{\Delta}{z}\right)}{P\left(\frac{\Delta}{L}\right)},$$

where $P(\Delta/L)$ is the fraction of data contained in each $\Delta/L$ bin. In this fashion the dependence on $\Delta/L$ is isolated, independent of the amount of data in different stability bins in our data set (there are much more near-neutral data than stably stratified data which biases the joint pdf $P(c^2_s, \Delta/L)$ towards low values of $\Delta/L$). To construct the pdf the range of $c^2_s$ ($-0.02 < c^2_s < 0.04$) is divided into 120 bins. The resulting conditional pdf of the coefficient is shown using color contours in Fig. 2-2a for the $c^2_s$ and $\Delta/L$-range where sufficient data are available. Repeating the procedure for a longer averaging time $T_c = 102.4$ s, corresponding to about $32\Delta/\langle u \rangle$, we obtain the conditional pdf shown in Fig. 2-2b.
Figure 2-2: Contour plots of conditional pdf of $c_s^2$, $P(c_s^2|\Delta/L)$. The contours are spaced logarithmically. In (a) the averaging time to compute $c_s^2$ is $T_c = 3.2 \, s \sim 10\Delta/\langle u \rangle$, whereas in (b) it is $T_c = 102.4 \, s \sim 32\Delta/\langle u \rangle$. Results are from array 2 with $\Delta/z \sim 2.1$. The solid line is an empirical fit described in Eq. 2.7. The dashed line shows $c_s^2 = 0$. 
Fig. 2-2a shows that the most likely value of $c_s^2$ depends strongly on stability. Specifically, $c_s^2$ decreases from values fluctuating around $\sim 0.015$ in neutral conditions to smaller values for increasing $\Delta/L$. $c_s^2$ is particularly sensitive to stability in the slightly stable region $0 < \Delta/L < 0.5$. For unstable conditions, there is a large spread in $c_s^2$ values around its conditional mean value, whereas for very stable conditions all $c_s^2$ fall within a narrower range. For unstable conditions there is a significant amount of negative $c_s^2$. These events are called backscatter events, because the resulting negative eddy viscosity causes an energy transfer from the SGS to the resolved scales during the time period $T_c$. When the averaging time $T_c$ for the computation of $c_s^2$ is increased (Fig. 2-2b), the spread in $c_s^2$ decreases significantly for near neutral conditions, while the pdf in stable regions is almost unchanged. The most likely value for $c_s^2$ is very similar to Fig. 2-2a. Moreover, there are fewer events of negative $c_s^2$.

The mean and the variability of $c_s^2$ around the most likely, or average, value and the statistics of backscatter events will be addressed in more detail in chapter 2.5. Next, we include the effects of distance to the ground (by considering results from different arrays).

Fig. 2-3 shows results for $c_s$ from averaging over segments of length $T_c = T_L = 13.7$ min $\sim 283\Delta(u)$ for the 4 different arrays. The data for arrays 3 and 4 are combined since they correspond to similar values of $\Delta/z$. As is visible, even after averaging over times corresponding to 283 filter length-scales, there is significant variability. Nevertheless, it is seen that for all stabilities, the $c_s$ values for large $\Delta/z$ tend to fall below those for low $\Delta/z$, a trend that is consistent with previous results (Mason 1994; Porté-Agel et al. 2000b, 2001b). No time segments of length $T_c = 13.7$ min yielded a negative coefficient after averaging. In order to identify more clearly the trends with $\Delta/L$ and $\Delta/z$, averages are performed over the entire data available.

Fig. 2-4 shows results for $c_s$ from averaging SGS energy dissipations over all segments within each $\Delta/L$-bin of Fig. 2-1. Thus, these results correspond to using $T_c$ equal to the times indicated in Fig. 2-1 in each case. A very clear dependence of the coefficient on $\Delta/L$ and $\Delta/z$ can be identified. Considering the heterogeneity of the data within one bin in respect to wind angle, turbulence intensity, mean velocity, etc. it is reassuring that such clear trends emerge from the data. From its
neutral value, $c_s$ decreases strongly under stable atmospheric conditions. Moreover, a larger $\Delta/z$ leads to a decrease in the model coefficient, consistent with the use of damping functions for $c_s$ close to the wall (see e.g. Mason and Thomson 1992), where $z$ becomes equal to or smaller than $\Delta$.

Based on the data in Fig. 2-4, a functional dependence of $c_s$ on both $\Delta/L$ and $\Delta/z$ is constructed. To establish a functional dependence of $c_s$ on $\Delta/z$, Eq. 1.15 for near-neutral stratification is written as

$$c_s = c_0 \left[ 1 + \left( \frac{c_0 \Delta}{\kappa z} \right)^n \right]^{-1/n} \tag{2.6}$$

In addition, for stable stratification $c_s$ has to be decreased compared to its value in neutral conditions. Considering the trends shown in Fig. 2-5a (which corresponds to Fig. 2-4 for $\Delta/L > 0$ but plotted in log-log coordinates to identify possible power-law scaling) we conclude that $c_s$ decreases as $c_s \sim (\Delta/L)^{-1}$ in very stable conditions for fixed $\Delta/z$. In other words, the length-scale $l = c_s \Delta$ scales as $L$ in stably stratified conditions. This is consistent with results presented in Sullivan et al. (2003) who show that $l$ scales with the peak in the spectrum of vertical velocity. That length-scale
Figure 2-4: Smagorinsky coefficient $c_s$ as a function of $\Delta/L$ and $\Delta/z$. Data segments of length $T_L = 6.8$ min are classified according to their $\Delta/L$ values, for each of the 4 arrays. Eq. 2.1 is applied to obtain $c_s$ using time averages of numerator and denominator over all segments. Depending on the availability of data in each $\Delta/L$-bin, the averaging time ranges from $T_c = 0.8$ hr to $T_c = 22.9$ hr. The symbols represent these experimental results, the lines are empirical fits described in Eq. 2.7. To test the fit for a different $\Delta/z$ value, $c_s$ is recomputed for a larger filter size $\Delta/z \sim 8.6$ using data from array 1 (downward facing triangles). Results obtained by Porté-Agel et al. (2001b) are included as open symbols.

is known to scale with $L$ (Nieuwstadt 1984).

Thus a correction factor appropriate for the stable range is $(1 + \frac{c_0 \Delta}{\kappa})^{-1}$, where $\alpha = O(c_0)$ is a model parameter. For large $\Delta/L$ this converges to $(\alpha/c_0) (\Delta/L)^{-1}$, whereas for small (but positive) $\Delta/L$ it approaches 1. Combining this expression with Eq. 2.6, and introducing the Ramp function $R(x) = x$ if $x > 0$ and $R(x) = 0$ if $x < 0$) to avoid difficulties in the unstable range where $L < 0$, we propose an expression of the form:

$$
c_s = c_0 \left[ 1 + \frac{c_0 \alpha \Delta}{\kappa} \right]^{-1} \left[ 1 + \left( \frac{c_0 \Delta}{\kappa \Delta z} \right)^n \right]^{-1/n}.
$$

(2.7)

To further examine the validity of the proposed expression we consider the simultaneous limit of large $\Delta/L$ and large $\Delta/z$. For this limit (and $n \geq 1$, say) Eq. 2.7 reduces to $c_s \sim (\Delta/L)^{-1} (\Delta/z)^{-1}$. 

26
Figure 2-5: (a) Same as Fig. 2-4 for $\Delta/L > 0$ but plotted in log-log coordinates to identify possible power-law scaling. The dashed line shows a $(\Delta/L)^{-1}$ scaling. (b) Smagorinsky coefficient $c_s$ as a function of $\Delta/L \times \Delta/z$ for an averaging time of $T_c = 13.7 \text{ min} \sim 283 \Delta \langle u \rangle$. The symbols represent experimental results, the dashed line shows a $c_s \sim (\Delta^2)^{-1}$ scaling.
To test this asymptotic trend, in Fig. 2-5b \(c_s\) is plotted vs. \(\Delta/z \times \Delta/L\) for all arrays. Indeed, for large \(\Delta/L\) and large \(\Delta/z\) \(c_s\) follows closely the line \(c_s \sim (\Delta^2/(Lz))^{-1}\) justifying the proposed fit in Eq. 2.7. This suggests that for \(\Delta \gg L\) and \(\Delta \gg z\) the value of \(c_s\) is determined by the product of the two length scales \(L\) and \(z\) rather than by the smaller of the two.

To fit the parameters of Eq. 2.7 to the data in Fig. 2-4 we set \(n = 3\) and fit \(c_0\) and \(\alpha\) using multidimensional unconstrained nonlinear optimization from MATLAB. Mason and Brown (1999) suggest \(n = 2\), but the small differences between the \(c_s\) of different arrays in neutral and unstable conditions are indication of a slower decrease of \(c_s\) with \(\Delta/z\), which requires a larger \(n\). From the optimization with \(n = 3\), we obtain \(c_0 = 0.1347\), and \(\alpha = 0.1289\). Since the difference between \(c_0\) and \(\alpha\) is within the range of experimental uncertainty, we assume \(\alpha = c_0 = 0.135\). The resulting equation is used for the fits in Fig. 2-4 as well as in the preceding Figs. 2-2 and 2-3.

The proposed fit is tested by comparison with a different set of data, namely from array 1 in which a box filter is applied on 4 adjacent sonics in the “s”-array and the corresponding sonics in the “d”-array. This results in a filter scale of \(\Delta = 26.8\) m and a value of \(\Delta/z = 8.6\). Using a one-sided derivative in the \(y\)-direction and a centered derivative in the \(x\)-direction, the quantities needed to compute \(c_s^2\) from Eq. 2.1 are obtained and the results are shown in Fig. 2-4 as downward facing triangles. We conclude that the proposed model fits these test-data quite well.

As a further test of the proposed fit, Fig. 2-6 compares the measured \(c_s\) for an averaging time \(T_c = T_L = 13.7\) min with the value obtained from Eq. 2.7. It can be concluded that the empirical fit represents the mean trends in the data also for the shorter (compared to Fig. 2-4) averaging time. However, for unstable conditions (large \(c_s\)) deviations between the modelled and the measured \(c_s\) occur due to the large variability of the measured \(c_s\), whereas the model fit yields a constant value of \(c_s\) for any given value of \(\Delta/z\). Also, for arrays 3 and 4 (\(\Delta/z < 0.7\)) the scatter in the data is larger than for arrays 1 and 2. This might be caused by the difference in setup geometry of array 3. There, the single filtered array is below the double filtered array (see table 2.1), which influences and possibly overestimates vertical derivatives compared to the other setups. For array 4, different filter types in the lateral direction are used for the single and double filtered arrays, as indicated in
Figure 2-6: Scatter plot of measured vs. modelled results for the Smagorinsky coefficient $c_s$ for an averaging time of $T_c = 13.7$ min. The symbols represent experimental results, the line marks $c_s^\text{meas} = c_s^\text{mod}$. The expression used to compute $c_s^\text{mod}$ is described in Eq. 2.7. Results obtained by Porté-Agel et al. (2001b) are included as filled symbols.

table 2.1.

Analysis by other investigators has revealed similar results. Deardorff (1971) and Piomelli et al. (1988) both found $c_s \approx 0.1$ for small $\Delta/z$. Porté-Agel et al. (2001a) found $c_s \approx 0.08$ which is about 35% smaller than ours, but the tendency of an increase of the coefficient with $\Delta/z$ is the same.

The proposed expression in Eq. 2.7 can be easily used in LES, since $\Delta/L$ and $\Delta/z$ are known parameters that are imposed in the simulations a priori by the choice of mesh-spacing, wall shear stress and heat flux at the boundary. If the dependence on stratification is to be expressed as a function of Richardson number, relationships between $Ri$ and $L/z$ can be used such as those appearing in Businger et al. (1971). However, most of the recent work dealing with stability of the lower atmosphere has tended to be in terms of $L$ (Brutsaert 1982).

Finally, we report the coefficient values that are obtained from matching momentum flux instead of dissipation, according to Eq. 2.3. Fig. 2-7 shows the coefficients so determined for various $\Delta/z$
Figure 2-7: Smagorinsky coefficient $c_{s\text{mom}} = \left[-\langle \tau_{13} \rangle / (2\Delta^2 \left| \vec{S} \right| \left| \vec{S}_{13} \right|) \right]^{1/2}$ as a function of $\Delta/L$ and $\Delta/z$. Averages are evaluated over the entire data set.

and $\Delta/L$. Comparing with Fig. 2-4, we see that the coefficients are much larger. LES with such values are known to be overly damped and thus we conclude that the condition of correct energy dissipation gives a better estimate of the true $c_s$. The impossibility to choose a $c_s$ which satisfies both the requirements of producing the correct rate of kinetic energy transfer from the resolved to the subgrid-scales II and the correct subgrid-scale stress $\tau_{ij}$ is a basic flaw of the eddy-viscosity model. For further information consult Meneveau (1994), Pope (2000, p. 603), and Juneja and Brasseur (1999).

## 2.4 Dependence of $c_s$ on local strain rate magnitude

The basic scaling inherent in the Smagorinsky model, predicated upon inertial-range dimensional arguments, assumes that the eddy-viscosity is linearly proportional to the local strain-rate magnitude $\left| \vec{S} \right|$ (see Eq. 1.12). Whether this concept is justified can be examined by evaluating $c_s$.
conditioned on \( |S| \). If the Smagorinsky scaling is correct, the measured value of \( c_s \) should be independent of strain-rate magnitude. Thus, in this section we further classify the available data according to the local strain-rate magnitudes for conditional sampling. Since the data must also be classified into different ranges of stabilities, the limited amounts of data under each condition become an issue. In order to assure sufficient amounts of data in each condition, data segments of \( T_L = 6.8 \) min are classified into 6 ranges of stability: unstable to neutral \((\Delta/L \leq 0)\), and several ranges of increasing stability: \((0 < \Delta/L < 0.1, 0.1 < \Delta/L < 0.5, 0.5 < \Delta/L < 1.5, 1.5 < \Delta/L < 3\) and \(\Delta/L > 3)\).

For each of the stability ranges, we consider the pdf of the filtered strain-rate magnitude \( |\tilde{S}| \) to decide how many bins of \( |\tilde{S}| \) to use for conditional sampling. As expected, the pdfs and ranges of variability of \( |\tilde{S}| \) depend on stability. We seek to collapse the range of pdfs by normalizing the strain-rate magnitude by a velocity scale \( u_\Delta \) and a length scale \( \ell \) appropriate to the values of \( \Delta/L \) and \( \Delta/z \). For consistency with the empirical fits of chapter 3.3, we use the length-scale

\[
\ell = \Delta \left[ 1 + R \left( \frac{\Delta}{L} \right) \right]^{-1} \left[ 1 + \left( \frac{c_0 \Delta}{\kappa z} \right)^n \right]^{-1/n}.
\]

(2.8)

Only when \( \Delta \ll z \) and \( \Delta \ll L \), one obtains the standard filter scale \( l \sim \Delta \). As velocity scale, we use the inertial-range scaling \( u_\Delta \sim u_\ast (\Delta/z)^{1/3} \) when \( \Delta < \min(z, L) \). Otherwise, when \( \Delta > \min(z, L) \), \( u_\ast \) is a reasonable velocity scale. The velocity scale \( u_\Delta = u_\ast [1 + \min(z, L)/\Delta]^{-1/3} \) combines these two scaling behaviors. The normalized strain-rate is then defined as

\[
S_{\text{norm}} = \frac{|\tilde{S}|}{u_\ast} \left( 1 + \frac{\min(z, L)}{\Delta} \right)^{1/3},
\]

(2.9)

with \( \ell \) given by Eq. 2.8. Fig. 2-8 shows the pdfs of \( S_{\text{norm}} \) for the various \( \Delta/L \) cases for array 1. It can be observed that the range of \( S_{\text{norm}} \) is roughly independent of \( \Delta/L \) with most of the data falling between \( S_{\text{norm}} = 1 \) and \( S_{\text{norm}} = 10 \), although the collapse of the different pdfs is not very good. The magnitude of the normalized strain-rate is smaller in unstable conditions and gradually
Figure 2-8: Probability density function of strain-rate magnitude normalized by $u_\Delta/\ell$ for different $\Delta/L$. The scales used to normalize $|\vec{S}|$ are $u_\Delta = u_* (1 + \min(z, L)/\Delta)^{-1/3}$ as velocity scale and the empirical fit of Eq. 2.8 as length scale $\ell$. The data are from array 1 ($\Delta/z \sim 4.3$). For clarity, a smooth beta-distribution is fit to the (unconditioned) pdf of $S_{\text{norm}}$ (solid line).

increases in slightly stable conditions. In very stable conditions the pdfs look similar for different ranges of $\Delta/L$. Of the many different normalizations of $|\vec{S}|$ we have attempted, Eq. 2.9 produces the best collapse of $P(S_{\text{norm}}|\Delta/L)$ vs. $S_{\text{norm}}$ in Fig. 2-8 for different stabilities. We conclude that our normalization is appropriate for present purposes.

The range of normalized strain-rates (between 0 and 15) is divided into 20 strain-rate bins, and the conditional Smagorinsky coefficient is computed from the data. The coefficient is evaluated as follows:

$$c_s^2(\Delta/L, S_{\text{norm}}) = - \frac{\langle \tau_{ij} \tilde{S}_{ij} | \Delta/L, S_{\text{norm}} \rangle}{\langle 2\Delta^2 | \tilde{S}_{ij} \tilde{S}_{ij} | \Delta/L, S_{\text{norm}} \rangle}. \quad (2.10)$$

The conditional averages are evaluated over the entire set of available data points within each bin. Fig. 2-9 shows $c_s^2$ as a function of normalized strain-rate for each of the stability ranges considered, for the case $\Delta/z \sim 4.3$ (array 1). As already shown in chapter 2.3, $c_s$ decreases with increasing stability. The observed trends with strain-rate magnitude are as follows: For unstable conditions
\[ \text{Figure 2-9: Smagorinsky coefficient } c_s^2 \text{ conditioned on normalized strain-rate magnitude } S^{\text{norm}} = \left| \frac{S}{\ell} \right| / u_\Delta \text{ for different } \Delta/L. \text{ The scales used to normalize } \frac{S}{\ell} \text{ are } u_\Delta = u_* (1 + \min(z, L)/\Delta)^{-1/3} \text{ as a velocity scale and the empirical fit of Eq. 2.8 as a length scale } \ell. \text{ The data are from array 1 } (\Delta/z \sim 4.3). \]

\[(\Delta/L < 0) \] \(c_s^2\) decreases with strain-rate magnitude but only by a factor of about 2: values decrease from \(c_s^2 \sim 0.02\) at low \(S^{\text{norm}}\) to \(c_s^2 \sim 0.01\) at high \(S^{\text{norm}}\). We remark that trends for \(S^{\text{norm}} < 2\) are rather inconclusive and appear noisy, probably due to the small amount of data available in these bins. In stable stratification (except for the case \(\Delta/L > 3\) which shows negligibly small coefficients from which no trend with strain-rate can be discerned), the coefficient decreases quite significantly with increasing local strain-rate magnitude. Typically the coefficient decreases about five-fold between \(S^{\text{norm}} = 2\) and \(S^{\text{norm}} = 10\).

In order to isolate the effect of strain-rate magnitude, the conditional \(c_s^2\) values are normalized by \(c_s^2(\Delta/L)\), the Smagorinsky coefficient conditioned on \(\Delta/L\) for each array obtained by summing over all strain-rate bins. Fig. 2-10 compares these normalized \(c_s^2\) for all three arrays, by considering different stability ranges. Figure 2-10a is for unstable cases, 2-10b is for slightly stable cases, and 2-10c is for very stable cases. For large strain-rate magnitudes, a scaling of \(c_s^2 \sim (S^{\text{norm}})^{-1}\) can be identified for \(1.5 < \Delta/L < 3\) in Fig. 2-10c. This slope becomes smaller in magnitude when
\( \Delta / L \) approaches zero (Fig. 2-10b) and \( c_s^2 \) is found to be almost constant in unstable atmospheric conditions (Fig. 2-10a). These trends are similar for all \( \Delta / z \)-values (arrays). In terms of normalized strain-rate magnitude, two regimes are identified. For large strain-rate magnitudes, \( c_s^2 \) decreases with \( S_{\text{norm}} \). The other regime concerns small strain-rate magnitudes and shows an almost constant Smagorinsky coefficient. The transition between these two regimes occurs at values of \( S_{\text{norm}} \) that depend on \( \Delta / L \) and \( \Delta / z \). The smaller \( \Delta / L \) and the smaller \( \Delta / z \), the smaller the transition value of \( S_{\text{norm}} \). Fig. 2-10b exemplifies this statement. For \( \Delta / z < 0.7 \) the transition region starts at \( S_{\text{norm}} \sim 4 \), for \( \Delta / z \sim 2.1 \) the value is \( S_{\text{norm}} \sim 3 \) and for \( \Delta / z \sim 4.3 \) we find \( S_{\text{norm}} \sim 2 \).

