8.5 SCALE DEPENDENCE AND SUBGRID-SCALE MODELING IN LES

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1. INTRODUCTION

Large-eddy simulation (LES) is becoming increasingly popular to study turbulent transport in the atmospheric boundary layer (ABL). LES explicitly resolves the dynamics of the flow for all turbulent scales larger than the grid size Δ_{LES} (on the order of 10 m in the ABL), while the contribution of the subgrid scale physics is parameterized. Subgrid-scale (SGS) modeling constitutes a major challenge in LES due to the fact that simulation results are very sensitive to *(a)* the subgrid-scale model formulation, and *(b)* the way the model coefficients are specified (Meneveau and Katz, 2000; Piomelli, 1999, 2002).

In LES the separation of scales between resolved and subgrid scales is achieved by filtering (with a filter of characteristic width $\Delta \geq \Delta_{LES}$) the equations describing the transport of momentum and scalar quantities. For a scalar θ, the effect of the unresolved scales (smaller than Δ) on the evolution of the filtered scalar concentration $\widetilde{\theta}$ appears through the SGS flux q_i, which is defined as

$$q_i = \widetilde{u_i\theta} - \widetilde{u}_i\widetilde{\theta}. \qquad (1)$$

Note that q_i needs to be parameterized (using a SGS model) as a function of the resolved (filtered) velocity and scalar fields. In the near-ground region of wall-bounded turbulent flows, such as the ABL, the characteristic eddy size is relatively small compared to the grid/filter scale, making the subgrid-scale fluxes a large fraction of the overall turbulent fluxes. Moreover, near the ground the flow becomes more anisotropic at all resolved scales (including the grid scale) as the filter scale falls near (or even outside) the upper limit of the inertial subrange. This is expected to affect the performance of most SGS models that assume, in one way or another, isotropic behavior at the subgrid scales and at the smallest resolved scales. In particular, dynamic models, used to optimize the value of the model coefficient(s) based on the information contained in the resolved scales, rely on the assumption of isotropy of the flow and scale invariance of the model coefficients at the smallest resolved scales (Germano et al, 1991; Moin et al, 1991; Lilly, 1992). In a recent *a priori* field study, Porté-Agel et al (2001) showed experimental evidence of scale dependence of the coefficient in the eddy-viscosity and eddy-diffusion models. They found that scale dependence is stronger near the ground. This is consistent with results from a numerical study (Porté-Agel et al, 2000) that shows scale dependence of the eddy-viscosity coefficient computed using the dynamic model.

In this paper, we address the issue of scale dependence in the eddy-diffusion model (for the SGS scalar flux). In Section 2 we show evidence from numerical simulations with the standard dynamic model that near the ground the model coefficient strongly depends on the grid/filter scale. In Section 3 we introduce a new dynamic procedure that accounts for the scale dependence of the coefficient based on information contained in the resolved field, thus not requiring any parameter specification. The new scale-dependent model is tested in simulations of a neutral atmospheric boundary layer with a constant surface flux of a passive scalar.

2. THE DYNAMIC MODEL

2.1 Model formulation

Eddy-diffusion models are widely used in LES of the atmospheric boundary layer. A common formulation of this model is

$$q_i^{ed} = -\left[Sc_{sgs}^{-1} C_S{}^2(\Delta)\right] \Delta^2 \left|\widetilde{S}\right| \frac{\partial \widetilde{\theta}}{\partial x_i}. \qquad (2)$$

where $|\widetilde{S}| = (2\widetilde{S}_{ij}\widetilde{S}_{ij})^{1/2}$ is the resolved strain-rate magnitude, $\widetilde{S}_{ij}$ is the resolved strain rate tensor. $Sc_{sgs}^{-1}C_S{}^2$ is a lumped coefficient that comprises the Smagorinsky coefficient C_S in the eddy-viscosity model, and the subgrid-scale Schmidt number Sc_{sgs}. Note that if θ is temperature, then $Sc_{sgs} = \mathrm{Pr}_{sgs}$ (subgrid-scale Prandtl number).

The value of the model parameters C_S and Sc_{sgs} (and therefore $Sc_{sgs}^{-1}C_S{}^2$) is well established for isotropic turbulence. In that case, if a cutoff filter is used in the inertial subrange and the filter scale Δ is equal to the grid size Δ_{LES}, then $C_S = C_o \sim 0.17$ and $Sc_{sgs} \sim 0.4$ (Lilly, 1967; Mason and Derbyshire, 1990). However, anisotropy of the flow and the presence of a strong mean shear near the surface in high Reynolds number boundary layers makes the optimum value of those coefficients depart from their isotropic counterparts.

