DEVELOPMENT OF STABLE BOUNDARY LAYER PARAMETERIZATIONS IN NUMERICAL WEATHER PREDICTION MODELS: A SCALE-DEPENDENT DYNAMIC LES MODELING APPROACH

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1. INTRODUCTION

Numerical weather prediction (NWP) modeling always involves boundary layer (BL) parameterization schemes to represent: (i) turbulent transfer of heat, momentum and moisture between the surface and the lowest computational level, and also (ii) turbulent transport of the same quantities across model levels inside the BL. Firstorder turbulent K-closure models are commonly used to specify the turbulent flux of a quantity ϕ at a given level proportional to the vertical gradient of that quantity using the concept of eddy-viscosity/diffusivity. The eddyviscosity/diffusivity coefficients (K_{ϕ}) strongly depend on prescribed stability functions ($f_{\phi}(Ri)$) and are typically computed as:

$$K_{\phi} = \lambda_{\phi}^2 S f_{\phi}(Ri), \tag{1}$$

where λ , *S*, and *Ri* denote mixing length, vertical wind shear and gradient Richardson number, respectively. The mixing length is customarily defined in terms of height (*z*), roughness length (*z*₀), von Karman constant (κ) and an asymptotic length scale (λ_0) as follows:

$$\frac{1}{\lambda} = \frac{1}{\kappa(z+z_0)} + \frac{1}{\lambda_0}$$
(2)

Unfortunately, the performance of field-observationsbased stability functions - like Monin-Obukhov (M-O) stability functions and their variants - in operational forecasting under very stable conditions have been found to be extremely poor because of decoupling and runawaycooling problems (Beljaars and Viterbo, 1998; Viterbo et al., 1999; King et al., 2001). This prompted ECMWF (European Centre for Medium-Range Weather Forecasts) among other operational forecasting centers to propose ad-hoc stability functions (e.g., Louis-Tiedtke-Geleyn -LTG scheme and its revised version), which are not physically based but "inspired by model performance" (Beljaars and Viterbo, 1998; Viterbo et al., 1999). Most of these ad-hoc stability functions (see Appendix for a short list) alleviate the temperature-drift problem by enhanced turbulent mixing, but at the same time create unphysical consequences, like unreasonably deep boundary layers (Viterbo et al., 1999). Till today, this critical issue is far from being resolved and duly became one of the key questions of the GABLS (Global Energy and Water Cycle Experiment Atmospheric Boundary Layer Study) initiative: "Why do (most) models like enhanced mixing in stable cases?" (Holtslag, 2003).

At this point, it has to be also emphasized that the shapes of the field-observations-based stability functions in the very stable regime are quite uncertain and a subject of ongoing debate. This ambiguity arises from the fact that stable boundary layer (SBL) measurements are rarely free from nonstationarities (e.g., bursting, mesoscale disturbances, wave activities) and the observations become increasingly uncertain with increasing stability. This inevitable limitation highlights the need for high-resolution spatio-temporal simulated information about these flows to supplement the observations. With the recent developments in computing resources, largeeddy simulation (LES) of atmospheric boundary layer (ABL) flows can provide this kind of information.

2. LARGE-EDDY SIMULATION

In high Reynolds number turbulent flows (such as ABL) computational limitations impose the choice of a grid size substantially larger than the smallest scale of motion (Kolmogorov scale). LES deals with this limitation by resolving the transport equations for all scales of motion larger than the grid size (Δ) while the contributions of the subgrid scales (SGS, smaller than Δ and presumably less important) on the resolved field is parameterized using a SGS model. The contributions of the unresolved scales on the evolution of resolved velocity (\tilde{u}_i) and potential temperature ($\tilde{\theta}$) appear in the SGS stress (τ_{ij}) and the SGS flux (q_i), respectively. Note that these SGS quantities are unknown and must be parameterized using a SGS model.

2.1 SGS Modeling

Eddy viscosity (eddy-diffusion) models are widely used in LES of the ABL. They parameterize the SGS stresses (fluxes) as being proportional to the resolved velocity (temperature) gradients. Particularly, the *ij*-component of the SGS stress tensor modeled with the eddy-viscosity model is of the form:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2[C_S\Delta]^2|\tilde{S}|\tilde{S}_{ij}$$
(3)

where, S_{ij} is the resolved strain rate tensor and |S| is the magnitude of the resolved strain rate tensor. C_S is the so-called Smagorinsky coefficient. Similarly, the SGS heat fluxes are modeled with the eddy-diffusion model as proportional to the temperature gradients

$$q_i = -\frac{C_S^2(\Delta)}{Pr_{sgs}} \Delta^2 |\tilde{S}| \frac{\partial \theta}{\partial x_i},\tag{4}$$

where, Pr_{sgs} is the SGS Prandtl number.