The implications for the Smagorinsky model are as follows. We conclude that the deeper \( \Delta \) is in the inertial range (\( \Delta \ll \min(z, L) \)) the more \( c_s^2 \) is constant with \( S_{\text{norm}} \) implying that the Smagorinsky scaling is valid. This becomes especially clear for the unstable to neutral data, for which the weak dependence of \( c_s^2 \) upon local strain-rate magnitude for all arrays provides support for the basic scaling of the Smagorinsky model. However, the data for the stable cases show that the Smagorinsky scaling is erroneous under conditions of stable stratification. As a consequence, one may conclude that to properly scale the eddy-viscosity one must not only change the basic length-scale (i.e. using \( \ell \) as opposed to \( \Delta \)) but also the velocity scale. More specifically, results suggest that at large \( S_{\text{norm}} \) and \( \Delta / L \), the coefficient of Eq. 2.7 should be multiplied by a factor \([1 + \beta(\Delta / L)S_{\text{norm}}]^{-1}\) where \( \beta(\Delta / L) \) is some function that describes at what \( S_{\text{norm}} \) the transition to a \((S_{\text{norm}})^{-1}\) scaling occurs. In the limit of large \( S_{\text{norm}} \), the eddy viscosity would then scale as \( c_0^2 \hat{\ell}^2 (S_{\text{norm}})^{-1} \left| \tilde{S} \right| \sim c_0^2 \hat{\ell} u_\Delta \) with \( u_\Delta = u_* \) (at large \( \Delta / L \)), instead of \( c_0^2 \hat{\ell}^2 \left| \tilde{S} \right| \). The reasonable collapse in our analysis suggests that the velocity scale \( u_\Delta \) may be more generally appropriate than the conventional choice of \( \ell \left| \tilde{S} \right| \). Finally, we recall that one has to differentiate between the scaling with local strain-rate as it is examined here and the dependence on global shear as examined in Hunt et al. (1988) and Canuto and Cheng (1997). In this thesis we consider the dependence on global shear in the case of near-wall ABL to be already subsumed by the dependence upon \( \Delta / z \) that was considered in chapter 2.3.
Figure 2-10: Log-log plots of Smagorinsky coefficient $c_s^2$ conditioned on normalized strain-rate magnitude $S_{\text{norm}}$ for different stabilities $\Delta/L$ and arrays. (a) unstable: $\Delta/L < 0$, (b) slightly stable: $0.1 < \Delta/L < 0.5$, (c) very stable: $1.5 < \Delta/L < 3$. In (b,c) the dashed line has a slope of -1, and shows an inverse power-law behavior.
2.5 Variability of $c_s$

In this section we address the question "how variable is $c_s$?". Results shown in chapter 2.3, specifically Figs. 2-2a and b, suggest that while the most likely value of $c_s^2$ does not change significantly with averaging time $T_c$, the variability of the coefficient decreases for increasing $T_c$, at least for the near-neutral and unstable cases. To quantify the dependence of the statistics of $c_s$ on $T_c$ and stability, pdfs of $c_s$ are computed for different values of $\Delta/L$ and $T_c$. Two stability bins are selected for the analysis. The first bin contains unstable atmospheric conditions characterized by $-2.0 < \Delta/L < 0.0$. The second bin groups data under very stable conditions. Since there are less overall data available for large $\Delta/L$, in order to obtain reasonably well-converged pdfs, we choose a wide bin of stabilities, namely $1.5 < \Delta/L < 5.5$. Five different values of $T_c$ are selected, ranging from $T_c = 3.2$ s to $T_c = 205$ s. Fig. 2-11a shows the resulting pdfs for the unstable data, while the very stable data are presented in Fig. 2-11b. Backscatter events are excluded from the analysis to focus on $c_s > 0$. The probability $P(c_s^2 < 0)$ is less than 0.2 (as will be shown later in Fig. 2-13).

Fig. 2-11a shows that the spread in the pdf of $c_s$ increases for decreasing $T_c$ for unstable atmospheric stability. Reassuringly, however, the most likely value of $c_s$ and the median (as shown in Fig. 2-12a) do not depend on $T_c$. For stable conditions (Fig. 2-11b), the most likely value and the median (Fig. 2-12a) of $c_s$ are constant with $T_c$ and smaller than for unstable conditions, in agreement with the findings in chapter 2.3. The fact that the medians of $c_s$ are independent of $T_c$ for stable and unstable conditions is encouraging for LES with dynamic SGS models which, as discussed in the introduction, often use some kind of averaging procedures, either in space (e.g. horizontal planes) or time (e.g. the Lagrangian dynamic model (Meneveau et al. 1996)) to compute the coefficient. Our results suggest that correct median coefficients can be obtained even for fairly short averaging time-scales. Rather surprisingly, however, in the case of stable conditions it appears that the spread in the pdf does not decrease for increasing $T_c$.

Fig. 2-12b presents a quantification of the width of the pdfs as a function of $T_c$. Instead of computing the rms value (which tends to be biased due to some outliers in the distribution), we
Figure 2-11: Pdf of Smagorinsky coefficient $c_s$ for different averaging times $T_c$ (see legend) for (a) unstable atmospheric stability conditions ($-2.0 < \Delta/L < 0.0$) and (b) very stable atmospheric stability conditions ($1.5 < \Delta/L < 5.5$). The advection time through one filter scale is roughly $\Delta/\langle u \rangle = 5.4$ s. The data are from array 1 ($\Delta/z \sim 4.3$).
quantify the spread of the pdfs with quartiles. The figure shows the difference between the third and first quartile of the distribution, normalized by the second quartile (thus giving a dimensionless measure of the variability that is not strongly affected by atypical outliers). The relative width of the pdf for the stable bin does not decrease as $T_c$ is increased. This result shows strong variability of the real and/or modelled SGS dissipation (in the numerator and denominator of Eq. 2.1) under stable atmospheric conditions indicating that fluctuations occur over very long time-scales. This may be related to the strong intermittency in stable atmospheric conditions.

The fraction of segments of length $T_c$ that display average backscatter (with negative $c_s^2$ over the time $T_c$) that were neglected in the preceding analysis of chapter 2.5 is shown in Fig. 2-13 as a function of $T_c$. As expected, the fraction diminishes with increasing $T_c$ because backscatter events tend to be cancelled by forward-scatter events within the time-interval $T_c$, yielding a positive $c_s^2$ on average. Consistent with Sullivan et al. (2003) we find that the fraction of time with backscatter events increases with $z/\Delta$ (not shown). Sullivan et al. (2003) report a ratio of backscattered energy to total transferred energy of 0.2 for this array configuration.

### 2.6 Results for coefficients in scalar models

As introduced in Eq. 2.2, the coefficient for the Smagorinsky model for the SGS heat flux $Pr_T^{-1}c_s^2$ can be computed by matching SGS dissipations of scalar variance. Similar to Fig. 2-2b, in Fig. 2-14a the conditional pdf of $Pr_T^{-1}c_s^2$ is presented. The data are from array 2 with averaging time $T_c = 102.4$ s. Similar to Fig. 2-2b, the coefficient decreases under stable conditions, and shows more variability in unstable conditions.

By dividing $c_s^2$ by $Pr_T^{-1}c_s^2$ for each data segment, the Prandtl number is obtained and plotted in Fig. 2-14b. Most values of $Pr_T$ lie between 0 and 1 independent of stability. For unstable to neutral conditions the most likely value of $Pr_T$ increases from $Pr_T \sim 0.3$ to $Pr_T \sim 0.8$, and over the stable range a clear tendency is not apparent. The spread in the conditional pdf does not change significantly with stability. In the following the dependencies of $Pr_T^{-1}c_s^2$ and $Pr_T$ are examined in
Figure 2-12: (a) Median of pdf of Smagorinsky coefficient $c_s$ and (b) width of pdf of $c_s$ quantified as $[q^i(c_s) - q^1(c_s)] / q^2(c_s)$ ($q^i$ means i-th quartile) as a function of averaging time $T_c$. To contrast unstable and very stable conditions, two stability bins for unstable ($-2.0 < \Delta/L < 0.0$) and very stable ($1.5 < \Delta/L < 5.5$) atmospheric conditions are selected. The data are from array 1 ($\Delta/z \sim 4.3$).
Figure 2-13: Fraction of segments of length $T_c$ with negative $c_s^2$ as a function of averaging time $T_c$ for unstable ($-2.0 < \Delta/L < 0.0$) and very stable ($1.5 < \Delta/L < 5.5$) conditions. The data are from array 1.

more detail.

Repeating the analysis of chapter 2.3, $Pr_T^{-1} c_s^2$ and $Pr_T$ are computed by averaging over the total available time for a given $\Delta/L$ and $\Delta/z$-bin. Fig. 2-15a supports the previous finding that $Pr_T^{-1} c_s^2$ decreases in stable conditions. For different $\Delta/z$, we observe that $Pr_T^{-1} c_s^2$ is smaller for $\Delta/z \sim 4.3$ than for $\Delta/z \sim 2.1$ and $\Delta/z < 0.7$. For $Pr_T$ the results presented in Fig. 2-15b are significantly more noisy. Due to the large spread of values for $Pr_T$, the $y$-axis is plotted in logarithmic units. No clear trend of variation with $\Delta/L$ can be discerned from the data, although for this very long averaging time there is a rise in $Pr_T$ between $\Delta/L \sim 1$ and $\Delta/L \sim 4$. However, this trend depends strongly on $T_c$. In almost all $\Delta/L$-bins the Prandtl number increases with increasing $\Delta/z$. In order to get a robust estimate on the value of $Pr_T$ for different $\Delta/z$, the Prandtl number is computed by averaging over all stabilities. The results are shown in table 2.2 and plotted in Fig. 2-14b and 2-15b as horizontal lines. Indeed, $Pr_T$ is increasing with $\Delta/z$. 

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Figure 2-14: Contour plot of conditional pdfs of (a) the Smagorinsky model coefficient for the SGS heat flux: \( P(Pr_T^{-1}c_s^2|\Delta/L) \) and (b) the turbulent Prandtl number: \( P(Pr_T|\Delta/L) \). The contours are spaced logarithmically. The averaging time is \( T_c = 102.4 s = 32\Delta/\langle u \rangle \) and the plots show data from array 2 with \( \Delta/z \sim 2.1 \). The dashed lines show \( Pr_T^{-1}c_s^2 = 0 \) and \( Pr_T = 0 \), respectively. In (b) the solid line depicts \( Pr_T(z/\Delta \sim 2.1) = 0.60 \) (from table 2.2), in (a) the solid line shows \( Pr_T^{-1}c_s^2 \), with \( c_s^2 \) taken from the empirical fit described in Eq. 2.7 and \( Pr_T = 0.60 \).
Figure 2-15: Smagorinsky model coefficients (a) $Pr_{T}^{-1}c_s^2$ and (b) $Pr_T$ as a function of $\Delta/L$ for different $\Delta/z$. Note that the $y$-axis in (b) is in logarithmic units. $T_L = 6.8$ min data segments are classified according to their $\Delta/L$ values, for each of the 4 arrays. For each $\Delta/L$ value, Eq. 2.2 is applied to obtain $Pr_{T}^{-1}c_s^2$ using time averages of numerator and denominator over all segments. $Pr_T$ is computed by dividing $c_s^2$ computed from Eq. 2.1 by $Pr_{T}^{-1}c_s^2$. Depending on the availability of data in each $\Delta/L$-bin, the averaging time ranges from $T_c = 0.8$ hr to $T_c = 22.9$ hr. The lines are empirical fits. The fits are constructed from Eq. 2.7 (for $c_s^2$) and from table 2.2 for $Pr_T$. Results obtained by Porté-Agel et al. (2001b) are included as open symbols.
\( \Delta/z \sim 4.3 \quad \Delta/z \sim 2.1 \quad \Delta/z < 0.7 \)

| \( Pr_T \) | 0.67 | 0.60 | 0.49 |

Table 2.2: Prandtl number \( Pr_T \) conditioned on \( \Delta/z \) computed from Eqs. 2.1 and 2.2 assuming that \( Pr_T \) is not a function of stability. The averaging time is the total time available for each array \( (T_c > 35 \text{ hours}) \).

In order to quantify the variability of \( Pr_T \), the analysis of chapter 2.5 is repeated. All data segments with \(-2.0 < \Delta/L < 0.0 \) (unstable bin) and \(1.5 < \Delta/L > 5.5 \) (stable bin) are selected and \( Pr_T(\Delta/L) \) is computed with varying averaging times \( T_c \). Then the quartiles of the resulting probability distribution of \( Pr_T \) are obtained and the median \( q^2 \) is plotted in Fig. 2-16a. In contrast to our findings concerning \( c_s \), the median of the Prandtl number is not constant, but increases with \( T_c \). This explains the difference between Fig. 2-15b and 2-14b, in which \( Pr_T \) computed from averages over several hours in Fig. 2-15b was significantly larger than \( Pr_T \) computed from 102.4 s averages in Fig. 2-14b. The increase with averaging time appears to level off for \( T_c > 10^2 \text{ s} \). For all \( T_c \), the median for very stable conditions is larger than the median for unstable conditions, but they seem to converge for large \( T_c \). A similar behavior (but with different magnitudes of Prandtl numbers) is observed for the other arrays. The dependence of the median of \( Pr_T \) on the averaging time and the large scatter in Fig. 2-14b complicate the development of empirical expressions for \( Pr_T \) and \( Pr_T^{-1}c_s^2 \). Thus we only present definitive results on the dependence of \( Pr_T \) upon \( \Delta/z \) (as shown in table 2.2), and refrain from attempting to fit the \( \Delta/L \) dependence.

In comparing with prior results, we can remark that for small \( \Delta/z \), Mason and Derbyshire (1990), Moin et al. (1991), and Porté-Agel et al. (2001a) found \( Pr_T \sim 0.4 \), which is within the range of uncertainty around our value of \( Pr_T(\Delta/z < 0.7) = 0.49 \). For large \( \Delta/z \), Porté-Agel et al. (2001a) examined two 30 min segments whose \( \Delta/z \) roughly correspond to the values for our arrays 1 and 2. For the setup similar to our array 2 they obtain \( Pr_T \sim 0.5 \) for \( \Delta/L = -0.26 \), their analysis of the setup similar to our array 1 results in \( Pr_T \sim 0.6 \) for \( \Delta/L = -1.18 \). Our results from table 2.2 suggest \( Pr_T = 0.60 \) and \( Pr_T = 0.67 \), which is qualitatively consistent and within the range of
Figure 2-16: (a) Median of pdf of Prandtl number $q^2(Pr_T)$ and (b) width of pdf of $Pr_T$ quantified as $[q^3(Pr_T) - q^1(Pr_T)]/q^2(Pr_T)$ ($q^i$ means i-th quartile) as a function of averaging time $T_c$. To contrast unstable and very stable conditions, two stability bins for unstable ($-2.0 < \Delta/L < 0.0$) and very stable ($1.5 < \Delta/L < 5.5$) atmospheric conditions are selected. The data are from array 1 ($\Delta/z \sim 4.3$).
The spread of the pdf of $Pr_T$ is shown in Fig. 2-16b as a function of $T_c$. For unstable atmospheric stability conditions, $(q^3 - q^1)/q^2$ decreases from a value of 1.7 to 0.3 for $T_c$ ranging from $T_c = 0.05$ s to 6.8 min. For very stable conditions the variability is constant between 0.3 and 0.6 for the entire range of $T_c$. This is in agreement to findings for the variability of $c_s$ in chapter 2.5. Possibly due to the intermittency in stable conditions the variability does not decrease for larger averaging times, while in unstable conditions the variability decreases significantly. The results for arrays 1, 3 and 4 are very similar.

### 2.7 Conclusions

Parameters of the Smagorinsky model for the SGS shear stress and the SGS heat flux have been studied based on a statistical analysis of a large data set (157 hours) of ABL turbulence. Model coefficients have been measured based on the condition of equivalence between real and modelled SGS dissipation of kinetic energy and scalar variance. Several trends have been identified. Consistent with prior results in the literature, near the ground it is found that $c_s$ depends on the ratio of filter length and height above the ground, $\Delta/z$, and decreases as $\Delta/z$ is increased. Moreover, $c_s$ depends strongly on atmospheric stability as parameterized by the length-scale ratio $\Delta/L$. The previously postulated decrease of $c_s$ in stable stratification and shear (Deardorff 1980; Canuto and Cheng 1997) is quantified from the data and an empirical formula (Eq. 2.7) for $c_s$ is proposed.

By varying the time $T_c$ over which the SGS energy dissipations are averaged, we find that the variability in $c_s$ decreases with increasing $T_c$ for unstable to neutral conditions, whereas in very stable conditions the variability in $c_s$ is independent of averaging time. The fact that in either case the median of $c_s$ is independent of averaging time confirms the robustness of the results. It also supports the assumption inherent in the Lagrangian dynamic SGS models that coefficients can be obtained from data by averaging over time-scales that are not overly long.

The dependence of $c_s$ on local strain-rate magnitude has also been studied here. Since the
Smagorinsky model already assumes proportionality of the eddy viscosity $\nu_T$ to strain-rate magnitude $|\bar{S}|$, $c_s$ should be independent of strain-rate magnitude. The data suggest that this is correct for unstable to neutral conditions or for small strain-rate magnitudes. However, in stable conditions and for large strain-rate magnitudes, $c_s$ decreases with strain-rate magnitude. In very stable conditions the data are consistent with a $c_s^2 \sim |\bar{S}|^{-1}$ scaling. The transition value of the strain-rate magnitude between these two regimes is found to depend on stability and $\Delta/z$. This result shows that the usual velocity scale, $\ell |\bar{S}|$, is inappropriate under stable conditions, even when correcting the length-scale from $\Delta$ to $L$ (i.e. using $\ell$). Instead, the friction velocity provides a better scale for prescribing the eddy-viscosity when the turbulence is limited by stable stratification, but one still has to account for the fact that the velocity scale has to be smaller than $u^*$ when $\Delta$ is in the inertial range.

A similar analysis is carried out for the coefficient of the SGS heat flux $Pr_T^{-1}c_s^2$ and the derived turbulent Prandtl number $Pr_T$. The strong decrease of $Pr_T^{-1}c_s^2$ in stable conditions comes mostly from the strong dependence of $c_s^2$ on stability, while we observe that $Pr_T$ depends only weakly on stability. A robust increase of $Pr_T$ with increasing $\Delta/z$, going from $Pr_T \sim 0.49$ for $\Delta/z < 0.7$, to $Pr_T \sim 0.67$ for $\Delta/z \sim 4.3$, is observed. The observed dependence of the median of $Pr_T$ on the averaging time $T_c$ and general variability of the results precludes us from stating unambiguous conclusions on the dependence of $Pr_T$ on stability. Results for the SGS heat flux models show more scatter than those for the SGS stress models, most likely because of larger experimental uncertainty in the temperature gradients than in the velocity gradients. In general, the coefficient of the SGS heat flux model $Pr_T^{-1}c_s^2$ behaves very similarly to $c_s^2$. Thus for the remainder of this thesis we concentrate on the coefficient in the momentum equations.