The so-called dynamic models avoid the need for *a priori* specification and consequent tuning of coefficients because they are evaluated directly from the resolved scales in LES (Germano et al, 1991; Moin et al, 1991; Lilly, 1992). For scalar fluxes, the dynamic procedure is based on the identity

$$K_i = Q_i - \overline{q}_i = \overline{\widetilde{u}_i\widetilde{\theta}} - \overline{\widetilde{u}}_i\overline{\widetilde{\theta}}, \qquad (3)$$

where $Q_i = \overline{\widetilde{u_i\theta}} - \overline{\widetilde{u}}_i\overline{\widetilde{\theta}}$ is the SGS flux at a test-filter scale (typically $\overline{\Delta} = 2\Delta$) and K_i is a 'resolved flux' vector that

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can be evaluated based on the resolved scales. Applying the eddy-diffusion model, Q_i is determined by

$$Q_i = -\left[Sc_{sgs}^{-1} C_S{}^2\left(\overline{\Delta}\right)\right] \overline{\Delta}^2 \left|\overline{\widetilde{S}}\right| \frac{\partial \overline{\widetilde{\theta}}}{\partial x_i}. \qquad (4)$$

Substitution of Eqs. (2) and (4) into (3) leads to the system

$$K_i = Sc_{sgs}^{-1} C_S{}^2 X_i, \qquad (5)$$

where, for $\overline{\Delta} = 2\Delta$,

$$X_i = \Delta^2 \left(\overline{\left|\widetilde{S}\right| \frac{\partial \widetilde{\theta}}{\partial x_i}} - 4\frac{Sc_{sgs}^{-1} C_S{}^2\left(2\Delta\right)}{Sc_{sgs}^{-1} C_S{}^2\left(\Delta\right)} \left|\overline{\widetilde{S}}\right| \frac{\partial \overline{\widetilde{\theta}}}{\partial x_i} \right). \qquad (6)$$

It is important to note that the traditional dynamic model assumes scale invariance of the model coefficient at the filter and test filter scales, i.e.,

$$Sc_{sgs}^{-1} C_S{}^2\left(\Delta\right) = Sc_{sgs}^{-1} C_S{}^2\left(\overline{\Delta}\right) = Sc_{sgs}^{-1} C_S{}^2, \qquad (7)$$

Minimizing the error associated with the use of the eddy-diffusion model in Eq. (3) over all three vector components as well as over some averaging region of statistical homogeneity or fluid pathlines (Meneveau et al, 1996), results in

$$Sc_{sgs}^{-1} C_S{}^2 = \frac{\langle K_i X_i \rangle}{\langle X_i X_i \rangle}. \qquad (8)$$

Although widely used in the engineering community, the dynamic model has not yet become common practice in simulations of atmospheric boundary layers. In a recent study, Porté-Agel et al (2000) applied the dynamic model to compute C_S in simulations of a neutral boundary layer. They showed that, as opposed to the traditional eddy-viscosity model that is too dissipative near the ground, the dynamic model is not dissipative enough, leading to velocity gradients that are too small near the ground. They also showed that the value of C_S obtained from simulations depends on resolution, which violates the assumption of scale invariance. Next, we apply the dynamic model to compute $Sc_{sgs}^{-1} C_S{}^2$ and study the issue of scale dependence.

2.2 Numerical simulations

We implement the standard dynamic eddy-viscosity and dynamic eddy-diffusion models in the simulation of a neutrally stable (no convective forcing) atmospheric boundary layer with a constant and uniform surface flux of a passive scalar. We use a modified version of the LES code described by Porté-Agel et al (2000). The dynamic coefficients are computed every 10 time steps.

Figure 1 shows the non-dimensional vertical gradient of the mean scalar concentration $\Phi_\theta = \frac{kz}{\theta_*}\frac{d\langle\widetilde{\theta}\rangle}{dz}$ as a function of distance to the ground z, normalized by the boundary layer depth H. k is the von Karman constant ($k = 0.4$), $\theta_* = -q_w u_*^{-1}$, q_w is the surface scalar flux, and u_* is the friction velocity. According to similarity theory (Businger et al, 1971) one expects that in the surface layer (approximately lower 10 % of the boundary layer) Φ_θ has a constant value of 0.74. The combination of the eddy-viscosity model and the eddy-diffusion model yields a value of Φ_θ that is too small near the ground, and increases too sharply in the surface layer (where Φ_θ is expected to remain constant).