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The values of the SGS model parameters C_S and Pr_{sgs} are well established for homogeneous, isotropic turbulence. However, the optimal value of C_S decreases with increasing mean shear. In order to account for this, application of the constant eddy-viscosity(diffusion) model in LES of ABL (with strong shear near ground and in the stably stratified layers) has traditionally involved the use of various types of ad-hoc wall-damping and stability functions (Mason, 1994).

An alternative approach would be to use the 'dynamic' SGS modeling approach (Germano, 1991; Lilly, 1992). The dynamic model computes the value of the coefficient in the eddy-viscosity model (C_S) at every time and position in the flow. By looking at the dynamics of the flow at two different resolved scales (typically the grid scale Δ and twice the grid scale, 2Δ) and assuming scale similarity as well as scale invariance of the model coefficient [i.e., $C_S(2\Delta) = C_S(\Delta)$], one can optimize the value of C_S . Thus, the dynamic model avoids the need for apriori specification and consequent tuning of the coefficient because it is evaluated directly from the resolved scales in an LES.

In a recent work, by relaxing the assumption of scale invariance of C_S , Porté-Agel et al. (2000) proposed an improved and more generalized version of the dynamic model: the 'scale-dependent dynamic' SGS model. In a later work (Porté-Agel, 2004), the same scale-dependent dynamic procedure was applied to estimate the SGS heat flux. In essence this procedure not only eliminates the need for any ad-hoc assumption about the stability dependence of the SGS Prandtl number (Pr_{sgs}), but also completely decouples the SGS flux estimation from SGS stress computation, which is highly desirable.

2.2 LES of SBL and NWP Parameterizations

The main weakness of any LES model is associated with our limited ability to accurately account for the SGS dynamics. Under very stable conditions - due to strong flow stratification - the characteristic size of the eddies becomes increasingly smaller with increase in atmospheric stability, which eventually imposes an additional burden on the SGS models. Not surprisingly, until now none of the traditional LES models have been sufficiently faithful to the physics of strongly stratified stable boundary layer flows. Furthermore, the recent GABLS LES intercomparison study (Beare et al., 2004) highlights that the LESs of even moderately stable BLs are quite sensitive to SGS models at a relatively fine resolution of 6.25 m. At a coarser resolution (12.5 m), a couple of SGS models even laminarised spuriously. These breakdowns of traditional SGS models undoubtedly calls for improved SGS parameterizations in order to make LES a more reliable tool to study stable boundary layers.

As a first step towards this goal, in this work we utilize the new-generation scale-dependent dynamic SGS model (Porté-Agel et al., 2000; Porté-Agel, 2004) to simulate the moderately stable GABLS LES case study at relatively coarse resolutions. In previous studies the performance of this SGS model in simulating neutral boundary layers (with passive scalars) was found to be superior (in terms of proper near-wall dissipation behavior, velocity spectra etc.) compared to the commonly used SGS models. As mentioned earlier, unlike NWP models and other standard LES-SGS models, the scale dependent dynamic SGS model is capable of dynamically adjusting (i.e., without tuning) model coefficients to account for atmospheric stability. In other words, this specific LES model does not require any ad-hoc prescription of stability functions for turbulent flux parameterizations inside the BL. Therefore, this fully dynamic LES model has the potential to come up with revised and improved yet physically-based stability formulations for NWP SBL parameterizations.¹

2.3 Description of Simulation

The GABLS LES intercomparison study is described in detail in Beare et al. (2004). Briefly, the boundary layer is driven by an imposed, uniform geostrophic wind (G = 8 m/s), with a surface cooling rate of 0.25 K/hour and attains a quasi-steady state in ~ 8-9 hours with a boundary layer depth of ~ 200 m. The initial mean potential temperature is 265 K up to 100 m with an overlying inversion of strength 0.01 K/m. The coriolis parameter is set to $f_c = 1.39 \times 10^{-4}$ s⁻¹, corresponding to latitude 73° N. The computational domain size is: ($L_x = L_y = L_z = 400$ m). It is divided into $N_x \times N_y \times N_z = 32 \times 32 \times 32$ nodes (i.e., $\Delta_x = \Delta_y = \Delta_z = 12.5$ m). Another slightly finer resolution simulation with $N_x \times N_y \times N_z = 32 \times 32 \times 64$ (i.e., $\Delta_x = \Delta_y = 12.5$ m and $\Delta_z = 6.25$ m) is also carried out to study the sensitivity of our results on vertical grid-resolution.