Finally the basic flaws of the eddy viscosity models need to be pointed out. Even perfect knowledge of the coefficient does not result in correct prediction of both energy transfer from the resolved scales to the subgrid-scales and the momentum fluxes associated with the SGS stress. Moreover, the basic proportionality assumption of the Smagorinsky model $\tau_{ij} \propto \Delta^2 |\bar{S}| \bar{S}_{ij}$ is contradicted by tensorial misalignment between SGS stress and strain-rate (Tao et al. 2002), independent of the value
of $c_s$. Even with these limitations, the eddy-viscosity closure is still the most-often used in practical applications, providing continued interest in the dependence of $c_s$ on physical flow parameters as studied here.
Chapter 3

Predictions from dynamic SGS models and comparisons with measured Smagorinsky coefficients

3.1 Dynamic SGS models

In the simplest SGS model the SGS stress defined in Eq. 1.9 can be expressed in terms of velocity gradients by the Smagorinsky model (Eq. 1.12, Smagorinsky 1963). Once the basic eddy-viscosity closure is accepted, the most crucial remaining parameter to choose is the Smagorinsky coefficient \( c_s^{(\Delta)} \). In traditional LES of atmospheric boundary layers, \( c_s^{(\Delta)} \) is deduced from phenomenological theories of turbulence (Lilly 1967, Mason 1994).

Along a fundamentally different line of thinking, Germano et al. (1991) proposed the “dynamic model”. Instead of prescribing \textit{a priori} a model for \( c_s^{(\Delta)} \) as a function of flow parameters, this approach is based upon the idea of analyzing the statistics of the simulated large-scale field (during LES) to determine the unknown model coefficient. The dynamic model is based on the Germano identity (Germano 1992),

\[
L_{ij} \equiv \overline{u_i u_j} - \overline{u_i} \overline{u_j} = T^{\alpha\Delta}_{ij} - \tau^{\alpha}_{ij}. 
\] (3.1)
Above, $L_{ij}$ is the resolved stress tensor and $T^\alpha_{ij} = \overline{u_iu_j} - \overline{u_i}\overline{u_j}$ is the stress at a test-filter scale $\alpha\Delta$ (an overline $(..)$ denotes test filtering at a scale $\alpha\Delta$). In simulations, $\alpha$ is typically chosen to be $\alpha = 2$. If one applies this dynamic procedure by replacing $T^\alpha_{ij}$ and $\tau^\Delta_{ij}$ by their prediction from the basic Smagorinsky model the result is:

$$L_{ij} - \frac{1}{3} \delta_{ij} L_{kk} = \left(c_s^{(\Delta)}\right)^2 M_{ij}, \quad \text{where} \quad M_{ij} = 2\Delta^2 \left(\overline{|\overline{S}_{ij}|} - \frac{\alpha c_s^{(\alpha\Delta)}}{\left(c_s^{(\Delta)}\right)^2} \overline{|\overline{S}_{ij}|}\right). \quad (3.2)$$

To proceed, the crucial assumption in the standard dynamic model (Germano et al. 1991) is scale invariance of the coefficient, namely

$$c_s^{(\Delta)} = c_s^{(\alpha\Delta)}. \quad (3.3)$$

This step allows the only remaining unknown parameter in Eq. 3.2, $c_s^{(\Delta)}$, to be obtained. The overdetermined system of equations can be solved by minimizing the square error averaged over all independent tensor components (Lilly 1992), and some spatial domain (Ghosal et al. 1995) or temporal domain (Meneveau et al. 1996). The result is:

$$\left(c_s^{(\Delta)}\right)^2 = \frac{\langle L_{ij}M_{ij} \rangle}{\langle M_{ij}M_{ij} \rangle}. \quad (3.4)$$

Here the symbol $(..)$ denotes ensemble, time or spatial averaging, depending on the context. The dynamic model has been successfully applied to a variety of engineering flows (see Meneveau & Katz 2000 and Piomelli 1999 for reviews). In general, it provides realistic predictions of $c_s^{(\Delta)}$ when the flow field is sufficiently resolved, i.e. the test-filter scale $\alpha\Delta$ is smaller than the local integral scale of turbulence.

In the context of ABL turbulence the dynamic Smagorinsky model has been implemented in an LES by Porté-Agel et al. (2000b). They examined the scale-invariance hypothesis and the dynamic
model with LES of a neutral ABL. They found that near the wall streamwise energy spectra decay too slowly, indicating that the dynamically determined coefficient is too small. In addition, by running four simulations at different resolutions they demonstrated a clear scale-dependence of the Smagorinsky coefficient \( c_s(\Delta) \neq c_s(\alpha \Delta) \), which violates the scale-invariance assumption of the dynamic model (Eq. 3.3). As a consequence Porté-Agel et al. (2000b) proposed a scale-dependent dynamic model. In addition to a test-filter at \( \alpha \Delta \), a test-filter at \( \alpha^2 \Delta \) (denoted by a hat below) delivers another equation similar to Eq. 3.2:

\[
Q_{ij} - \frac{1}{3} \delta_{ij} Q_{kk} = \left( c_s(\Delta) \right)^2 N_{ij}, \quad \text{where} \quad Q_{ij} = \hat{u}_i \hat{u}_j - \bar{u}_i \bar{u}_j
\]

\[
N_{ij} = 2\Delta^2 \left( \overline{\hat{S}_{ij}} - \left( \frac{\alpha^2 c_s(\alpha^2 \Delta)}{c_s(\Delta)} \right)^2 \overline{\hat{S}_{ij}} \right).
\]

With this additional equation the scale-invariance assumption can be relaxed. A new parameter, \( \beta \), is defined according to

\[
\beta = \frac{\left( c_s(\alpha \Delta) \right)^2}{\left( c_s(\Delta) \right)^2}.
\]

Under the assumption that \( \beta \) is constant independent of \( \Delta \), which is equivalent to assuming a power-law behavior \( c_s(\Delta) \sim \Delta^\Phi \), the two equations 3.2 and 3.6 can be solved for the two unknowns \( c_s(\Delta) \) and \( \beta \) (Porté-Agel et al. 2000b). The solution procedure for \( \beta \) is detailed in Appendix B.

Porté-Agel et al. (2000b) applied the scale-dependent dynamic SGS model to an LES of a neutral boundary layer and obtained realistic results for mean velocity gradients and streamwise energy spectra.

The objective of the present study is to examine field data at various length scales and determine whether the dynamic model yields realistic predictions of the coefficient \( c_s(\Delta) \) and its dependencies upon distance to the ground and atmospheric stability. Both the scale-invariant (Germano et al. 1991) and the more elaborate scale-dependent form (Porté-Agel et al. 2000b) of the dynamic model will be examined. The current chapter uses the field data presented in chapter 2.2 but processed at a different set of length scales to perform the various filtering operations required for the dynamic
models. We also investigate how the averaging time scale influences the results. As indicated in Eq. 3.4 the dynamic model requires averaging of data. Knowledge of an appropriate averaging time scale is relevant for the Lagrangian SGS model (Meneveau et al. 1996) which determines the model coefficient by accumulating weighted averages over fluid path lines. However, due to the experimental conditions, only Eulerian averaging can be used in this study.

The present chapter is organized as follows: In chapter 3.2, we describe the field experiment and the data processing techniques. Chapter 3.2 also contains a brief review of the results in chapter 2.3: measured distributions of \( c_s^{(\Delta)} \) as a function of height and stratification. In chapter 3.3 the ability of the scale-invariant dynamic and scale-dependent dynamic SGS models to reproduce the behavior of \( c_s^{(\Delta)} \) is studied. Conclusions are presented in chapter 3.4.

3.2 Data set and processing

3.2.1 The HATS data set for dynamic models

The HATS experiment was described in detail in chapter 2.2 and Horst et al. (2004). In chapter 2.3, the dependence of \( c_s^{(\Delta)} \) on different relevant length scales was examined: height above ground, \( z \), filter scale \( \Delta \), and the Obukhov length \( L \) (Eq. 1.1).

Out of a total of four field setups with different geometrical arrangements, only two had sensor arrangements so that they can be used to dynamically determine Smagorinsky coefficients. These setups are presented in Table 3.1.

Figure 3-1 shows a schematic of the instrument setup for arrays 1 and 2. To compute SGS quantities, the velocity fields have to be spatially filtered in two dimensions at a scale \( \Delta \). Since the velocities will also be filtered at two larger scales, \( \alpha \Delta \) and \( \alpha^2 \Delta \), \( \Delta \) is chosen to be smaller than the values used in chapter 2. Here we use \( \Delta = 2\delta_y \) where \( \delta_y \) is the lateral spacing of the sonic anemometers. Discrete versions of a trapezoidal filter function are applied in the lateral \((y)\) direction and a smoother Gaussian filter is used in the streamwise \((x)\) direction. For details see chapter 2.2.
Table 3.1: Array properties for the HATS experiment. “d”: double filtered array, “s”: single filtered array, $d_0$: displacement height, $\delta_y$: lateral instrument spacing, $\Delta$: filter size.

Gradients are calculated with finite differences (FD). In the vertical direction ($x_3 = z$), the setup necessitates a first order one-sided FD $\partial \tilde{u}/\partial z |_{z_d} = (z_s - z_d)^{-1} [\tilde{u}(z_s) - \tilde{u}(z_d)]$. In the horizontal directions, a 2nd-order centered FD scheme is used, e.g. for the $y$-direction: $\partial \tilde{u}_i / \partial y |_{y_0} = (2 \delta_y)^{-1} [\tilde{u}_i(y_0 + \delta_y) - \tilde{u}_i(y_0 - \delta_y)]$. Assuming Taylor’s hypothesis, the same formula with $\delta_x = \delta_y$ is used in the streamwise direction to compute $\partial \tilde{u}_i / \partial x$.

In order to depict the available data as a function of stability and array, in chapter 2 the data was divided into segments of length 6.8 min. These segments were classified according to stability, parameterized as Obukhov length $L$ non-dimensionalized by the filter size $\Delta$. The distribution of data by stability can be seen in Fig. 2-1, for various heights (parameterized as $\Delta/z$). In the present chapter we use the same procedure and data classification. In the following, the procedures to compute the model coefficient as a function of the parameters will be described in more detail.

### 3.2.2 Empirically determined Smagorinsky coefficient: procedures and results

The “real” value of $c_s^{(\Delta)}$ for LES is determined from the field data by matching mean measured and modeled SGS dissipations $\Pi_\Delta$ (Eq. 2.1). In this case we use our time series of some particular length, a time scale $T_c$. In chapter 2.3 we analyzed the behavior of $c_s^{(\Delta,emp)}$ from HATS data as a function of parameters $\Delta/z$ and $\Delta/L$. A fit to the data for $c_s$ as a function of $\Delta/L$ and $\Delta/z$ was proposed in Eq. 2.7.
In the present chapter, the filter size is only half of that in chapter 2. Figure 3-1a provides a sketch of the filtering procedures in the transverse (y or $x_2$) direction. A three-point trapezoidal filter with weights [0.25, 0.5, 0.25] is used in the lower array and a two-point filter with weights [0.5, 0.5] is used in the upper array. In the streamwise direction, the Gaussian filter is used as described in the preceding section. Thus filtered velocities $\tilde{u}_i$, and SGS stresses $\tau_{ij}$, at a scale $\Delta = 2\delta_y$ are available at locations 7 - 13 and between locations 1 - 5 (Fig. 3-1b). As a result, the filtered strain rate tensors can be obtained at locations 9 and 11, using 2nd order centered FD in the horizontal and 1st order one-sided FD in the vertical directions, respectively. Since $\tau_{ij}$ is available at these locations as well, the Smagorinsky coefficients $c_s^{(\Delta, \text{emp})}$ are evaluated at locations 9 and 11. The results from these two locations are essentially identical and only results from location 9 are presented.
A first question to address is whether the data analyzed at scale $\Delta = 2\delta_y$ provide results that are consistent with those of chapter 2 that were obtained at a larger scale, using more sensors from each array. To compare the current results with chapter 2, data from array 2 ($\Delta/z \sim 1.1$) is divided into stability bins from $\Delta/L = -1$ to $\Delta/L = 5$ and further divided into subsegments of length $T_c = 3.2$ s. This corresponds roughly to a length scale $T_c(u) \sim 8.7$ m which is on the order of twice the filter scale $\Delta \sim 4.3$ m. The empirically determined Smagorinsky model coefficient $c_s^{(\Delta, \text{emp})}$ is obtained by evaluating the averages in Eq. 2.1 over time $T_c$. In order to isolate the dependence on $\Delta/L$, we compute the conditional pdf of $(c_s^{(\Delta, \text{emp})})^2$, $P\left(\frac{c_s^2}{\Delta}, \frac{\Delta}{L}\right) = P\left(c_s^2, \frac{\Delta}{L}\right) / P\left(\frac{\Delta}{L}\right)$, where $P(\Delta/L)$ is the fraction of data contained in each $\Delta/L$ bin. The $(c_s^\Delta)^2$ range $(-0.03 < (c_s^\Delta)^2 < 0.1)$ is divided into 260 bins. Figure 3-2 shows the conditional pdf of $(c_s^{(\Delta, \text{emp})})^2$ using color contours. The figure confirms the results of chapter 2: $c_s^{(\Delta, \text{emp})}$ decreases in stable conditions and its pdf shows a large spread in unstable conditions with a considerable number of negative values. The most likely value of $c_s^{(\Delta, \text{emp})}$ corresponds well to the empirical fit of chapter 2. Liu et al. (1995) obtained the eddy viscosity field without averaging and also found a highly variable eddy viscosity field with negative values, which causes numerical instabilities in LES.

The comparison with chapter 2 is repeated using a larger averaging time scale $T_c$. Fig. 3-3a shows a direct comparison of data from array 1 ($\Delta/z \sim 2.1$) of the present chapter with data from a better resolved filter but same $\Delta/z$ from array 2 of chapter 2 for an averaging time scale of $T_c = 6.8$ min. The results agree very well, even though they are obtained from two different arrays. The agreement confirms that the curves collapse for a given $\Delta/z$, independent of the dimensional values of $\Delta$ or $z$. Finally, in Fig. 3-3b we perform a comparison based on the global time averages of SGS dissipations. Here we average the terms in Eq. 2.1 over all data available in each $\Delta/L$ bin, obtaining a single measured value of $c_s^{(\Delta, \text{emp})}$ in each bin. The coefficients are very close to the lines which are the predictions from the fit of chapter 2. Only in unstable conditions are the predictions about $\sim 10\%$ too small. Besides confirming the collapse of the data, this comparison shows that despite the coarse filter resolution in the lateral direction (using only two or three sensors) the resulting measured coefficients agree with the results of using finer lateral resolutions.
Figure 3-2: Contour plots of conditional pdf of $(c_{s}^{\Delta, \text{emp}})^{2}$, $P(c_{s}^{2}|\Delta/L)$, for array 2 ($\Delta/z \sim 1.1$). The contours show $\log_{10}P(c_{s}^{2}|\Delta/L)$. The averaging time to compute $c_{s}^{(\Delta)}$ is $T_{c} = 3.2 s \sim 2.0 \Delta/\langle u \rangle$. The solid line is the empirical fit of Eq. 2.7. The dashed line shows $(c_{s}^{\Delta})^{2} = 0$.

To provide a systematic description of the effects of averaging time $T_{c}$ upon the statistics of $c_{s}^{(\Delta, \text{emp})}$, the main aspects of the pdf of $c_{s}^{(\Delta, \text{emp})}$ are documented as a function of $T_{c}$. Fig. 3-4 displays the median of $c_{s}^{(\Delta, \text{emp})}$ as a function of $T_{c}$ for different stabilities. As reported in chapter 2, the median of $c_{s}^{(\Delta, \text{emp})}$ is constant with averaging time and much smaller in stable conditions than in unstable and neutral conditions. In unstable conditions the median increases slightly with averaging time. A measure of the spread of the pdf is documented in terms of the difference between third and first quartile normalized by the second quartile. As expected, this measure decreases with increasing $T_{c}$, in neutral and unstable conditions. As reported in chapter 2, the decrease is weaker in stable conditions, which can be attributed to larger intermittency in stable conditions.
Figure 3-3: (a) Comparison of $c_s^{(\Delta, \text{emp})}$ from array 1 of the present chapter ($z = 3.13 \text{ m}, \Delta = 6.7 \text{ m}$) with $c_s^{(\Delta, \text{emp})}$ from array 2 of chapter 2 ($z = 4.01 \text{ m}, \Delta = 8.68 \text{ m}$). The averaging time is $T_c = 6.8 \text{ min}$. (b) Comparison of $c_s^{(\Delta, \text{emp})}$ from the present chapter (symbols) with empirical fits of Eq. 2.7. Parameter $c_s^{(\Delta, \text{emp})}$ is obtained from Eq. 2.1 by averaging over the total time in each stability bin.
Figure 3-4: Median $q^2$ and spread $(q^3 - q^1)/q^2$ of the $(c_s^{\Delta,\text{emp}})^2$ distribution as a function of averaging time scale $T_c$ for different stabilities: unstable ($-0.5 < \Delta/L < -0.25$), near neutral ($0 < \Delta/L < 0.25$), and stable ($2 < \Delta/L < 2.5$). The data are from array 2.

### 3.2.3 Scale-invariant dynamic Model: procedures

In order to obtain the dynamic model coefficient from Eq. 3.4, filtered strain-rate tensors and velocity vectors at a scale $\Delta$ have to be filtered at $\alpha\Delta$ to evaluate $L_{ij}$ and $M_{ij}$. Usually $\alpha = 2$, but the limited maximum filter width in the lateral direction requires us to use $\alpha = 1.75$ in the present study. As shown in Germano et al. (1991), the sensitivity of the dynamic coefficient to $\alpha$ is not expected to be important. Figure 3-1b shows that $\tilde{S}_{ij}$ at a scale $\Delta$ can be obtained at locations 7, 9, 11, and 13. At locations 9 and 11, $\tilde{S}_{ij}$ is computed from centered horizontal FD and one-sided vertical FD. At locations 7 and 13, the horizontal and the vertical FD are one-sided. A filter of size $1.75\Delta$ is applied on $\tilde{u}_i$, $\tilde{S}_{ij}$, $|\tilde{S}|$, and $|\tilde{S}|\tilde{S}_{ij}$. The filter weight $w_i$ associated with a variable (already filtered at scale $\Delta$) at location $y_i$, used to compute a test-filtered variable at location $y_{\alpha\Delta}$ is evaluated as follows: $w_i^* = |[y_i - \Delta/2, y_i + \Delta/2] \cap [y_{\alpha\Delta} - \alpha\Delta/2, y_{\alpha\Delta} + \alpha\Delta/2]|$, where $[y_i - \Delta/2, y_i + \Delta/2]$ is the segment of length $\Delta$ surrounding the point $y_i$, and $[y_{\alpha\Delta} - \alpha\Delta/2, y_{\alpha\Delta} + \alpha\Delta/2]$ is the segment of
length $\alpha\Delta$ surrounding the point $y_{\alpha\Delta}$. Variables $y_i$ and $y_{\alpha\Delta}$ are the $y$ coordinates of the instrument at location $i$ and the test-filtered variable, respectively. Weights $w_i^*$ are normalized so that they sum up to 1: $w_i = w_i^*/\sum_i w_i^*$. This procedure gives weights of $w_i = [0.214, 0.571, 0.214]$ for locations $i=[7, 9, 11]$ and $i=[9, 11, 13]$. Using the test-filtered variables, the time series of $L_{ij}M_{ij}$ and $M_{ij}M_{ij}$ are computed at locations 9 and 11, averaged over a time scale $T_c$, and divided to obtain $c_s^{(\Delta,\text{dyn})}$ using Eq. 3.4.

### 3.2.4 Scale-dependent dynamic Model: procedures

The scale-dependent dynamic coefficient is obtained similarly to procedures described in section 3.2.3. The filtered strain rate tensors and filtered velocity vectors of Fig. 3-1b are now, however, filtered at $\alpha^2\Delta = 1.75^2\Delta$. The same weighting scheme as in chapter 3.2.3 produces weights of $w_i = [0.18, 0.32, 0.32, 0.18]$ for strain-rate tensors at locations $[7, 9, 11, 13]$. The resulting $\hat{S}\tilde{S}_{ij}$, and $\hat{\tilde{S}}\tilde{S}_{ij}$ are used to compute $N_{ij}$, while $\hat{u}_i\tilde{u}_j$, and $\hat{\tilde{u}}_i$ are used to compute $Q_{ij}$.

It is important to note that $N_{ij}$ is a function of $\beta$. Parameter $\beta$ is computed using procedures identical to those in Porté-Agel et al. (2000b, hereafter POR). Six coefficients of a fifth order polynomial in $\beta$ are obtained from averaging products of strain rates and resolved stresses over $T_c$, as described in Appendix B (Eqs. 6.4-6.12). Then the roots of the polynomial in $\beta$ are determined by the “roots” function in MATLAB (The Mathworks Inc.). As argued in POR, only the largest real root is physically meaningful. A time series of $Q_{ij}$ and $N_{ij}$ is obtained from Eq. 3.6 using the $\beta$ value which was derived from quantities averaged over $T_c$. Finally, the scale-dependent dynamic procedure yields the coefficient at a scale $\Delta$ as $(c_s^{(\Delta,\text{sd-dyn})})^2 = \langle Q_{ij}N_{ij} \rangle / \langle N_{ij}N_{ij} \rangle$ or $(c_s^{(\Delta,\text{sd-dyn})})^2 = \langle L_{ij}M_{ij} \rangle / \langle M_{ij}M_{ij} \rangle$. 58
3.3 Smagorinsky coefficients determined from dynamic SGS models

3.3.1 Scale-invariant dynamic model: results

To begin, the scale-invariant, dynamically determined Smagorinsky model coefficient $c_s^{(\Delta, \text{dyn})}$ is obtained according to chapter 3.2.3 by evaluating the averages over time $T_c = 3.2$ s for array 2. Figure 3-5 shows the pdf of $(c_s^{(\Delta, \text{dyn})})^2$ conditioned on $\Delta/L$ using color contours. It is apparent that the most likely value of $(c_s^{(\Delta, \text{dyn})})^2$ depends on stability. It is very close to zero for $\Delta/L > 1$ and increases strongly in near neutral conditions ($\Delta/L \sim 0$). In neutral and unstable conditions, the spread in the pdf is large with a considerable number of negative values. These trends are consistent with those of the empirical coefficient reported in chapter 3.2.2. However, comparing the color contours with the line from the fit in Eq. 2.7 and with the conditional pdf of $c_s^{(\Delta, \text{emp})}$ in Fig. 3-2, it can be seen that the dynamically determined coefficients are too small, especially in conditions of stable stratification ($\Delta/L > 0$).

Figure 3-6 shows the empirically and dynamically determined coefficient for a longer averaging time $T_c = 6.8$ min and for arrays 1 and 2. At this averaging scale too, the results confirm that the dynamic model predicts a coefficient which is significantly smaller than $c_s^{(\Delta, \text{emp})}$. Finally, the same results are obtained when performing the averages over all available data as shown in Fig. 3-7, where one value of $c_s^{(\Delta, \text{dyn})}$ is plotted for each $\Delta/L$-bin.

The dynamic procedure predicts the correct basic trends of the coefficient with stability ($\Delta/L$) and height ($\Delta/z$), but the magnitudes of the coefficients are too small by significant factors. In unstable and neutral conditions, factors range from 2-5. In very stable conditions this factor is as large as an order of magnitude or more. Thus the energy transfer ($\Pi_\Delta$) from resolved scales to SGS is too small, and in LES using such a model one would expect a high-wavenumber pile-up of energy in the spectra near the wall. This weakness of the dynamic model was already observed in LES of the ABL in neutral conditions (POR), and present results suggest that this weakness would be acerbated in conditions of stable stratification.

The variability of $c_s^{(\Delta, \text{dyn})}$ is examined in Fig. 3-8 by plotting the quartiles of the $(c_s^{(\Delta, \text{dyn})})^2$
Figure 3-5: Contour plots of the pdf of \((c_s^\Delta)^2\) conditioned on \(\Delta/L\) for array 2 \((\Delta/z \sim 1.1)\). The contours show \(\log_{10} P(c_s^2|\Delta/L)\). The averaging time to compute \(c_s^\Delta\) is \(T_c = 3.2 \text{s} \sim 2.0\Delta/\langle u \rangle\). The solid line is the empirical fit of Eq. 2.7. The dashed line shows \((c_s^\Delta)^2 = 0\).

distribution for different averaging times \(T_c\). The median of \(c_s^{(\Delta,\text{dyn})}\) is very similar for \(T_c\) ranging from 0.05 s (no averaging) to hours. The relative spread of the pdf decreases with averaging time which agrees with results from chapter 2 and Fig. 3-4 for \(c_s^{(\Delta,\text{emp})}\).

In summary, the results for \(c_s^{(\Delta,\text{dyn})}\) consistently show that the dynamic procedure under-predicts the Smagorinsky coefficient when \(\Delta\) is close to, or exceeds \(L\), or \(z\), or both. This deficiency is not surprising. As suggested by the very same empirical fit through the available data for \(c_s^{(\Delta,\text{emp})}\) (Eq. 2.7), for any fixed value of \(z\) or \(L\) the coefficient is dependent upon \(\Delta\) unless \(\Delta \ll L\) and \(\Delta \ll z\). Thus, the expected behavior of the coefficient contradicts the basic assumption of scale-invariance underlying the dynamic model. This was already noted in POR for the neutral case but \(\Delta > z\). The scale-dependent dynamic model described in chapter 3.2.4 addresses this problem. In the following section we analyze the data to study whether the scale-dependent model yields more realistic predictions of the coefficient compared to the standard dynamic model.
Figure 3-6: Smagorinsky coefficient $c_s^{(\Delta,\text{dyn})}$ as a function of $\Delta/L$ for arrays 1 and 2 and an averaging time of $T_c = 6.8$ min.

Figure 3-7: Comparison of $c_s^{(\Delta,\text{dyn})}$ (symbols) with empirical fits for $c_s^{(\Delta,\text{emp})}$ (Eq. 2.7). Variables are averaged over all segments in each stability bin.
3.3.2 Scale-dependent dynamic model: results

Analysis for the scale-dependent dynamic model first requires computation of the parameter describing scale-dependence of the Smagorinsky coefficient, \( \beta = \left( c_s^\Delta \right)^2 / \left( c_s^\Delta \right)^2 \). Again, data from array 2 \((\Delta / z \sim 1.1)\) are divided into bins of different stabilities ranging from \( \Delta / L = -1 \) to \( \Delta / L = 5 \), and divided into subsegments of length \( T_c \). Parameter \( \beta \) is obtained according to chapter 3.2.4. Specifically, we use Eqs. 6.4-6.12. Averages such as \( \langle \left| \bar{S}_{ij} \right| \bar{S}_{ij} \rangle \) or \( \langle \left| \tilde{S} \right|^2 \tilde{S}_{ij} \tilde{S}_{ij} \rangle \) are evaluated over a time scale \( T_c \). Figure 3-9 shows a few representative polynomials \( P(\beta) \) for the case \( T_c = 6.8 \) min, for three values of \( \Delta / L \). The largest root is the value of \( \beta \) that solves the condition of Eq. 6.3 and 6.4 (POR).

Parameter \( \beta \) is computed for the short duration averaging time of \( T_c = 3.2 \), and \( \beta \) is obtained in each segment. The conditional pdf of \( \beta \) is presented in Fig. 3-10a, where the \( \beta \) range \((0 < \beta < 1.5)\) is divided into 150 bins. Note that \( \beta \) also depends on stability. In very stable conditions most \( \beta \)
Figure 3-9: Representative fifth order polynomials $P(\beta)$ from Eq. 6.4 for different stabilities and $\Delta/z \sim 1.1$. The squares mark the largest roots $\beta = 0.593, 0.442, \text{and} 0.330$.

values are close to 0.3. The lower bound of $\beta$ can be explained by considering the limit of $c_s^{(\Delta)}$ for small $L$: $c_s^{(\Delta)} \propto (\Delta/L)^{-1}$. Consequently,

$$\beta = \left(\frac{c_s^{(1.75\Delta)}}{c_s^{(\Delta)}}\right)^2 \rightarrow \left(\frac{1/1.75\Delta}{1/\Delta}\right)^2 = \left(\frac{1}{1.75}\right)^2 \approx 0.327.$$  (3.8)

For $\Delta/L < 0.5$, $\beta$ increases and reaches a most likely value of $\beta \sim 0.5$. Recall that for scale-invariance one would expect a limiting behavior of $\beta \sim 1$. Here we obtain $\beta < 1$ since even in the neutral case $\Delta > z$ and thus $\beta < 1$ for the reasons explored in POR. The data analysis is repeated by increasing the averaging time $T_c$ to cover segments of length $T_c = 6.8 \text{ min}$, as well as over very long averaging times covering all data segments in each stability bin. Results are shown in Figs. 3-11a and 3-12a. The observations from results for $T_c = 3.2 \text{ s}$ (Fig. 3-10a) are confirmed since $\beta$ is close to its lower bound 0.327 for $\Delta/L > 1$ and increases to values between 0.5 and 0.7 in neutral and unstable conditions. Parameter $\beta$ is very similar for $\Delta/z \sim 2.1$ and for $\Delta/z \sim 1.1$. The
Figure 3-10: Contour plots of conditional pdf of (a) $\beta$ and (b) $(c_{\Delta,sd-dyn})^2$ from the scale-dependent dynamic model. The contours show (a) $\log_{10} P(\beta|\Delta/L)$ and (b) $\log_{10} P(c_{\Delta,sd}^2|\Delta/L)$. The averaging time to compute $c_{\Delta,sd}$ and $\beta$ is $T_c = 3.2\, s \sim 2.0\Delta/\langle u \rangle$. The dashed line in (a) shows $\beta = 0.327$ (cf. Eq. 3.8). The dashed and solid lines in (b) show $(c_{\Delta,sd}^2)^2 = 0$ and the empirical fit of Eq. 2.7, respectively.
magnitude of $\beta$ in the present analysis compares well with Fig. 10 in POR. They obtain a significant increase from $\beta \sim 0.5$ at $\Delta/z = 2$ to $\beta \sim 0.65$ at $\Delta/z = 1.1$ in neutral conditions ($\Delta/L = 0$), quite consistent with present field measurement results. The limit of large $z/\Delta$ ($\Delta << z$), where the turbulence is better resolved, cannot be verified with the HATS data for which $\Delta$ is comparable or larger than $z$. Figure 3-13 shows that the median of $\beta$ is constant with averaging time and the variability decreases with $T_c$.

The model coefficient, $c_s^{(\Delta, sd-dyn)}$, predicted from the scale-dependent dynamic model, is obtained by replacing the measured $\beta$ value in the expression for $N_{ij}$ (see chapter 3.2.4). The analysis is performed again using several averaging times $T_c = 3.2$ sec, $T_c = 6.8$ min, as well as a large $T_c$ encompassing all available data in each bin. As before, results for $T_c = 3.2$ s are presented in terms of a conditional pdf for $c_s^{(\Delta, sd-dyn)}$, for the case $\Delta/z \sim 1.1$, and $-1 < \Delta/L < 5$ in Fig. 3-10b. The general trend in the relationship with stability is similar to that observed for $c_s^{(\Delta, dyn)}$ in Fig. 3-5, but the spread in the pdf is considerably larger. The most likely value of the coefficient seems to be larger (and hence more accurate) than the scale-invariant dynamic model coefficient. However, the large variability in $c_s^{(\Delta, sd-dyn)}$ prevents us from stating this as a definitive conclusion at this short averaging time scale.

Results from the intermediate time scale $T_c = 6.8$ min, in which $\beta$ computed at that time scale is used, are shown in Fig. 3-11b. Results clearly show that the scale dependent dynamic model predicts $c_s^{(\Delta, emp)}$ quite well in unstable and neutral conditions. In stable conditions, the prediction is still improved compared to the dynamic model (Fig. 3-6), but significant scatter persists. Finally, we present results using the longest $T_c$, by averaging over the entire data set in each stability bin. Results are shown in Fig. 3-12b. As can be seen $c_s^{(\Delta, sd-dyn)}$ obtained from long-time averaging predicts $c_s^{(\Delta, emp)}$ and its dependence on stability and height quite accurately.

The variability of $c_s^{(\Delta, sd-dyn)}$ is examined in Fig. 3-13b. The variability is larger than for $c_s^{(\Delta, emp)}$ and $c_s^{(\Delta, dyn)}$ and for all stability bins more than 25% of the recorded $(c_s^{(\Delta, sd-dyn)})^2$ are negative. The variability reduces subsequently for $T_c > 3.2$ s. Also, in unstable conditions the median increases significantly with averaging time for $T_c > 3.2$ s. If a reasonable criterion is introduced which
Figure 3-11: (a) $\beta$ and (b) $c_s^{(\Delta, sd-dyn)}$ as a function of $\Delta/L$ for arrays 1 and 2. The averaging time is $T_c = 6.8$ min.
Figure 3-12: (a) Scale-dependence parameter $\beta$ for array 1 ($\Delta/z \sim 2.1$) and array 2 ($\Delta/z \sim 1.1$). (b) Comparison of $c_s^{(\Delta,\text{sd-dyn})}$ (symbols) with empirical fits for $c_s^{(\Delta,\text{emp})}$ (Eq. 2.7). Variables are averaged over all segments in each stability bin.
Figure 3-13: Median $q^2$ and spread $(q^3 - q^1)/q^2$ of the (a) $\beta$ and (b) $(c_{s}^{\Delta,sd-dyn})^2$ distributions as a function of averaging time scale $T_c$ for different stabilities: unstable ($-0.5 < \Delta/L < -0.25$), near neutral ($0 < \Delta/L < 0.25$), and stable ($2 < \Delta/L < 2.5$). The data are from array 2.
requires the median of $c_s^{(\Delta,sd-dyn)}$ to differ less than 10% from the median of $c_s^{(\Delta,emp)}$, then Fig. 3-13b suggests that the Eulerian averaging time scale $T_c$ should correspond to at least 12.8 s, or about eight filter scales ($8 \approx 12.8(u/\Delta)$).

To confirm that we have obtained results that are unique to turbulence signals under the present physical conditions and do not occur for any time series of random numbers, the procedure to compute dynamic and scale-dependent dynamic coefficients is tested with a time series of random velocity vectors. We generate random velocity fluctuations by distributing 3d vectors whose length is sampled from a uniform distribution in [0, 1] m s$^{-1}$, and whose direction is uniformly distributed over a sphere. Both white-noise and colored-noise signals (with a -5/3 energy spectrum for each velocity component) are used. The resulting $c_s^{(\Delta,emp)}$, $c_s^{(\Delta,dyn)}$, $c_s^{(\Delta,sd-dyn)}$ feature symmetric pdfs with a strong peak at $(c_s^{(\Delta)})^2 = 0$, i.e. as expected random signals do not have the correlations between $L_{ij}$ and $M_{ij}$ associated with net energy flux to smaller scales and a non-zero value of the coefficient. The resulting pdf for $\beta$ is positively skewed, increasing for $\beta > 0.327$ and but reaching a peak at $\beta \sim 0.45$. This is significantly different from the results of the present chapter, where e.g. the peak in $P(\beta|\Delta/L)$ for stable conditions in Fig. 3-10a is narrow and much closer to 0.327.

### 3.4 Conclusions

Predictions of the scale-invariant dynamic SGS model (Germano et al. 1991) and the scale-dependent dynamic SGS model (Porté-Agel et al. 2000b) for the Smagorinsky coefficient $c_s^{(\Delta)}$ have been tested a priori with a large data set from two horizontal arrays of fourteen 3D-sonic anemometers in the atmospheric surface layer. Figures 3-14a and 3-14b summarize the results by comparing the empirically determined $c_s^{(\Delta,emp)}$ with predictions from scale-invariant dynamic and scale-dependent dynamic models, for both values of $\Delta/z$ considered. Clearly, the scale-invariance assumption of the dynamic model breaks down when the filter size is large ($\Delta > z$ or $\Delta > L$), resulting in coefficients that are too small. In LES of the ABL this is expected to lead to unrealistic velocity profiles near the surface and a pile-up of energy reflected in flat velocity spectra.
Figure 3-14: Smagorinsky coefficient $c_s^{(\Delta)}$ as a function of $\Delta/L$ for different SGS models. Variables are averaged over all segments in each stability bin. (a) array 1, $\Delta/z \sim 2.1$ (b) array 2, $\Delta/z \sim 1.1$. 
The scale-dependent dynamic model accounts for scale-dependence of the coefficient. As a result the predicted coefficient is close to the real measured value. Note that despite the success of the scale-dependent dynamic model in predicting the coefficient which produces the correct SGS dissipation, it is reiterated that even “perfect” prediction of the coefficient does not necessarily result in correct prediction of the SGS stress tensor, for reasons discussed in the introduction.

The data suggest that the Eulerian averaging time scale of the scale-dependent dynamic model should be at least $\sim 8$ times the time scale associated with the filter scale. Such a time scale is somewhat larger than averaging time scales usually employed in the Lagrangian dynamic model (Meneveau et al 1996). However, due to the fundamental differences between Lagrangian and Eulerian averaging the applicability of the result to Lagrangian averaging is uncertain and remains to be explored in simulations.
Chapter 4

Dynamic subgrid-scale models in Large Eddy Simulation

4.1 Introduction

A Large Eddy Simulation (LES) with dynamic SGS models is performed in order to study the accuracy of the predicted mean flow velocities, and compare the predictions of \( c_s \) with those measured in the field. Specifically, the prediction of the coefficient from the dynamic procedure introduced in chapter 3.2 applied in LES is compared to \textit{a priori} tests from the HATS experiment.

In that way the applicability of \textit{a priori} results in field experiments to \textit{a posteriori} settings in LES can be studied. As in chapter 3, both the scale-invariant and scale-dependent dynamic models will be examined. The main difference between the experimental analysis and the simulations is the type of averaging employed to measure the coefficients: In the \textit{a priori} analysis of chapter 3, Eulerian time averaging over times \( T_c \) was performed. In the simulations, we use time averaging along fluid pathlines (Lagrangian averaging). Lagrangian averaging is required for the general applicability of dynamic models to flows in complex geometries which do not possess directions of statistical homogeneity.

In chapters 2 and 3, stability parameter \( \Delta/L \) accurately characterized the experimental data from the lowest 10 m in the ABL. The Obukhov length \( L \) is a surface layer length scale and the
surface layer \((z < 10 \text{ m at night, } z < 100 \text{ m during the day})\) quickly responds to changes in surface boundary conditions (heat flux and friction velocity). This assumption is confirmed by the good collapse of measurements of \(c_s\) with \(\Delta/L\) in the HATS experiment. The LES domain, however, extends beyond the surface layer and spans the entire height of the ABL \((\sim 2 \text{ km})\). There, \(\Delta/L\) is not expected to be an appropriate length scale. The Richardson number, on the other hand, is expected to be a parameter that may be applicable throughout the ABL. Hence, before showing the simulations and results, we begin by recasting the HATS measured results in terms of the Richardson number, in addition to the Obukhov length \(L\) used before.