In this study, we have used a modified version of the LES code described in Porté-Agel et al. (2000) and Porté-Agel (2004). The salient features of this code are as follows:

- Solves Navier-Stokes equations written in rotational form.
- Derivatives in the horizontal directions are computed using the Fourier Collocation method, while vertical derivatives are approximated with second-order central differences.
- Explicit second-order Adams-Bashforth time advancement scheme.
- Scale dependent dynamic SGS model. The model coefficients are obtainted dynamically by averaging in the spanwise direction.
- Stress/flux free upper boundary condition.
- M-O similarity based lower boundary condition.

¹There have been a few recent attempts to extract stability functions from traditional LES-SGS models-generated databases (see for example, Beare and MacVean 2004; Beare et al. 2004). However, almost all these SGS models in one way or another require some kind of apriori prescriptions for stability dependence of the SGS model coefficients (C_S and Pr_{sgs}). One common approach consists of using ad-hoc pointwise Richardson number based correction functions for C_S and also assumes a constant Pr_{sgs} . Thus, in our opinion, extraction of stability functions for NWP parameterizations from databases generated by these artific ially-tuned traditional LESs has fundamental limitations.

- Periodic lateral boundary condition.
- · Coriolis terms involving horizontal wind.
- Forcing imposed by Geostrophic wind.
- Staggered vertical grid.
- Rayleigh damping layer near the top of the domain.

3. RESULTS

The mean profiles of wind speed, potential temperature, momentum flux and heat flux, averaged over the final hour (8-9 hours) of simulation, are shown in Figures 1 and 2, respectively. The shapes and features of these profiles (e.g., super-geostrophic nocturnal jet near the top of the boundary layer, linear heat flux profile) are in accordance with Nieuwstadt's theoretical model for 'stationary' stable boundary layers (Nieuwstadt, 1985; Beare et al., 2004). A comprehensive set of turbulence statistics obtained from these simulations, as well as from several field campaigns (with diverse field conditions and wide range of stabilities) and wind-tunnel experiments also support the 'local scaling hypothesis' of Nieuwstadt (Nieuwstdat, 1984). These results will be reported elsewhere (Basu et al., 2004).



FIG. 1: (Left) Mean wind speed and (right) potential temperature profiles.



FIG. 2: (Left) Mean longitudinal momentum flux (\overline{uw}) and (right) heat flux $(\overline{w\theta})$ profi les for the 32 x 32 x 64 simulation.

The boundary layer height²(h), Obukhov length (L) and other characteristics of the simulated SBLs (averaged over the final hour of simulation) are given in Table 1.

In Figure 3, the averaged dynamic SGS coefficients (C_S and Pr_{sgs}) are plotted. C_S is found to decrease with atmospheric stability, consistent with recent field observational findings (Kleissl et al., 2003). The SGS Prandtl number is more or less constant (~ 0.5) inside the boundary layer and gradually increases to ~ 1 in the inversion layer, as commonly assumed.

Table 1: Basic characteristics of the simulated SBLs during the last hour of simulation

Grid Points	h (m)	L (m)	u_* (m/s)	$ heta_*$ (K)
32 x 32 x 32	217	98	0.27	0.051
32 x 32 x 64	187	93	0.25	0.046

Next, we extract the stability functions ($f_m(Ri)$ and $f_h(Ri)$) from the LES model simulated results using Equations (1), and (2). The tunable asymptotic length scale (λ_0) is assumed to be equal to 40 m following the recommendation of UK Met Office (Beare et al., 2004). From Figure 4, it is evident that the LES-derived stability functions are very similar to the observational M-O stability functions, which is perhaps expected, given the idealized terrain conditions (flat, homogeneous) for both LES and field campaigns. Now, it is known that the M-O stability functions do not include the effects of surface heterogeneity, global intermittency, katabatic flows, gravity waves etc. This also means that in order to extract some kind of 'effective' stability functions for NWP parameterizations, the underlying LES models should also be able to capture these processes and phenomena.