### 4.2 HATS results in terms of Richardson number

The Richardson number is a stability parameter measuring the ratio of buoyant to mechanical production of turbulent kinetic energy. Flux and gradient Richardson numbers are defined as

\[
Ri_f = \frac{\langle w'\theta' \rangle}{\langle uu' \rangle + \langle vv' \rangle \frac{\partial \langle \theta \rangle}{\partial z}} \tag{4.1}
\]

\[
Ri_g = \frac{\partial \langle \theta \rangle}{\partial z} \left( \frac{\partial \langle u \rangle}{\partial z} \right)^2 + \left( \frac{\partial \langle v \rangle}{\partial z} \right)^2 \tag{4.2}
\]

respectively. Dynamic stability criteria state that laminar flows become turbulent for \(Ri_g < 0.25\) and turbulent flows become laminar for \(Ri_g > 1.0\) (Stull 1997). Unstable flows are characterized by \(Ri_f < 0\) and \(Ri_g < 0\). In LES, the Richardson number has often been used to parameterize \(c_s\) as a function of stability in simulations. For instance, Lilly (1962) parameterizes the eddy viscosity as \(\nu_T = \lambda_r^2 \left| \bar{S} \right| (1 - Ri_f^p)\) where \(\lambda_r\) is a characteristic subgrid length scale and \(Ri_f^p\) is the pointwise flux Richardson number (without the averaging operation of Eq. 4.1). Lilly (1962) proposed this model with \(\lambda_r = \lambda\), where \(\lambda\) is the “basic mixing length”, i.e. the height-dependent mixing length in neutral conditions. This approach only considers the direct influence of buoyancy on the energy production and it was intended for unstable conditions only. In our notation Lilly’s model implies that \(\lambda = c_s(\Delta/z, Ri_f^p = 0)\Delta\) and thus \(c_s(\Delta/z, Ri_f^p) = c_0 \left[1 + \left( \frac{\Delta}{\lambda} \right) \right]^{1/n} (1 - Ri_f^p)^{\gamma}\).

Brown
et al. (1994, hereafter BDM) also account for the influence of buoyancy on the length scales by making $\lambda_r$ dependent on $Ri_g$

$$
\nu_T = \lambda^2 \left| \tilde{S} \right| f_m(Ri_g^p)
$$

From field experimental data in the surface layer, they propose a functional dependence of the length scale on stability by expressing the function $f_m$ in Eq. 4.3 as

$$
f_m = (1 - 16 Ri_g^p)^{0.5} \quad \text{for} \quad Ri_g^p < 0
$$

$$
f_m = \left( 1 - \frac{Ri_g^p}{Ri_g^c} \right)^4 \quad \text{for} \quad 0 < Ri_g^p < Ri_g^c
$$

$$
f_m = 0 \quad \text{for} \quad Ri_g^p > Ri_g^c.
$$

Since $\lambda^2 f_m(Ri_g^p) = c_s^2(\Delta/z, Ri_g^p) \Delta^2$, we can write BDM’s model as

$$
c_s(\Delta/z, Ri_g^p) = c_0 \left[ 1 + \left( \frac{c_0}{\kappa} \frac{\Delta}{z} \right)^n \right]^{-1/n} \left[ f_m(Ri_g^p) \right]^{0.5}.
$$

To compare with this model, the HATS data is plotted against $Ri_g$ in (Fig. 4-1). HATS data from array 1 (upper plots) and array 2 (lower plots) for two different filter size $\Delta = 2\delta$ and $\Delta = 4\delta$ are presented and compared to the proposed model by BDM and the fit of chapter 2 (Eq. 2.7).

For this purpose, empirical relationships by Businger et al. (1971) have been used to express $L$ as a function of $Ri_g$:

$$
Ri_g = z/L \quad \text{when} \quad L < 0
$$

$$
Ri_g = \frac{z}{L} \left( 0.74 + \frac{4.7z}{L} \right) \quad \text{when} \quad L > 0.
$$

Since Eq. 2.7 has been fit to the very same data, the good agreement between data and fit in Fig. 4-1 only supports the validity of the empirical conversion relationships (Eqs. 4.8 and 4.9). In Fig. 4-1 it can be observed, that when $Ri_g$ is larger than the critical Richardson number ($Ri_g^c \sim 0.25$), $c_s^2$ is close to 0. For $0 < Ri_g < Ri_g^c$, $c_s^2$ increases dramatically. The model of Eq. 2.7 (which has
been fit to the very same data) agrees very well with the data in stable conditions ($Ri_g > 0$). Thus it can be used to represent the HATS data in comparisons with results from LES in chapters that follow. BDM’s model also fits the data well, but underpredicts $c_s^2$ for $\Delta/z \sim 1$. Clearly, BDM strongly overpredict $c_s^2$ under unstable conditions ($Ri_g < 0$).

The rest of this chapter is organized as follows: The LES code is described in chapter 4.3. In chapter 4.4 the Lagrangian dynamic model and different procedures for averaging the numerators and denominators needed to calculate the dynamic coefficient in the simulation are presented. Two test cases in stable and unstable conditions are analyzed in chapter 4.5. A simulation with a heat flux and geostrophic wind forcing corresponding to a diurnal cycle is presented in chapter 4.6.
Predictions for $c_s$ from the simulation are compared to HATS results in chapter 4.7. Conclusions follow in chapter 4.8.

### 4.3 Numerical simulations

The boundary conditions for the simulation are selected to resemble as much as possible the measured conditions during HATS on September 6, 2000. This day is selected because it includes typical features that are representative to the entire data set. Various meteorological variables measured in the field are presented in Fig. 4-2 as a time series of 5 minute averages. A typical diurnal heat flux variation is observed with a maximum $\langle w'\theta' \rangle_s$ of 0.3 K m s$^{-1}$ and a minimum of 0.03 K m s$^{-1}$. As can be seen, wind speeds at a height $z = 3.45$ m are significantly lower at nighttime than at daytime. The weak winds lead to low friction velocity $u_*$, which in turn creates a very stably stratified boundary layer (e.g. $\Delta/L$ up to 10).

A 64 x 64 x 64 grid staggered in the vertical, and spanning a domain of 6283 m x 6283 m x 2000 m is simulated. The filtered Navier-Stokes equations are integrated over time based on the numerical approach described in Albertson and Parlange (1999, 2000).

\[
\partial_t \tilde{u}_i = 0 \tag{4.10}
\]

\[
\partial_t \tilde{u}_i + \tilde{u}_j (\partial_j \tilde{u}_i - \partial_i \tilde{u}_j) = -\frac{1}{\rho_0} \partial_i \tilde{p}^* - g \frac{\tilde{\theta}'}{\theta_0} \delta_{i3} - \partial_j \tau_{ij} + f(\tilde{u}_2 - v_g)\delta_{i1} + f(u_g - \tilde{u}_1)\delta_{i2} \tag{4.11}
\]

\[
\partial_t \tilde{\theta} + \partial_j (\tilde{\theta} \tilde{u}_j) = -\partial_j q_j. \tag{4.12}
\]

Variable $\tilde{\theta}' = \tilde{\theta} - \langle \tilde{\theta} \rangle$ describes temperature fluctuations and $q_j$ is the SGS heat flux

\[
q_i = -Pr_T^{-1} c_s^2 \Delta^2 \left| S \right| \frac{\partial \tilde{\theta}}{\partial x_i}, \tag{4.13}
\]

where $Pr_T$ is the turbulent SGS Prandtl number, which is set to $Pr_T = 0.4$. The Coriolis parameter $f = \sin \Phi \times 1.45 \times 10^{-4}$ s$^{-1}$ is imposed, using $\Phi \sim 36^\circ$ N for the latitude of the HATS array. The velocity field is forced by a geostrophic wind velocity $(u_g, v_g)$ (Eq. 4.12).
Figure 4-2: Observed meteorological conditions on 9/6/2000 in Kettlemen City, CA. The measurement height is $z = 3.45\, \text{m}$. The time is PST (Pacific Standard Time). The wind direction perpendicular to the array is marked by a solid line, deviations of $\pm 30^\circ$ are marked by dashed lines.
The horizontal boundary conditions are periodic and the vertical boundary conditions are zero vertical velocity and imposed stress at the bottom and no-stress at the top. The surface shear stresses are prescribed using the Monin-Obukhov similarity law:

\[
\tau_{13} = -\left( \frac{\kappa}{\ln z/z_o - \psi_m} \right)^2 \left( \overline{u^2} + \overline{v^2} \right)^{0.5} \overline{u},
\]

\[
\tau_{23} = -\left( \frac{\kappa}{\ln z/z_o - \psi_m} \right)^2 \left( \overline{u^2} + \overline{v^2} \right)^{0.5} \overline{v},
\]

where \( \overline{() \overline{}} \) represents a local average from filtering the velocity field at 2\( \Delta \). The roughness length at the surface is set to \( z_o = 0.02 \) m, equivalent to the value determined from the HATS data, and \( \kappa = 0.4 \). The flux-profile functions in unstable conditions are given by Dyer (1974) with the correction by Hogstrom (1987). In stable conditions we use the formulation by Cheng and Brutsaert (2004, personal communication):

\[
\phi_m = \begin{cases} 
(1 - 15.2z/L)^{-1/4} & \text{when } L < 0 \\
1 + 6.1 \frac{z/L + (z/L)^{2.5} \left( 1 + \left( z/L \right)^{2.5} \right)^{-1/2.5}}{z/L + \left( z/L \right)^{2.5}} & \text{when } L > 0
\end{cases}
\]

(4.16)

(4.17)

The \( \psi_m \) functions are determined as

\[
\psi_m(z/L) = \int_{z_o/L}^{z/L} \left[ 1 - \phi_m(x) \right] \frac{dx}{x}
\]

(4.18)

A sponge at the four levels below the top is applied to dissipate energy of gravity waves before they reach the upper boundary of the domain (Nieuwstadt et al. 1993). Pseudospectral treatment is used in horizontal planes and second-order finite finite differencing is implemented in the vertical direction. The second order accurate Adam-Bashforth scheme is used for time-advancement. Nonlinear convective terms and the SGS stress are dealiased using the 3/2 rule (Orszag 1970). The simulations are forced with prescribed geostrophic velocity \( (u_g, v_g) \) and surface heat flux \( \langle w'\theta' \rangle_s \). Figure 4-3 shows the initial mean temperature and mean velocity profile of the simulations. A
stably stratified layer with a large temperature gradient $\langle \partial \theta / \partial z \rangle = 0.012 \text{ K m}^{-1}$ is created at the top to limit the growth of the boundary layer in daytime. The boundary layer height $z_i$ is used as a characteristic length scale.

4.4 The Lagrangian dynamic SGS model

First we consider the scale-invariant model with $c_s^\Delta = c_s^\Delta$. As reviewed in chapter 1.3, the Smagorinsky coefficient $c_s^2$ in LES needs to be averaged over homogeneous areas or over time in order to prevent negative eddy viscosities that lead to numerical instabilities. Typically in channel flow, or ABL flow, $c_s^2$ is computed from quantities averaged over horizontal planes. However, over heterogeneous surfaces, spatial averaging over large planes is not appropriate, whereas time averaging in a Lagrangian sense can be physically motivated (Meneveau et al. 1996). The Lagrangian dynamic model is based on Germano’s identity (Eq. 3.1) which upon replacing the stresses with
the Smagorinsky model expression yields

\[ L_{ij} = \left( c_s^{(\Delta)} \right)^2 M_{ij}. \]  

(4.19)

To determine the ideal value of \( c_s \) (\( c_s \) has to match five independent tensor components), Lilly (1992) defines an error function

\[ \epsilon = L_{ij} - \left( c_s^{(\Delta)} \right)^2 M_{ij}. \]  

(4.20)

In the traditional formulation, the square error is minimized by averaging over horizontal planes (Eq. 3.4). Here, the coefficient \( c_s^{(\Delta)} \) is obtained by minimizing the weighted time average of the square error over fluid pathlines

\[ E = \int_{-\infty}^{t} \epsilon_{ij} (x(t'), t') \epsilon_{ij} (x(t'), t') W(t - t') dt', \]  

(4.21)

where \( x(t') \) are the positions of the fluid elements at time \( t' \), and \( W(t) \) is a weighting function. The minimum of \( E \) occurs when

\[ \left( c_s^{(\Delta)} \right)^2 = \frac{I_{LM}}{I_{MM}}, \]  

(4.22)

where \( I_{LM} \) and \( I_{MM} \) are defined as

\[ I_{LM} = \int_{-\infty}^{t} L_{ij} M_{ij} (x(t'), t') W(t - t') dt', \]  

(4.23)

\[ I_{MM} = \int_{-\infty}^{t} M_{ij} M_{ij} (x(t'), t') W(t - t') dt'. \]  

(4.24)

When the weighting function \( W(t) \) is chosen to be an exponentially decreasing function, \( I_{MM} \) and \( I_{LM} \) are the solutions to two relaxation transport equations which can be easily implemented in LES. These transport equations read:

\[ \frac{\partial I_{LM}}{\partial t} + \bar{u} \cdot \nabla I_{LM} = \frac{1}{T} (L_{ij} M_{ij} - I_{LM}) \]  

(4.25)
\[
\frac{\partial I_{MM}}{\partial t} + \bar{u} \cdot \nabla I_{MM} = \frac{1}{T} (M_{ij} M_{ij} - I_{MM})
\]

(4.26)

The model uses \(W(t - t') = T^{-1} \exp\left[ (t - t') / T \right]\), where the time scale \(T\) is chosen based on several criteria (see Meneveau et al. 1996) according to

\[
T = 1.5 \Delta (I_{LM} I_{MM})^{-1/8}.
\]

(4.27)

Among others, this choice ensures that in regions where \(L_{ij} M_{ij}\) is negative (and would produce negative coefficients without averaging), the time-scale increases inhibiting the average \(I_{LM}\) from ever becoming negative. For further details see Bou-Zeid et al. (2004) and Meneveau et al. (1996).

### 4.4.1 Inclusion of scale-dependence in the Lagrangian dynamic SGS model

The Lagrangian SGS model described above relies on scale-invariance of the Smagorinsky coefficient. This was proven to be an incorrect assumption in conditions of small turbulence integral scales (see chapter 3 and POR). A dynamic scale-dependent version of the Lagrangian SGS model is currently under development (Bou-Zeid et al. 2004 - personal communication), but not yet operational at the time of writing of this thesis. As a pragmatic compromise, following the approach of Bou-Zeid et al. (2004), in this work we employ a non-dynamic procedure to account for scale-dependence.

Instead of computing parameter \(\beta = c_s^2(2\Delta) / c_s^2(\Delta)\) dynamically from the resolved scales as outlined in chapter 3, an empirical expression is used for \(\beta\), as obtained from our field experimental data. Specifically, from the fit in Eq. 2.7 a functional form of \(\beta\) is derived as follows:

\[
\beta = \left[ \frac{1 + R(\Delta/L)}{1 + R(2\Delta/L)} \right]^2 \left[ \frac{1 + \left( \frac{L}{\kappa} \frac{\Delta}{\varepsilon} \right)^3}{1 + \left( \frac{L}{\kappa} \frac{\Delta}{\varepsilon} \right)^3} \right]^{2/3},
\]

(4.28)

where \(R(x)\) is the ramp function.

In summary, in the present simulations the Lagrangian scale-dependent dynamic SGS model with the prescribed (non-dynamic) \(\beta\) of Eq. 4.28 is used. Parameter \(c_s\) is computed from Eq. 4.22.
4.4.2 Effects of time-averaging on the coefficient

To illustrate some features of the different averaging procedures, the averages over $L_{ij} M_{ij}$ and $M_{ij} M_{ij}$ are computed in two different ways. Using the Lagrangian formalism (Eq. 4.22), $L_{ij} M_{ij}$ and $M_{ij} M_{ij}$ are accumulated along fluid pathlines and named $I_{LM}$ and $I_{MM}$. Alternatively, $c_s^2$ is computed from the same subroutine by averaging $L_{ij} M_{ij}$ and $M_{ij} M_{ij}$ over horizontal planes. The comparison between these two averaging procedures is made in the context of stable and unstable flow over a homogeneous surface. Figure 4-4 compares the $c_s^2$ determined from plane averaging ($c_s^2 = \langle L_{ij} M_{ij} \rangle_{x,y}/\langle M_{ij} M_{ij} \rangle_{x,y}$) and Lagrangian averaging ($c_s^2 = \langle I_{LM} \rangle_{x,y}/\langle I_{MM} \rangle_{x,y}$) in stable and unstable conditions. The time-series of $c_s^2$ shows that in unstable conditions plane-averaging yields a slightly smaller coefficient than Lagrangian averaging and, as expected, the coefficient determined from Lagrangian averaging fluctuates less. In stable conditions the two methods give close results with plane-averaging giving a slightly larger coefficient.

To understand these differences, in Fig. 4-5 and Fig. 4-6 contour plots of $L_{ij} M_{ij}$, $M_{ij} M_{ij}$, $I_{LM}$, and $I_{MM}$ are presented together with the horizontal and vertical velocity fields in one horizontal plane at $t = 0.5$ h in the simulations. The plane-averaged mean of the quantity under consideration is indicated in the title of each subplot. In unstable conditions (Fig. 4-5) large values of all quantities predominantly occurs along vertical buoyant updrafts occur. While $I_{LM}$ is rarely negative, large negative values of $L_{ij} M_{ij}$ are observed next to large positive values. The areas of negative $L_{ij} M_{ij}$ reduce the plane-average significantly (here $\langle L_{ij} M_{ij} \rangle_{x,y} < 0.5(\langle I_{LM} \rangle_{x,y})$), while the spatial means of $M_{ij} M_{ij}$ and $I_{MM}$ are on the same order. Conversely, the Lagrangian SGS model is structured to not yield negative values for $I_{LM}$. This is achieved by increasing the Lagrangian averaging time scale in such conditions (see Eq. 4.27). In stable conditions (Fig. 4-6) it is hard to identify any large structures in the velocity fields. Negative $L_{ij} M_{ij}$ again decrease the plane-average to less than one-half of the plane-average of $I_{LM}$. However, $\langle M_{ij} M_{ij} \rangle$ is also less than one half of $\langle I_{MM} \rangle$ such that the resulting $c_s^2$ is of the same magnitude. Overall the Lagrangian averaging seems to be beneficial since the coefficient can adjust to structures in the flow, gives a smoother field of coefficients, and
avoids the occurrence of negative values of $\mathcal{L}_{LM}$. We remark that strong backscattering degrades the performance of plane averaging in unstable conditions. (For lower resolutions ($32^3$) and unstable conditions it was even observed that negative $L_{ij}M_{ij}$ dominated the plane-average. In that case (when the plane-averaged dynamic formulation for $c_s$ is used) $c_s$ became negative and had to be artificially clipped to zero in the entire plane to avoid numerical instabilities.) Thus, Lagrangian time averaging displays important advantages compared to planar averaging.

### 4.5 Unstable and stable test cases

We recall (see Bou-Zeid et al. 2004) that the LES model using the Lagrangian scale-dependent dynamic model with prescribed $\beta$ gives excellent results in neutral conditions. Non-dimensional velocity gradients and velocity energy spectra confirm well known experimental results such as the $k^{-5/3}$ slope in the inertial range and $\Phi_m = \kappa z u_*^{-1} \partial u / \partial z = 1$ in the surface layer.

To study the effects of stability, and to quantify the effects of using $\beta = 1$ (scale-invariant approach) or $\beta \neq 1$ (scale-dependent approach), in this section we compare simulations in unstable and stable conditions with constant heat fluxes and Coriolis forcing. Subsequently in the following sections, a prescribed surface heat flux that forces a daily boundary layer cycle is studied.

Results from a $64^3$, 1 hour simulation with $\langle w'\theta' \rangle_s = 0.1$ K m s$^{-1}$ and $(u_g, v_g) = (10, 0)$ m s$^{-1}$ are shown in Fig. 4-7. The stability parameter $L$ is about -60 m during the time span, characteristic of very unstable conditions. Two variations in the SGS model, described in the previous chapter, are considered. In the first, the scale-invariance assumption uses $\beta = 1$. In the second $\beta \neq 1$, and the fit from experimental data (Eq. 4.28) is employed.

In Fig. 4-7a it can be seen that the prescribed $\beta$ decreases close to the surface for the latter option. This in turn causes an increase in $c_s^2$ (Fig. 4-7b) close to the surface as compared to the $\beta = 1$ option. Above $\sim 1000$ m, $c_s^2$ decreases and reaches a value of $c_s^2 \sim 0.002$ in the stable region above the capping inversion. The height of the capping inversion $z_i$ is often defined as the location of maximum negative heat flux (Fig. 4-7c). It occurs at $z_i \sim 1200$ m for $\beta = 1$ and $z_i \sim 1170$ m.
Figure 4-4: Time series of plane averaged and Lagrangian averaged $c_s$ from LES. (a) unstable conditions, $z = 603$ m $\sim 0.5z_i$; (b) stable conditions, $z = 95$ m.
Figure 4-5: Horizontal slice of quantities used for calculating Smagorinsky coefficients at $z = 603$ m $\sim 0.5z_i$ in LES of an unstable boundary layer with $\langle u'\theta' \rangle_s = 0.1$ K m s$^{-1}$. 
Figure 4-6: Horizontal slice of quantities used for calculating Smagorinsky coefficients at $z = 95$ m in LES of a stable boundary layer with $\langle w'\theta' \rangle_s = 0.005$ K m s$^{-1}$
for $\beta \neq 1$. Above the inversion height, the stresses and variances are close to zero. The shear stress (Fig. 4-7d) increases linearly with proximity to the ground and it is slightly smaller for $\beta \neq 1$. The velocity variances are also smaller for $\beta \neq 1$, especially near $z = 0$ (Fig. 4-7e). Ideally, the non-dimensional velocity gradient (Fig. 4-7f) should follow empirical functions (Eq. 4.16) in the surface layer ($z < 100$ to 200 m). Indeed, the agreement is good up to $z \sim 200$ m, except for a region of small $\Phi_m$ around $z \sim 50$ m.

While the unstable boundary layer grows steadily into the inversion region, the stable boundary layer is shallow and largely unaffected by the inversion region. Therefore, in Figs. 4-8(a-f) only the lower half of the simulation domain is presented. To reach stationary conditions, the simulation with $\langle w'\theta' \rangle_s = -0.005$ K m s$^{-1}$ had to be spun-up for 1 hour and averages of the hour thereafter are shown. The Obukhov length is $L \sim 500$ m, characterizing weakly to moderately stable conditions. Again, in the scale-dependent version, $\beta$ decreases near the surface (Fig. 4-8a). In stable conditions $\beta$ is also reduced at greater heights. However, the decreased $\beta$ causes $c_s^2$ to increase only up to a height of $z \sim 400$ m (Fig. 4-8b). Heat fluxes (Fig. 4-8c), stresses (Fig. 4-8d), and variances (Fig. 4-8e) decrease to zero at $z \sim 600$ m, indicating the height of the stable boundary layer. The magnitudes of stresses and variances are much smaller than in unstable conditions and the variances are smaller for $\beta \neq 1$. In comparison to the empirical results for $\Phi_m$ (Fig. 4-8f, dotted line), a deviation similar to what was observed in unstable conditions exists at $z \sim 50$ m. There, $\Phi_m$ is too small in the simulation. It increases parallel to the empirical line at larger heights.

We conclude that the LES with the Lagrangian scale-dependent dynamic SGS model captures the main features of stable and unstable boundary layers. The improvement of the scale-dependent model in comparison to a scale-invariant model is hard to quantify in the unstable case, where both predict essentially similar mean velocity gradients $\Phi_m$. In stable conditions scale-dependence of $c_s$ slightly improves the results.
Figure 4-7: Profiles of quantities averaged over 30 min during LES with $\langle w'\theta' \rangle_s = 0.1$ K m s$^{-1}$. (a) Scale-dependence parameter $\beta$, (b) Smagorinsky coefficient $c_s^2$, (c) total vertical heat flux $\langle \tilde{w}'\tilde{\theta}' \rangle + q_3$, (d) total resulting horizontal shear stress $\left(\langle \tilde{u}'\tilde{w}' \rangle + \tau_{13}\right)^2 + \left(\langle \tilde{v}'\tilde{w}' \rangle + \tau_{23}\right)^2$, (e) resolved velocity variances $\sigma^2(\tilde{u})$ and $\sigma^2(\tilde{w})$. (f) non-dimensional velocity gradient $\Phi_m = \kappa z u_z^{-1} \partial u / \partial z = 1$ and empirical functions (Eq. 4.16) for $\beta = 1$ and $\beta \neq 1$ as dotted line and dots, respectively.
Figure 4-8: Profiles of quantities averaged over 1 h during a LES with $\langle w'^{\prime} \theta^{\prime} \rangle_s = -0.005 \text{ K m s}^{-1}$. (a) Scale-dependence parameter $\beta$, (b) Smagorinsky coefficient $c_s^2$, (c) total vertical heat flux $\langle w'^{\prime} \theta^{\prime} \rangle + q_3$, (d) total resulting horizontal shear stress $\left[ \left( \langle u'^{\prime} w'^{\prime} \rangle + \tau_{13} \right)^2 + \left( \langle v'^{\prime} w'^{\prime} \rangle + \tau_{23} \right)^2 \right]^{0.5}$, (e) resolved velocity variances $\sigma^2(\bar{u})$ and $\sigma^2(\bar{w})$. (f) non-dimensional velocity gradient $\Phi_m = \kappa z u_{*}^{-1} \partial u/\partial z = 1$ and empirical functions (Eq. 4.17) for $\beta = 1$ and $\beta \neq 1$ as dotted line and dots, respectively.
4.6 Simulation of the diurnal cycle of the ABL

Here our goal is to simulate a diurnal cycle and compare with the diurnal cycle of the HATS data (see Fig. 4-2). In order to generate a realistic turbulent flow field, the simulation initialized as in Fig. 4-3 is spun-up for one hour with a constant heat flux of \(<w'\theta'>_s = 0.1 \text{ K m s}^{-1}\) and a geostrophic velocity of \(u_g = 8 \text{ m s}^{-1}\). Then the simulation is run for 24 h with time-dependent surface heat flux and geostrophic velocity boundary conditions shown in figure 4-9a,b. The simulation is forced to follow a ground heat flux which resembles the daily cycle of 9/6/2000 during HATS. The minimum is \(<w'\theta'>_s = -0.005 \text{ K m s}^{-1}\). The velocity field is forced with a geostrophic velocity. In order to replicate weaker winds at night, the geostrophic velocity \(u_g\) is decreased at night time. Time series of simulated variables at the first grid point \((z = 15.9 \text{ m})\) are presented in figure 4-9c,d,e,f. Note that some of the variables in the simulation differ quantitatively from the field experiment although qualitative trends are maintained. The priority in the simulation was to create a range of stability conditions similar to the experiment rather than exactly reproduce the measured day and night boundary layer properties. In fact, reproduction would be an impossible task since the initial and boundary conditions throughout the simulation domain are not known from the field measurements at the surface (e.g. inversion height and strength, geostrophic velocity).

The main difference between HATS and the simulation is that the range of stable conditions is smaller in the simulation. It was found that the most negative (most stable) heat flux which could be sustained in a simulation is limited. When the simulated flow field becomes too stable, anomalies (such as unphysical oscillatory behavior and instabilities) were observed with simultaneous sudden drops in \(u_*, L\), and \(\psi_m\). As an example of such behavior, in Fig. 4-10 we show the results using a lower imposed heat flux \((\min((w'\theta')_s) = -0.01 \text{ K m s}^{-1})\). (This run was for \(\beta = 1\), but similar results are obtained for \(\beta \neq 1\)). A physical reason might be laminarization of the simulated flow or a decrease of the integral scale of turbulence significantly below the grid size, i.e. no turbulence was resolved. The problem might also stem from the empirical flux-profile functions which are not well established for very stable conditions (Mahrt 1998, Poulos and Burns 2003). Thus the most
Figure 4-9: Forcing variables and output results for the simulation with $\beta \neq 1$ in LST (local standard time). The minimum of $\langle u^2 \theta^2 \rangle_s$ is -0.005 K m s$^{-1}$. 
stable conditions in our simulation are only moderately stable with \( L \sim 128 \text{ m}, \Delta/L \sim 0.77, \) and \( z/L \sim 0.12 \) at the first grid point.

Time series of profiles of different variables in the simulation are shown in Fig. 4-11. Typical inertial oscillations of the geostrophic velocity are observed. The forcing at the top requires \( \sim 1 \) h to affect the boundary layer, because the strong capping inversion limits vertical exchange of momentum. A weak low-level jet is observed at \( \sim 400 \text{ m} \) between 0200 h and 0730 h. The horizontal velocity close to the surface decreases significantly when the surface cooling starts at 1800 h. During the simulated daytime (0700 h-1600 h), the horizontal velocity is almost constant with height in the mixed layer. A cold nocturnal boundary layer can be seen in the temperature profiles starting at 2100 h and reaching up to \( \sim 400 \text{ m} \) at 0700 h. From the profiles of temperature and resolved and subgrid resulting horizontal shear stress the breakdown and growth of the daytime boundary layer can be seen in more detail. From the shallow nocturnal boundary layer (\( z \sim 400 \text{ m} \)), the daytime convective layer grows up to the inversion height within less than 1 hour after sunrise. This phase of rapid growth is called free encroachment (Sorbjan 1997). Then the growth of the ABL height is slowed by the stable inversion and penetrative convection dominates. The shear stress shows more variations in time in the daytime boundary layer than the turbulent kinetic energy. The simulation done with \( \beta = 1 \) (the scale-invariant SGS model) yields very similar results to Fig. 4-11. This is expected since scale-dependence will most strongly influence near-surface properties of the flow, while the bulk ABL parameters are largely unaffected.

Figure 4-12 shows instantaneous vertical slices of the lower boundary layer during the evening transition period. In unstable conditions \( (t = 1700 \text{ h}) \) large thermal plumes can be seen which introduce strong variations in temperature and vertical velocity. The turbulent structures decrease in size in neutral conditions upon sunset \( (t = 1730 \text{ h}) \) and become very small and vertically elongated in weakly stable conditions \( (t = 1800 \text{ h}) \), 30 min after solar heating ceased. The temperature field is then well mixed, but some large structures can still be observed at larger heights \( (z > 300 \text{ m}) \).
Figure 4-10: Forcing variables and output results for a $32^3$ simulation with $\beta = 1$ in LST (local standard time). The minimum of $\langle w' \theta' \rangle_s$ is $-0.01 \text{ K m s}^{-1}$. 

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Figure 4-11: Daily evolution of resulting horizontal velocity, temperature, turbulent kinetic energy, total vertical heat flux ($\langle \tilde{w} \tilde{\theta}' \rangle + q_3$), and total (resolved + subgrid) resulting horizontal shear stress ($\langle (\tilde{u} \tilde{v}')^2 + (\tilde{v} \tilde{w}')^2 \rangle^{0.5} + \langle (\tau_{13})^2 + (\tau_{23})^2 \rangle^{0.5}$) averaged over $x$ and $y$ for the simulation with $\beta \neq 1$. 
Figure 4-12: Vertical slices of $\tilde{w}$ and $\tilde{\theta}$ during the evening transition period between 1700 h and 1800 h in the simulation with $\beta \neq 1$. The time from the start of the simulation at 1600 h and the current value of the heat flux are given in the titles.
4.7 Smagorinsky coefficient as a function of $\Delta/L$ and $Ri_g$

A plot of the evolution of $c_s^2(z)$ from the simulation with $\beta \neq 1$ as a function of time and height is shown in figure 4-13a. As observed in the experiment, the coefficient decreases after sunset ($\sim 1730h$) and remains very low during stable conditions at night. Conversely, $c_s$ increases in unstable daytime conditions. Above the daytime boundary layer, the stable capping inversions produces a smaller $c_s$. Fig. 4-14 focuses on the evening and morning transitions. During the evening transition, large $c_s^2$ persist at mid-ABL heights ($\sim 600$ m) until $\sim 45$ min after stable conditions set in at the surface. This indicates that mixed layer turbulence prevails at upper heights in the first hours of the night.

During the morning transition, the first strong increase in $c_s$ occurs $\sim 30$ min after sunrise ($\sim 0630h$) at $z \sim 100$ m. With the rapidly increasing ABL height, $c_s$ also quickly increases at greater heights. Comparing to the simulation with $\beta = 1$ (Figs. 4-13b and 4-14c,d) it is observed that during daytime, the scale-dependent $c_s$ is only slightly larger than the scale-invariant $c_s$ at $z > 200$ m, but that close to the surface the differences become greater. At nighttime the scale-dependent coefficient is larger at distances up to $z = 700$ m. This persists until very stable conditions set in at after 2100 h. While $c_s$ during the morning transition is similarly predicted by the two approaches, the evening transition from large $c_s$ to small $c_s$ is prolonged when using the scale-dependent formulation.

In Fig. 4-15 time series of $c_s^2$ (a) and $Ri_g$ (b) are plotted for three heights together with $\Delta/L$. In Figs. 4-16 the same is plotted for $\beta \neq 1$. As observed in Fig. 4-13 the coefficient decreases rapidly after sunset, stays low during the night and increases dramatically upon sunrise. The scale-dependent model produces a larger $c_s$ and the coefficient is more stability dependent in stable conditions. In unstable conditions the scale-dependent coefficient depends less on the strength of instability, while the scale invariant $c_s$ decreases with decreasing $\Delta/L$. Next, the LES results are compared to the HATS data fit (Eq. 2.7) in Figs. 4-15c,d,e,f and 4-16c,d,e,f. While the LES predictions capture the decrease of $c_s$ in stable conditions qualitatively, $c_s$ from the scale-invariant
Figure 4-13: Daily evolution of $c_s^2(z)$ averaged over $x$ and $y$. (a) $\beta \neq 1$, (b) $\beta = 1$.

The model is too small (4-15c,d,e,f). The coefficient computed from the scale-dependent procedure is closer to the value from field measurements. In stable conditions the scale-dependent $c_s$ decreases more rapidly with stability than the scale-invariant $c_s$. In unstable conditions the scale-dependent $c_s$ reaches a plateau for $\Delta/L < -1$, which is quite realistic, while the scale-invariant $c_s$ continues to increase with growing unstable atmospheric conditions.

The other important observation from Figs. 4-15 and 4-16 is a delay in the response to changing surface conditions at larger heights (smaller $\Delta/z$). In Figs. 4-15c and 4-16c $\Delta/L$ collapses the data for $z = 15$ m ($\Delta/z = 6.19$) reasonably well. At greater heights, however, two different values are obtained for $c_s$ in unstable conditions depending on time of the day (Figs. 4-15d,e,f and 4-16d,e,f). This behavior is called hysteresis. If one considers an example of early morning and late afternoon conditions, the hysteresis becomes more intuitive. In the early morning the instability increases...
rapidly with time. Since it takes some time for the turbulence at a larger height to adjust to the new conditions at the surface, the stability conditions at greater heights are less unstable than those close to the surface. This difference is extreme when a gridpoint at a greater height is still outside of the turbulent boundary layer and thus dynamically disconnected from the unstable regime near the surface. This can be observed in Figs. 4-15b and 4-16b, where $\Delta/L$ at the surface decreases earlier than $Ri_g$ decreases, and earlier than $c_s$ increases at $\Delta/z \leq 1.0308$. Conversely, in the late afternoon the stability conditions become slowly less unstable (decaying turbulence), and thus the turbulence has more time to adjust to changing surface conditions. It is expected that a change in surface conditions needs several large eddy turnover times ($\sim 100m/u_* \sim 400$ s) to effect the entire surface layer.

Thus, the observed hysteresis behavior indicates that the surface layer length scale $L$ is not a good stability parameter for larger heights, above the surface layer, especially during the morning transition. Another parameter such as the Richardson number might be more appropriate. Whether the Richardson number is a universal parameter will be studied later. Note that in HATS the
measurements were taken closer to the surface \( z \sim 5 \) m and no hysteresis for \( c_s(\Delta/L) \) was observed.

Next, the predicted values of \( c_s \) in the surface layer are examined by comparing \( c_s \) from the simulation to values from the field experiment. In Fig. 4-17 the predictions for the coefficient from the simulations \( (c_s^{\text{LES}}) \) are compared to the measured coefficients from HATS described in chapter 2 \( (c_s^{\text{emp}}) \) and the predicted dynamic coefficients from HATS in chapter 3 \( (c_s^{\text{dyn}}, c_s^{\text{sd-dyn}}) \).

In very unstable conditions (Fig. 4-17a, \( \Delta/L \sim -4 \)), there is insufficient field experimental data available to allow comparison with LES results. Still, we observe that \( c_s \) is larger than in neutral conditions (Fig. 4-17b). Also, the scale-invariant dynamic model computes a coefficient which is smaller than the coefficient from the scale-dependent dynamic model. The difference between the SGS models with \( \beta = 1 \) and \( \beta \neq 1 \) vanishes for \( z/\Delta > 3 \).

At times when the near-ground is near neutral conditions, the hysteresis behavior of the coefficient in Figs. 4-15 and 4-16 has to be taken into account when plotting the results. Consequently in Fig. 4-17 for \( \Delta/L \sim 0 \) (b) and \( \Delta/L \sim 0.25 \) (c), two datasets are plotted for each of the two \( \beta \) cases: The larger values are recorded during the evening transition. The smaller values occur during the morning transition, when - as outlined earlier - \( \Delta/L \) is not an appropriate scaling parameter. In neutral conditions \( (\Delta/L \sim 0) \) the data from HATS and from LES agree well for the scale-invariant case, \( c_s^{\text{dyn}} \) although, as noted before, the values fall significantly below the real, measured coefficient \( c_s^{\text{emp}} \). The predictions of the scale-dependent dynamic SGS model agree well with measured values near the surface, but simulation results \( c_s^{\text{sd-dyn}} \) fall below \( c_s^{\text{emp}} \) (circles) at greater heights, even during the evening transition.

In weakly stable conditions (Fig. 4-17c, \( \Delta/L \sim 0.25 \)) \( \beta \) is always less than one in the scale-dependent version of the SGS model. Thus \( c_s^{\text{sd-dyn}} \) is larger than \( c_s^{\text{dyn}} \) at all heights during the evening transition. The scale-dependent coefficient converges to \( c_s \sim 0.1 \) and the scale-invariant coefficient approaches \( c_s \sim 0.08 \) for \( z/\Delta > 2.5 \). Field experiment and simulation results agree well, except for large \( z/\Delta \). In the most stable conditions in the simulation (Fig. 4-17d, \( \Delta/L \sim 0.75 \)), the scale-dependent formulation shows little difference to the scale-invariant version close to surface,
Figure 4-15: Results for the simulation with $\beta = 1$: (a,b) Time series of $c^2_s$, $\Delta/L$, and $Ri_g$ for three heights. (c,d,e,f) $c^2_s$ as a function of $\Delta/L$ for four heights. The circle with the arrow in (f) indicates the clockwise time sequence of the hysteresis.
Figure 4-16: Results for the simulation with $\beta \neq 1$: (a,b) Time series of $c_s^2$, $\Delta/L$, and $Ri_g$ for three heights. (c,d,e,f) $c_s^2$ as a function of $\Delta/L$ for four heights. The circle with the arrow in (f) indicates the clockwise time sequence of the hysteresis.
but they converge to different values for \( z/\Delta > 2 \). LES prediction follow the same qualitative trends as the \textit{a priori} results from HATS; quantitatively they are larger than \( c_s^{\text{dyn}} \) from HATS, but smaller than the empirically determined HATS value, \( c_s^{\text{emp}} \).

Since in LES the scale-dependent dynamic model shows improved results compared to the scale-invariant model, for the remainder of this chapter we will focus on results from the scale-dependent SGS model. Also, since it was shown that \( L \) is not a good parameterization for stability conditions at heights above the surface layer, we examine the dependence of \( c_s \) on the Richardson number.

The evolution of \( Ri_f \) and \( Ri_g \) (introduced in Eqs. 4.1 and 4.2) during the simulation is presented in figure 4-18. In stable conditions the Richardson numbers are greater than zero. The growth
of the stable boundary layer through the night up to \( \sim 700 \) m can be seen. During daytime \( Ri_g \) and \( Ri_f \) are smaller than zero and decrease with height close to the surface. Above \( z \sim 400 \) m the vertical velocity gradients in the mixed layer become very small. Thus \( Ri_f \) shows very strong oscillations between positive and negative values while \( Ri_g \) exhibits large positive values above this height. In Fig. 4-19 \( c_s \) is plotted as a function of \( Ri_g \) rather than \( \Delta/L \), for various heights above the ground. It can be immediately observed that the hysteresis effect is reduced, especially at greater heights (smaller \( \Delta/z \)). We also note that during the simulation \( c_s \) does not become zero when \( Ri_g > Ri_c = 0.25 \), as can be seen in Fig. 4-19. This differs from the HATS data which yields \( c_s \sim 0 \) for \( Ri_g > 0.25 \). We also observe that the model of BDM overpredicts \( c_s \) in unstable conditions, while the fit from HATS captures the LES data for the evening transition well, except for an underprediction for \( \Delta/z = 6.185 \).