4. SUMMARY AND PERSPECTIVES

In the present study, we utilize a new-generation tuningfree SGS scheme to simulate a moderately stable boundary layer. The simulated statistics support the local scaling hypothesis. Also, the extracted stability functions closely resemble the empirical M-O stability functions, as anticipated.

The next logical step would be to check the performance of this new-generation as well as the traditional LES SGS schemes in simulating very stable boundary layers (VSBLs). This would of course require extensive validation against existing profiles of various turbulence statistics measured during different field campaigns. One of the characteristics of VSBLs is the existence of global intermittency (turbulent burstings in the midst of a laminar flow). In contrast to the constant coefficient eddyviscosity model, the dynamic model has the correct behavior in laminar and transitional flows (Germano et al., 1991). This makes us believe that the dynamic model and its generalized version, the scale-dependent dynamic model, will be able to model the complex intermittency behavior. Another interesting feature of VSBLs is the presence of gravity waves. Conceptually, LES is capable of simulating gravity waves, provided the domain size is large enough. Unfortunately, the present computational power dictates that in such cases one must have a coarser resolution making thus the scale dependent dynamic model more desirable than the laminarizationprone traditional SGS models.

Several other advances must be made in LES modeling (e.g., inclusion of the effects of surface heterogeneity, sloping/complex terrain induced katabatic flows) in order to successfully extract 'effective' stability functions from LES generated databases. Stability functions are integral parts of several present-day NWP models and from a

²Following Beare et al. (2004), the boundary layer height is defined as (1/0.95) times the height where the mean local stress falls to five percent of its surface value.



FIG. 3: (Left) Mean Smagorinsky coefficient (C_S) and (right) SGS Prandtl number (Pr_{sgs}) profiles.

scientific perspective, specifying them in an ad-hoc manner is not satisfactory. If LES can be made more robust and reliable, it could be effectively used to develop better stability function formulations. These are expected to substantially improve turbulent parameterizations under stable stratification and, consequently, the accuracy of regional and large-scale NWP model forecasts.

ACKNOWLEDGEMENTS

This work was partially funded by NSF and NASA grants. One of us (SB) was partially supported by the Doctoral Dissertation Fellowship from the University of Minnesota. All the computational resources were kindly provided by the Minnesota Supercomputing Institute. All these supports are greatly appreciated.

APPENDIX

The following stability functions are commonly used in operational NWP models. The subscripts m and h denote momentum and heat, respectively.

• Louis-Tiedke-Geleyn (LTG, Viterbo et al., 1999):

$$f_m(Ri) = \frac{1}{1 + 10Ri(1 + 5Ri)^{-0.5}} \quad Ri > 0$$

$$f_h(Ri) = \frac{1}{1 + 15Ri(1 + 5Ri)^{+0.5}} \quad Ri > 0$$

• Revised LTG (Viterbo et al., 1999):

$$f_m(Ri) = \frac{1}{1+10Ri(1+Ri)^{-0.5}} \quad Ri > 0$$

$$f_h(Ri) = \frac{1}{1+10Ri(1+Ri)^{+0.5}} \quad Ri > 0$$

SHARP (Beare et al., 2004):

$$f_m(Ri) = f_h(Ri) = \begin{cases} & (1 - 5Ri)^2 & 0 \le Ri < 0.1\\ & (\frac{1}{20Ri})^2 & Ri \ge 0.1 \end{cases}$$

• Long Tail (Beare et al., 2004):

$$f_m(Ri) = f_h(Ri) = \frac{1}{1+10Ri}$$
 $Ri > 0$

• The observational data-based Monin-Obukhov stability function reads as follows (Derbyshire, 1999; King et al., 2001):

$$f_m(Ri) = f_h(Ri) = \begin{cases} & (1 - \alpha Ri)^2 & Ri < 1/\alpha \\ & 0 & Ri \ge 1/\alpha \end{cases}$$

where, α is an empirical constant (\sim 5).



FIG. 4: (Left) momentum $(f_m(Ri))$ and heat $(f_h(Ri))$ stability functions.

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