The continued presence of a hysteresis effect in the scale-dependent model strongly suggest that neither \( \Delta/L \) nor \( Ri_g \) appear to be appropriate stability parameters to parameterize \( c_s \) uniquely throughout the boundary layer, including heights above the surface layer. In the surface layer, \( Ri_g \) collapses the data better than \( \Delta/L \) but there are still hysteresis effects for \( c_s \) during the morning and evening transitions.

### 4.8 Conclusions

We conclude that Lagrangian dynamic SGS models in LES of ABL flow of varying stability are able to predict trends of the Smagorinsky coefficient \( c_s \) that agree well with the trends measured \( a \ priori \) in the HATS experiment of chapters 2 and 3. When the surface is approached, or in stable conditions, \( c_s \) decreases. The scale invariant dynamic procedure (Germano et al. 1991) underpredicts the field experimental value of \( c_s \). \( c_s \) predicted from the scale-dependent dynamic model (Porté-Agel et al. 2000b) agrees better with field experimental measurements of \( c_s \) in different atmospheric stabilities. However, \( c_s \) increases faster with \( z/\Delta \) in the field measurements than in LES. We also observe that \( c_s \) (and also the mixing length) is reduced in the stable region above the
inversion layer.

We have also shown that $c_s$ obtained dynamically are different during the morning and evening transitions, and that they are not unique functions of $L$, or $Ri$ (although the latter provides a slightly better agreement). Hence, explicit parameterizations of $c_s$ as a function of such parameters appear to be impossible unless other parameters are included that can somehow distinguish between morning and evening transitions (for instance). Instead, the dynamic model does not require such expressions (except for the expression for $\beta$ in the currently used version of the Lagrangian model - but recall that a fully dynamic version is being developed). The dynamic model therefore appears to be an approach of great promise, as compared to parameterizations with prescribed dependencies on flow parameters.

Finally, insofar as the conclusions from the LES and the field experimental study are qualitatively quite similar, results in this chapter confirm the applicability of a priori studies to gain insights into development and testing of SGS parameterizations for LES.
Figure 4-19: $c_s$ as a function of $Ri_g$ for six heights in the simulation with $\beta \neq 1$. The circle with the arrow indicates the clockwise time sequence of the hysteresis.
Chapter 5

Summary and conclusions

LES is an important tool for the study of the turbulent transport of momentum and scalar quantities (e.g. heat, water vapor, pollutants) in the atmospheric boundary layer. ABL simulations using the Smagorinsky model require specification of the model coefficient $c_s$. When the $c_s$ derived from theoretical arguments in isotropic turbulence is used in a simulation, significant overprediction of SGS dissipation occurs when the turbulence length scales $z$ or $L$ are small compared to the filter or grid-scale $\Delta$.

The HATS experiment was described in chapter 2 in which $c_s$ was measured under a variety of flow conditions in the atmospheric surface layer. The experimental data was processed in chapter 3 further so as to derive predictions from dynamic SGS models for $c_s$. In chapter 4, a simulation of flow over a homogeneous surface with a prescribed diurnal surface heat flux was used to compare experimental measurements of $c_s$ to predictions from a numerical simulation.

The main conclusions from chapter 2 are listed below:

- The Smagorinsky coefficient is measured as $c_s \sim 0.14$ in near-isotropic conditions high above the ground. $c_s$ decreases when the integral scale of turbulence decreases, such as in stable conditions (small $L$) or near the ground (small $z$). The proper parameter to non-dimensionalize these length scales is $\Delta$. If $L$ and $z$ are small, then $c_s$ decreases with $(\Delta/L \times \Delta/z)^{-1}$. 

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In order to represent the measured data an empirical fit is proposed in Eq. 2.7.

The median of $c_s$ is independent of time scale $T_c$ over which the dissipations are averaged. However, the variability of $c_s$ decreases with increasing $T_c$ in unstable conditions, while it remains constant in stable conditions.

When the dependence of $c_s$ on the strain rate magnitude $|\tilde{S}|$ is examined, the assumption inherent in the Smagorinsky model is found to hold in neutral and unstable conditions, but $c_s$ decreases for large $|\tilde{S}|$ in stable conditions. Consequently, in stable conditions the velocity scale in the mixing length model $\ell \, |\tilde{S}|$ may have to be replaced by the friction velocity. This observation has, so far, not been explored further, since it would involve significant changes in the structure of the model.

The Prandtl number $Pr_T$ depends only weakly on stability. A robust decrease of $Pr_T$ with decreasing $\Delta/z$ is observed.

In chapter 3 the scale-invariant and scale-dependent versions of the dynamic model are studied.

It becomes clear that the scale-invariant dynamic model (Germano et al. 1991) underpredicts the Smagorinsky coefficient, especially in very stable conditions.

The scale-dependent dynamic model (Porté-Agel et al. 2000b) predicts $c_s$ correctly, when the time scale $T_c$ times the mean velocity is greater than 8 filter scales.

Chapter 4 of this thesis yields the following results:

LES with the Lagrangian scale-dependent dynamic SGS model gives good results for moderate levels of stability, $\Delta/L < 1$, only. For more stable conditions, simulations displayed unphysical instabilities even if physically realistic values of the Smagorinsky coefficient were being used. These observations suggest that for stable flows the basic structure of the model might have to be changed. More field experimental and computational evidence is needed on how to parameterize surface fluxes from velocity and temperature gradients under these conditions.
The stability parameter $\Delta/L$ becomes less useful to characterize the behavior of $c_s$ as a function of stratification with increasing distance from the surface. The gradient Richardson number $Ri_g$ seems to be advantageous since its application is not restricted to the surface layer. To compare with the results from the simulation, the fits for $c_s$ from HATS are recast in terms of $Ri_g$.

The simulation with the Lagrangian dynamic models yields a smooth and stable field of Smagorinsky coefficients. Qualitatively, $c_s$ predicted from the resolved scales in the simulation behaves very similarly to the $c_s$ measured from all scales in the experiment. $c_s$ decreases in stable conditions and close to the wall. The scale-invariant dynamic model in LES under-predicts the measured value of $c_s$ from the field experiment by about the same magnitude as the dynamic model in HATS.

The scale-dependent dynamic model in LES causes an increase in $c_s$ compared to the scale-invariant model. The resulting $c_s$ is similar to the coefficient measured in HATS, but $c_s$ does not increase with height as strongly as in the field study. From the wide range of unstable conditions in the simulation it can be concluded that $c_s$ increases in weakly unstable conditions beyond its neutral value and levels off for $\Delta/L > 1$.

The good agreement between $c_s$ determined from simulation and experiment confirms the applicability of a priori tests from field experiments to numerical simulations with LES.

The observations of hysteresis behavior when using either $L$ or $Ri$ to parameterize the effects of stability upon $c_s$ suggest that such explicit parameterizations may be impossible unless many other parameters are included that can somehow distinguish between different conditions (such as morning and evening transitions). This provides strong support for the dynamic model which does not require specifying such explicit dependencies.
5.1 Suggestions for future work

Although this dissertation has provided significant evidence from field experiments for the good performance of scale-dependent dynamic SGS models compared to scale-invariant dynamic SGS models, a fully dynamic version of the model (in which $\beta$ and $Pr_T$ are determined dynamically) has yet to be implemented and tested in LES. Of special interest will be the performance of a fully dynamic model in very stable conditions, where the current version of the model showed oscillations in $L$ and $u_*$. In order to determine all parameters dynamically during the simulation, a dynamic SGS model for the SGS heat flux needs to be implemented. Such a model determines the turbulent Prandtl number depending on the flow conditions and has been proposed by Moin et al. (1991). The procedure is based on Germano’s procedure for the momentum equations. The procedure by Moin et al. (1991) using the least-square estimation of $Pr_T$ similar to that conducted by Lilly (1992), has been coded in a fortran subroutine but has not yet been sufficiently tested. A Lagrangian implementation is desirable and might even give a smoother field of $Pr_T$ with less unphysical negative values.

From the HATS experiment predominantly stable and very stable conditions were analyzed, since during daytime the wind changed to less favorable directions. Other data sets (e.g. Davis 1999 in Porté-Agel et al. 2001b and Utah 2002 in Higgins et al. 2002) could be explored further to clarify the dependence of $c_s$ on $\Delta/L$ in very unstable conditions. In the simulations presented in this thesis $c_s$ increased between $-1 < \Delta/L < 0$ (see Fig. 4-16c,d,e,f). However, since Lagrangian averaging is not possible in field experiments, the abundance of backscatter events might reduce $c_s$ computed from Eulerian averaging as shown in chapter 4.3.

There exist a great amount of possible applications of the Lagrangian scale-dependent dynamic procedure in LES of the ABL. In the literature on numerical simulations of atmospheric flows, the dynamic procedure has not been used (except for Porté-Agel et al. 2000b). In ABL research, LES is typically still used to study steady state problems with periodic, homogeneous boundary
conditions, not much different from the early work of Deardorff in 1970. The time is ripe to use new dynamic SGS models to study daily evolution of the ABL, evening and morning transition, heterogeneous surfaces, and many other real world phenomena.
Appendix A: Test of filtered velocity gradient accuracy

In order to assess the data accuracy, in addition to the tests described in Horst et al. (2004), one can check how closely the measured filtered velocity gradients obey the divergence-free condition,

$$\frac{\partial \tilde{u}}{\partial x} + \frac{\partial \tilde{v}}{\partial y} + \frac{\partial \tilde{w}}{\partial z} = 0. \quad (6.1)$$

Since the equality cannot hold exactly, we must compare the magnitude of the divergence with typical velocity gradient magnitudes. Similar to Zhang et al. (1997) we examine the dimensionless parameter $\eta$ defined according to:

$$\eta = \frac{\left(\frac{\partial \tilde{u}}{\partial x} + \frac{\partial \tilde{v}}{\partial y} + \frac{\partial \tilde{w}}{\partial z}\right)^2}{\left(\frac{\partial \tilde{u}}{\partial x}\right)^2 + \left(\frac{\partial \tilde{v}}{\partial y}\right)^2 + \left(\frac{\partial \tilde{w}}{\partial z}\right)^2}. \quad (6.2)$$

This divergence-parameter $\eta$ vanishes if the divergence-free condition is obeyed exactly. Moreover, for random data where the individual gradient terms are uncorrelated, $\eta = 1$. $\eta$ is bound by $0 < \eta < 3$. For our data, $\eta$ varies from one data sample to another and so no unique value of $\eta$ exists. Instead, as in Zhang et al. (1997) we measure the probability density function (pdf) of $\eta$ and thus document the frequency of occurrence of different values of $\eta$. $\eta$ is computed for the four different arrays over the entire data set and pdfs are plotted in Fig. 6-1. Clearly $\eta = 0$ (satisfaction of continuity) is the most likely value. Between 50% (for array 1) and 65% (for array 4) of the data are between $0 < \eta < 0.5$. Comparing the pdfs with each other one can state that accuracy of gradients decreases with increasing $\Delta/z$. No conclusions can be made about relative errors of $x$-, $y$- or $z$-gradients, but we expect the largest contribution to the error to be from the first-order one-sided derivatives in the $z$-direction. The level of error in evaluating derivatives apparent from this test can be considered reasonable (although it is not small).
Figure 6-1: Probability density distribution of divergence parameter $\eta$ (Eq. 6.2) for the four HATS arrays with different values of $\Delta/z$. $\eta = 0$ for perfect data (satisfying mass continuity), $\eta = 1$ for pseudorandom data, and $\eta$ is bound by $\eta \leq 3$. All data specified in column 2 of table 2.1 are used for the pdf (over $2.5 \times 10^6$ data points per array).

Appendix B: Evaluation of $\beta$

From chapter 3.1 it is known that $(c_s^{(\Delta)})^2 = \langle L_{ij}M_{ij} \rangle / \langle M_{ij}M_{ij} \rangle = \langle Q_{ij}N_{ij} \rangle / \langle N_{ij}N_{ij} \rangle$. This equality can be rewritten as

$$\langle L_{ij}M_{ij} \rangle \langle N_{ij}N_{ij} \rangle - \langle Q_{ij}N_{ij} \rangle \langle M_{ij}M_{ij} \rangle = 0,$$

(6.3)

which has two unknowns, $\beta = (c_s^{(\alpha\Delta)})^2 / (c_s^{(\Delta)})^2$ and $\theta = (c_s^{(\alpha^2\Delta)})^2 / (c_s^{(\Delta)})^2$. As shown in POR, one unknown can be eliminated by assuming a basic functional form of the scale dependence of the coefficient. A power law assumption $(c_s^{(\alpha\Delta)})^2 = (c_s^{(\Delta)})^2 \alpha^\phi$ yields $\theta = \beta^2$. After substituting, Eq. 6.3 can be written as a fifth order polynomial in $\beta$:

$$P(\beta) \equiv A_0 + A_1\beta + A_2\beta^2 + A_3\beta^3 + A_4\beta^4 + A_5\beta^5 = 0.$$

(6.4)
Above,

\begin{align*}
A_0 &= b_2 c_1 - b_1 c_2, \quad A_1 = a_1 c_2 - b_2 e_1 \quad \text{(6.5)} \\
A_2 &= b_2 d_1 + b_1 e_2 - a_2 c_1, \quad A_3 = a_2 e_1 - a_1 e_2 \quad \text{(6.6)} \\
A_4 &= -a_2 d_1 - b_1 d_2, \quad A_5 = a_1 d_2, \quad \text{(6.7)}
\end{align*}

where

\begin{align*}
a_1 &= -2\alpha^2 \Delta^2 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{L}_{ij} \right\rangle, \quad a_2 = -2\alpha^4 \Delta^2 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{Q}_{ij} \right\rangle \quad \text{(6.8)} \\
b_1 &= -2\Delta^2 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{L}_{ij} \right\rangle, \quad b_2 = -2\Delta^2 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{Q}_{ij} \right\rangle \quad \text{(6.9)} \\
c_1 &= 4\Delta^4 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{S}_{ij} \right\rangle, \quad c_2 = 4\Delta^4 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{S}_{ij} \right\rangle \quad \text{(6.10)} \\
d_1 &= 4\alpha^4 \Delta^4 \left\langle \left| \bar{S} \right|^2 \bar{S}_{ij} \bar{S}_{ij} \right\rangle, \quad d_2 = 4\alpha^8 \Delta^4 \left\langle \left| \bar{S} \right|^2 \bar{S}_{ij} \bar{S}_{ij} \right\rangle \quad \text{(6.11)} \\
e_1 &= 8\alpha^2 \Delta^4 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{S}_{ij} \right\rangle, \quad e_2 = 8\alpha^4 \Delta^4 \left\langle \left| \bar{S} \right| \bar{S}_{ij} \bar{S}_{ij} \right\rangle. \quad \text{(6.12)}
\end{align*}

**Appendix C: Taylor’s hypothesis**

Taylor’s hypothesis \((\partial / \partial x = -\langle U_c \rangle \partial / \partial t)\) assumes that frozen turbulence is advected by a convection velocity \(U_c\) past a sensor. Taylor’s hypothesis (Taylor, 1938) has often been used in turbulence research to convert a time series at a fixed point in space to a spatial signal at a fixed instant in time. The latter is desirable, because we want spatial information about the scales of motion in the boundary layer, but difficult to achieve with traditional measurement techniques, i.e. point sensors. For this purpose, Taylor (1938) introduced the hypothesis of frozen turbulence. This hypothesis states that eddies are only advected by the flow but do not evolve dynamically. The mathematical formulation of Taylor’s hypothesis for any variable \(\Phi\) is:

\[
\frac{\partial \Phi}{\partial t} = -u_1 \frac{\partial \Phi}{\partial x_1} - u_2 \frac{\partial \Phi}{\partial x_2} - u_3 \frac{\partial \Phi}{\partial x_3}.
\]  

(6.13)
Wyngaard and Clifford (1977) expressed the relation in terms of wavenumber \( \kappa \), frequency \( f \) and the magnitude of the convection velocity, \( U_c \): \( \kappa = f / U_c \). Conditions for the acceptable error when applying Taylor’s hypothesis have usually been expressed in terms of the turbulence intensity.

\[
TI = \sigma_u / \langle u \rangle,
\]

(6.14)

i.e. standard deviation of the velocity divided by its mean. TI decreases with height and is generally larger in convective (unstable) conditions, where buoyancy induced turbulence enhances turbulence created by mechanical wind shear. Willis and Deardorff (1976) suggested \( TI < 0.5 \) as a necessary condition for Taylor’s hypothesis to hold.

A lot of work has already been dedicated to quantifying the validity of Taylor’s hypothesis in turbulence research. Most of the work has concentrated on the impact on energy spectra. For instance, Lumley (1965) showed that for the high frequency part of the energy spectrum, conversion from time spectra to space spectra is problematic because of convection velocity fluctuations. Based on this insight and a few assumptions, Lumley (1965) constructed a model for the effect of a fluctuating convection velocity on the one-dimensional streamwise spectrum. Wyngaard and Clifford (1977) tested Lumley’s (1965) assumptions with an alternate approximation. Comparing Lumley’s model to a model with Gaussian convection velocity fluctuations and looking at spectral moments they found good agreement between spatial and temporal spectra at \( \langle u'^2 \rangle / \langle u \rangle^2 \leq 0.1 \) (\( u' \) are the fluctuations of the streamwise velocity). Extending Lumley’s model to anisotropic turbulence and considering several cases for atmospheric stability situations Wyngaard concluded that the spectral error increases with wavenumber, because at large wavenumbers energy from faster moving lower \( k \) eddies is aliased into the measured spectrum. Convection velocity fluctuations can thus introduce local anisotropy.

In the context of measurements of SGS stresses, the accuracy of Taylor’s hypothesis has been considered first by Murray et al. (1996) using direct numerical simulations (DNS) of low Reynolds number channel flow. They found that one-dimensional temporal filtering can introduce significant
errors in SGS variables compared to 1D spatial filtering in the streamwise direction in channel flow. They also concluded that due to the anisotropy of the structures present near the wall (blocked eddies) 1D spatial filtering in the streamwise direction compares well with 2D spatial filtering only above \( y^+ \sim 50 \). Due to the strong viscous effects in the DNS, Murray et al.’s results are not directly applicable to the high-Reynolds number case of ABL.

Tong et al. (1998) used LES of a moderately convective boundary layer in order to evaluate filter performance for field data. They used a spectral cutoff filter with two cutoff wavenumbers \( k_c z = 1.68 \) and \( k_c z = 0.84 \), representing 1/5 and 1/10 of the LES cutoff wavenumber, respectively. Using the equivalence \( k_c = \frac{\pi}{\Delta} \), these scales correspond to \( z/\Delta = 0.53 \) and \( z/\Delta = 0.27 \), respectively. The data were taken from the 10th vertical grid point (height: 39 m). The results show high correlations for the true and surrogate velocities \( \rho(\tilde{u}, \tilde{u}^T) \sim 0.9 \) for both heights) but significantly lower correlations for the true and surrogate SGS stresses \( \rho(\tau_{13}, \tau_{13}^T) \sim 0.7 \) for \( z/\Delta = 0.53 \) (Surrogate quantities are computed using Taylor’s hypothesis). According to the authors this is due to the low correlation coefficient for time vs. streamwise filtering of the velocity product \( u_1u_3 \). Further analysis suggested that the aliasing of energy contained in wavenumbers slightly higher than the cutoff wavenumber into the resolved scales is responsible for the weaker correlation, because the stress spectra increase at the cutoff wavenumber, while the velocity spectra decrease. In section C.1 we examine the validity of Taylor’s hypothesis using pairs of sonic anemometers on two towers displaced in the streamwise direction. These data can be used to find the eddy convection velocity from unfiltered field measurements. This is of particular importance to the HATS analysis in chapters 2 and 3 since there it is assumed that the convection velocity of turbulence is equal to the mean velocity. If this were not the case then the actual filter size in the streamwise direction \( \Delta_x = U_c \Delta_y / \langle u_1 \rangle \) would be different from the filter size in the crosstream direction. Thus filtered variables could be contaminated with unresolved motions or could contain only a fraction of the resolved motions, depending on ratio of convection velocity to mean velocity.

However, since these single sonic anemometer data cannot be filtered in the lateral direction, they are not suitable for addressing the validity of Taylor’s hypothesis in the specific context of
determining filtered turbulence statistics and SGS stresses. Thus, in section C.2 we employ numerical simulation results from LES using spatial and temporal filtering at a scale larger than the simulation grid size. Specifically, we compare filtered velocities and SGS stresses determined from purely spatial horizontal filtering, with the SGS stresses obtained from a combination of time filtering (that corresponds to streamwise filtering using Taylor’s hypothesis) and spatial filtering in the lateral direction. Henceforth, a superscript “T” will denote quantities with streamwise filtering evaluated using Taylor’s hypothesis.

C.1 Eddy convection velocity from spatial cross-correlations

Spatial cross-correlation of velocity signals is a useful tool for examining the validity of Taylor’s hypothesis and for determining the eddy convection velocity (Powell and Elderkin, 1974). As illustrated in Hinze (1975, p. 422), Taylor’s hypothesis suggests a peak in the spatial cross-correlation at a time lag $dt = dx/\langle u_1 \rangle$, where $dx$ is the distance at which the spatial cross-correlation is evaluated and $\langle u_1 \rangle$ is the mean streamwise velocity. If Taylor’s hypothesis holds exactly, the value of the correlation function $\langle u'_i(x_0, t_0)u'_i(x_0 + dx, t_0 + dt) \rangle / \langle u'_i^2 \rangle$ at the peak should be equal to 1.

Fig. 6-2 shows representative results of spatial cross-correlation as a function of time lag, obtained from two sonics separated in the streamwise direction. Two curves are shown for the two different heights where measurements were taken. A third curve shows results from LES (described in the next section). To a first approximation, the figure shows that the peak correlation indeed occurs near $dt \approx dx/\langle u_1 \rangle$, with increasing correlation peaks at larger heights. More precisely, the peak in cross-correlation occurs left of the vertical line at $dt \langle u_1 \rangle/dx = 1$. Defining the “eddy convection velocity” $U_c$ as the velocity implied by the peak correlation time $dt_{\text{max}} (U_c = dx/dt_{\text{max}})$, the results in Fig. 6-2 show that $U_c$ is slightly higher than the mean velocity.

For statistically more meaningful results, the eddy convection velocity and peak cross-correlation value are measured as in Fig. 6-2 for 47 records of 27 minute periods of data for near-neutral stability.

Ideally, for the two towers to measure a correlation of the same flow structures, the horizontal
velocity should be parallel to a line spanned by the two towers. In order to correct for deviations of mean wind-direction from this line, instead of their actual displacement $dx$ we compute the effective distance $dx_{eff}$ using $dx_{eff} = dx \cos(\alpha)$ (where $\alpha$ is the angle of the mean velocity during each 27-minute period). Further investigation reveals that the peak correlation does not change considerably for an angle $-15^\circ < \alpha < 15^\circ$, i.e. data in this $\alpha$-range can be considered for the analysis given that $dx_{eff}$ is used to obtain $U_c$.

Also evaluated for each segment of data is the turbulence intensity (Eq. 6.14). Fig. 6-3 shows the measured convection velocities plotted vs. turbulence intensity. No apparent trend of eddy convection speed with TI can be observed. From these results we compute for each velocity component and sampling height the median and the quartiles of the ratio of eddy convection velocity
and mean streamwise velocity

\[ R_i = \frac{U_c}{\langle u_1 \rangle} \]  

(6.15)

(in order to give a sense of the spread around the mean value from one 27 minutes sample to another). The average peak in the correlation function is also computed for each case. The results are summarized in table 6.1.

Figure 6-3: Ratio of eddy convection velocity and mean streamwise velocity \( R_i = U_c/\langle u_1 \rangle \) vs. turbulence intensity \( u'_1/\langle u_1 \rangle \). \( U_c \) is obtained from maxima of spatial cross-correlations of velocity vector components \( u, v, \) and \( w \). A subscript “l” labels data from sonics at lower height \((z-d_0 = 4.01 \text{ m})\), likewise “u” means upper height \((z-d_0 = 8.34 \text{ m})\).

Significant differences for relative convection velocities of different velocity components are observed \((R_1 > R_3 > R_2, \text{ in agreement with Powell and Elderkin, 1974})\). The spread around these values (say mean of \( \left| R_i^{q3} - R_i^{q1} \right|/2 \)) is about 0.04. The maximum of spatial cross-correlation \( \rho_i^{\text{max}} \) is dependent on velocity component \((\rho_1^{\text{max}} > \rho_2^{\text{max}} >> \rho_3^{\text{max}})\) and increases with height.

A general conservative estimate for the error in using the mean velocity as turbulence convection velocity is taken to be the third quartile of the convection velocities of all velocity components at
Table 6.1: First quartile \( R_{q1} \), median \( R_{med} \), third quartile \( R_{q3} \) of the ratio of eddy convection velocity and streamwise velocity \( R_i \), and mean of the maxima of spatial cross-correlation \( \rho_{max} = \max(\langle u'_i(x_0, t_0)u'_i(x_0+dx, t_0+dt)\rangle/\langle u'_i^2 \rangle) \) (no summation over \( i \)) determined at the peak of the spatial cross-correlation of \( u_i \) velocities.

Both heights, \( R_{q3} = 1.1 \). Among others, these differences affect our estimate of the filter size in the streamwise direction, which is based on Taylor’s hypothesis. Roughly speaking, we may conclude that the effective streamwise filter scale in our data analysis is up to 10% smaller than the cross-stream filter scale.

It can also be concluded that the validity of Taylor’s hypothesis depends significantly on which quantity is being considered. Results for different velocity components differ from each other, and differences also occur among filtered or unfiltered quantities. Thus to examine Taylor’s hypothesis with regard to 2-d spatially filtered quantities (e.g. SGS stresses) we examine simulation results which can mimic spatial filtering of crosswind arrays of sensors.

C.2 Taylor’s hypothesis for subgrid-scale stresses

C.2.1 LES of a neutral boundary layer

The LES is based on the numerical approach described in Albertson & Parlange (1999) and extended in Albertson & Parlange (2000) which uses pseudospectral treatment in horizontal planes (periodic boundary conditions) and second-order finite differencing in the vertical direction.

A neutral ABL is simulated on a \( N^3 = 120^3 \) grid, which is staggered in the vertical direction. In
the output, the vertical velocity is linearly interpolated from the staggered grid nodes for vertical velocities to the horizontal velocity nodes. Nonlinear convective terms and SGS stress are dealiased using the 3/2 rule (Orszag 1970). The flow is driven by a constant pressure gradient in the streamwise direction, implying a prescribed friction velocity \( u_* \). The domain size is \( H \times 2\pi H \times 2\pi H \), with grid-size \( \delta = (2\pi H/N) \). The top boundary at \( z = H \) is a stress-free boundary. At the ground \((z = 0) \) a traditional log-layer boundary condition is used in which the wall shear stress is prescribed (Moeng, 1984). The roughness parameter on the ground is chosen to be \( z_0/H = 10^{-4} \).

As a subgrid-scale parameterization for scales smaller than \( \delta \) we use the scale-dependent dynamic model (Porté-Agel \textit{et al.}, 2000b), which determines the Smagorinsky coefficient self-consistently from the resolved scales in the simulation. The model thus adjusts to local conditions, without assuming that the coefficient is scale invariant. For further details about the model, see Porté-Agel \textit{et al.} (2000b). In this appendix we use the plane-averaged results, as opposed to the more advanced Lagrangian approach of chapter 4.

Fig. 6-4 documents basic features of the simulation, showing that the dynamic coefficient \( c_s \) yields an approximately constant value in the more isotropic turbulence region away from the ground, whereas it decreases close to the wall. Moreover, the dimensionless velocity gradient \( \Phi = 1 \) remains near unity (Monin-Obukhov scaling) near the ground, while the energy spectra show the expected \( k^{-1} \) and \( k^{-5/3} \) slopes for large scales and the inertial range, respectively. The mean velocity at the top of the simulation domain is \( \langle u_1(z = H) \rangle / u_* = 21.94 \).

For the analysis of Taylor’s hypothesis, velocity vectors \( u_i(x, y, z, t) \) at each height \( z \) are stored every \( t = 1.6 \times 10^{-4} H/u_* \) for a total duration of 0.08\( H/u_* \) (500 samples over about 0.3 domain crossing times at the mean velocity at the top of the domain). In order to obtain a “temporal” field invoking Taylor’s hypothesis, we first choose a reference plane at a fixed streamwise distance, \( x_0 \). We use \( x_0/H = \pi \), i.e. a vertical plane transverse to the mean flow at the center of the domain (corresponding to horizontal gridpoint no. \( N/2 = 60 \)). A horizontal line aligned in the \( y \)-direction on this plane mimics a horizontal array of sensors placed in the cross-stream direction at height \( z \). The velocities \( u_i(x_0, y, z, t) \) (with \( t - t_0 \in [-0.88H/u_*, +0.88H/u_*] \)) provide a time series which is
Figure 6-4: (a) Smagorinsky coefficient $c_s$ obtained from the scale-dependent dynamic model in LES (dots and solid line, bottom scale), and nondimensional velocity gradient $\Phi = \frac{\partial u}{\partial z} \frac{u^*}{\kappa z}$ (dots and dashed line, top axis) as a function of height $z$, normalized by simulation domain height $H$ (left axis) or filter size $\delta$ (right scale). (b) Energy spectrum of streamwise velocity vs. wavenumber $k$ for heights (from top to bottom) $z/H = 0.004, 0.021, 0.038, 0.063, 0.105, 0.156, 0.248, 0.332, 0.458$. The dashed lines show $E_u \propto k^{-1}$ and $E_u \propto k^{-5/3}$.

used to obtain a new “spatial” signal $u^T_i(x, y, z, t_0) \equiv u_i(x_0 - U_c(t - t_0), y, z, t_0)$ (with $x = x_0 - U_c(t - t_0)$, using Taylor’s hypothesis). As the convection velocity $U_c$ we choose the mean velocity of the spatial field, averaged over the $x$-direction over the entire domain, $U_c(y, z, t) = \langle u_1(x, y, z, t) \rangle_x$. Thus, along each $x$-direction, the spatial velocity field $u_i(x, y, z, t_0)$ is compared to the velocity field from the Taylor’s hypothesis signal $u^T_i(x_0 - U_c(t - t_0), y, z, t_0)$.

C.2.2 SGS stresses at zero displacement

We extend the analysis of Tong et al. (1998) to a wider range of the height parameter $z/\Delta$, thus also considering the effects of increasing isotropy of turbulence and decreasing turbulence intensity with height. Moreover, we use filters that mimic closely those used in the analysis of field data. Specifically, we use a Gaussian filter in the streamwise direction, and a box filter in the lateral direction.

The SGS stresses $\tau_{ij}(x, y, z, t_0) = \bar{u_i} \bar{u_j} - \bar{u_i} \bar{u_j}$ and $\tau^T_{ij}(x_0 - U_c(t - t_0), y, z, t_0) = \bar{u^T_i} \bar{u^T_j} - \bar{u^T_i} \bar{u^T_j}$
are obtained by applying the horizontal 2d-filter of size $\Delta$ to the velocities and velocity products. For the surrogate stress, $\tau_{ij}^T$, a temporal filter in the streamwise direction is combined with a spatial filter in the lateral direction (just as in field data analysis). In order to quantify the effects of not including the entire range of turbulent fluctuations at scales below $\Delta$ (only scales between $\Delta$ and $\delta$ are considered in this analysis - scales below $\delta$ are taken into account only by the SGS parameterization), the analysis is repeated for two filter sizes, $\Delta = 4\delta$ (or $\Delta/H = (8\pi/120) \sim 0.21$) and $\Delta = 8\delta$ (or $\Delta/H = (16\pi/120) \sim 0.42$). $\delta$ is the LES filter-size, $\Delta$ is the filter-size used in postprocessing the LES output. While these ratios of filter scale to boundary-layer height are significantly larger than those of the field experiments, the typical turbulence intensity levels of the simulation will be shown to be comparable to those of the field experiments. Most results presented will be normalized with filter scale $\Delta$ and the applied friction velocity $u_*$.

Two instantaneous examples of the SGS stress distribution in two representative horizontal planes at $z/\Delta = 2.27$ and $z/\Delta = 0.26$ are presented as contour plots in Fig. 6-5. From comparing contours of the true (Fig. 6-5a,c) and surrogate (Fig. 6-5b,d) stress fields it can be seen that when the distance to the ground is larger than the filter size (Fig. 6-5a,b), there is good overall correlation among features of the stress distributions, i.e. Taylor’s hypothesis is a good approximation for advection of turbulence at this height. Specifically, for zero displacement (near $x_0$, black vertical line), the correlation is high (the correlation coefficient $\rho(\tau_{13}, \tau_{13}^T) = 0.998$). At the lower plane near the ground (Fig. 6-5c,d), the agreement between $\tau_{13}$ and $\tau_{13}^T$ is slightly decreased ($\rho = 0.976$). The correlation worsens as one moves farther away from the reference location. This is quantified in Fig. 6-7.

We repeat the analysis for all horizontal planes and the 1-1 and 3-3 normal stresses, and compute correlation coefficients $\rho(x, y, z)$ between the time series of $\tau_{13}(x, y, z, t)$ and $\tau_{13}^T(x, y, z, t)$ at identical gridpoints. Averaging the correlation coefficients in $y$-direction results in $\rho(x, z) = \langle \rho(x, y, z) \rangle_y$. The correlation coefficients among stresses at zero displacement ($\rho(x_0, z)$) as a function of height are plotted in Fig. 6-6a. They are larger than 0.95 for $z/\Delta > 0.1$ for all examined stress components and even at the lowest gridpoint ($z/\Delta = 0.02$) significant correlations are still achieved ($\rho = 0.89$).
Since there are no significant differences among the results for $\Delta/\delta = 8$ and $\Delta/\delta = 4$, we conclude that the range of scales between $\delta$ and $\Delta$ used to measure the SGS stresses from the present simulations is sufficiently large. Also, the correlation coefficients for $\tau_{13}$ are slightly lower than those for the 1-1 and 3-3 components. Since the 1-3 component is of greatest interest in determining the momentum flux, for the remainder of the analysis we concentrate on the 1-3 component of the SGS stress and consider this a conservative estimate for correlations of the 1-1 and 3-3 components.

Examining the terms contributing to $\tau_{13}$ it turns out that the correlation for the filtered streamwise velocity $\tilde{u}_1$ is largest ($\rho > 0.995$ for all $z/\Delta$). High correlation is also observed for the filtered vertical velocity $\tilde{u}_3$ ($\rho > 0.95$) for all $z/\Delta$. The correlation for the filtered velocity product $\tilde{u}_1 \tilde{u}_3$
is similar but slightly higher than the one for the $\bar{w}_3$-velocity. These values are larger than those presented in Tong et al. (1998). The main reason is that their 2d-spectral filter function is less smooth in physical space than our combination of box and Gaussian filters. Using a 2-d spectral filter for our analysis, we obtain similar results as Tong et al. (1998).

While the present analysis coincides with the field measurements in terms of $z/\Delta$, it does not cover the same range in terms of $z/H$ (field experiments involve much lower $z/H$). Hence, it is of interest to compare the correlations in terms of turbulence intensity, which are more comparable between the simulation and field experiment. Although it has been shown before (Fig. 6-3) that turbulence intensity does not influence the ratio of convection velocity and mean streamwise velocity, it has been considered a crucial parameter for the validity of Taylor’s hypothesis in (unfiltered) turbulence by various investigators (Wyngaard and Clifford 1977, Willis and Deardorff 1976). The correlation coefficients are plotted versus turbulence intensity in Fig. 6-6b. In the simulation, the turbulence intensity is computed from the rms velocity of the resolved velocity, which in the field should be compared to the turbulence intensity of the filtered velocity. Over all data segments of near-neutral field experiments, the mean turbulence intensity was 0.137 with a standard deviation of about 0.051, i.e. most of the data fall within the two horizontal lines at 0.086 < $TI$ < 0.188 (filtered turbulence intensity). In this range the correlation coefficient is larger than 0.95, which also supports Taylor’s hypothesis.

The correlation coefficient alone does not provide complete information about the level of agreement between two variables. In order to assure that also the magnitude of the stresses is similar, the normalized square error, defined as $E(x, z) = \langle ((\tau_{11} - \tau_{11}^T)^2) \rangle_t / \langle \tau_{11}^2 \rangle_{tu}$ and the normalized rms error $\sqrt{E}$ are computed. The symbol $\langle . \rangle$ denotes averaging. These errors are $E \approx 0.06$ ($\sqrt{E} \approx 0.24$) at the smallest $z/\Delta$ and decreasing to $E < 0.02$ ($\sqrt{E} < 0.14$) for $z/\Delta > 0.1$. 

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C.2.3 Correlation functions between $\tau_{ij}$ and $\tau_{ij}^T$ at different displacements in the streamwise direction

Next, we examine the accuracy of Taylor’s hypothesis when it is used to interpret a temporal signal of measured SGS stress as a streamwise spatial signal. This type of use of Taylor’s hypothesis is important when calculating spatial auto-correlation functions or spectra of SGS stress signals. Specifically, we pose the question whether frequency spectra of SGS stresses can be treated as wavenumber spectra at wavenumbers below $\pi/\Delta$. Fig. 6-7 shows the correlations of true and surrogate SGS stress as a function of their displacement $(x - x_0)/\Delta$ from the measurement location $x_0$, for different $z/\Delta$.

The correlation value at $(x - x_0)/\Delta = 0$ (zero displacement) was already discussed above. In Fig. 6-7 it is seen that the correlation decreases with increasing distance from the measurement location, while it increases with increasing $z/\Delta$. An important question is up to which horizontal distance (or time) one may consider Taylor’s hypothesis valid. This question can be addressed...
Figure 6-7: Correlation function between $\tau_{13}(x-x_0, y, z, t)$ and $\tau_{13}^T(x-x_0, y, z, t)$ as a function of normalized displacement $(x-x_0)/\Delta$ for different heights $z/\Delta$ (see legend). $\Delta = 4\delta$.

by finding the distance at which the correlation coefficient falls below a chosen threshold. This distance is a multiple of the filter size, and is an increasing function of $z/\Delta$. For instance, if we set a threshold of $\rho = 0.7$ to consider Taylor’s hypothesis as approximately valid, from Fig. 6-7 we can deduce that the hypothesis holds up to distances equal to about $4\Delta$ when $z > \Delta$, but that for smaller $z/\Delta$ (e.g. $z/\Delta = 0.3$) the assumption is reasonable only for displacements of about $1.3\Delta$.

C.3 Conclusions

In summary, the validity of Taylor’s hypothesis for the analysis of field measurement data, which aims at evaluating the SGS stresses and fluxes in ABL, was examined from measurements at two towers displaced in streamwise direction and LES-generated fields. Both the correlations at zero displacement and at finite distances from the measurement point were considered. At zero displacement the correlation between the SGS stress component $\tau_{13}$ and $\tau_{13}^T$ above $z/\Delta = 0.25$ is sufficiently large ($> 0.97$) to justify the assumption. However, if we take the correlation at displaced points into account, we have to limit the displacement at different $z/\Delta$ to $x \sim r\Delta$, where $r$ is $O(1)$ for
$z < \Delta$ and increases above unity for larger distances from the ground. Field-experimental data from sensors displaced in the streamwise direction led to the conclusion that the eddy convection velocity $U_c$ is up to 20% larger than the mean streamwise velocity, which leads to a decrease in effective streamwise filter size. The value at the maximum in spatial cross-correlation, which indicates the validity of Taylor’s hypothesis, depends strongly on the velocity component of interest. Present results apply to neutral stability. For convective conditions, in which the resolved turbulence intensity increases, one expects the accuracy of Taylor’s hypothesis to degrade (Powell and Elderkin, 1974).
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