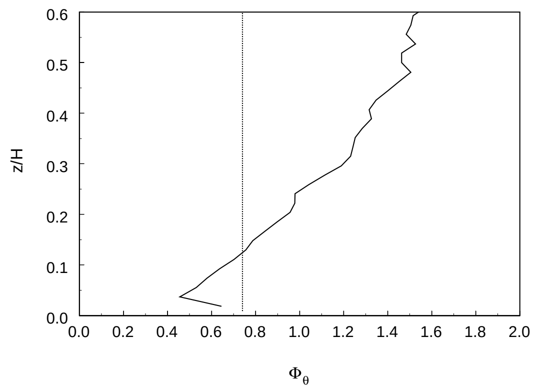

FIGURE 1. Non-dimensional vertical gradient of the mean scalar concentration ($\Phi_\theta = \frac{kz}{\theta_*}\frac{d\langle\widetilde{\theta}\rangle}{dz}$) from simulations with the traditional (scale-invariant) dynamic model.

The value of the model coefficient $Sc_{sgs}^{-1} C_S{}^2$ returned by the dynamic model (Eq. 8) is presented in Figure 2. In order to examine the dependence of the dynamic coefficient on Δ we show results from four simulations that use the dynamic model with different resolutions ($24 \times 24 \times 24$, $36 \times 36 \times 36$, $54 \times 54 \times 54$, and $80 \times 80 \times 80$ nodes, respectively). The value of the eddy-diffusion coefficient $Sc_{sgs}^{-1} C_S{}^2$ from the four simulations is presented in Figure 2 as a function of the distance to the surface z, normalized by Δ. The collapse of the four curves indicates that the model coefficient is dependent on z/Δ. For any given Δ, we observe the expected reduction of the coefficient with decreasing z. However, at a fixed height z, $Sc_{sgs}^{-1} C_S{}^2$ depends on Δ, which is consistent with the results found by Porté-Agel et al (2001) (also shown in Figure 2) using data from an *a priori* field study. Scale dependence appears to extend higher up in the boundary layer for $Sc_{sgs}^{-1} C_S{}^2$ than for C_S, which remains approximately scale invariant away from the ground (Porté-Agel et al, 2000). It is important to note that scale dependence of the model coefficient constitutes an internal inconsistency in the standard dynamic model since Figure 2 is obtained by assuming scale invariance. Therefore, it is of interest to generalize the dynamic models to include scale-dependence.

3. THE SCALE-DEPENDENT DYNAMIC MODEL

3.1 Model formulation

Without assuming that $Sc_{sgs}^{-1} C_S{}^2\left(\Delta\right) = Sc_{sgs}^{-1} C_S{}^2\left(2\Delta\right)$ we can still apply the dynamic model given by Eqs. (3), (5) and (6). Note that this change introduces a new unknown $\beta_\theta \equiv Sc_{sgs}^{-1} C_S{}^2\left(2\Delta\right)/Sc_{sgs}^{-1} C_S{}^2\left(\Delta\right)$. For scale-invariant situations, $\beta_\theta = 1$. In order to compute $Sc_{sgs}^{-1} C_S{}^2$ using Eq. (8) we need to estimate β_θ. A dynamic value

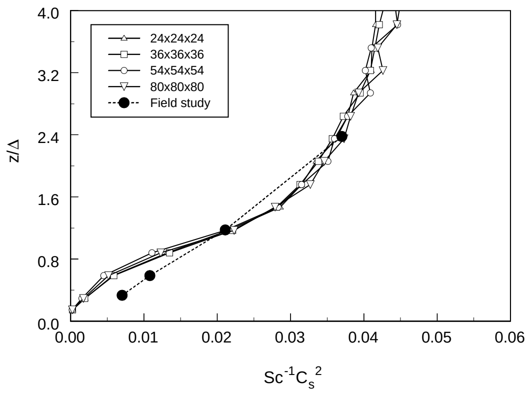

FIGURE 2. Dynamic coefficient as a function of z/Δ, obtained from simulations with different resolutions (open symbols) and from an a-priori field study (Porté-Agel et al, 2001).

for β_θ can be obtained using a second test-filter at scale $\widehat{\Delta} > \overline{\Delta}$. For simplicity, and without loss of generality, we take $\widehat{\Delta} = 4\Delta$, and denote variables filtered at scale 4Δ by a caret ($\widehat{\ }$). Writing the Germano identity between scale Δ and 4Δ yields

$$K_i' = Sc_{sgs}^{-1} {C_S}^2 X_i', \tag{9}$$

where

$$K_i' = \widehat{\widetilde{u}_i \widetilde{\theta}} - \widehat{\widetilde{u}}_i \widehat{\widetilde{\theta}}, \tag{10}$$

and

$$X_i' = \Delta^2 \left(\widehat{\left| \widetilde{S} \right| \frac{\partial \widetilde{\theta}}{\partial x_i}} - 4^2 \frac{Sc_{sgs}^{-1} {C_S}^2 (4\Delta)}{Sc_{sgs}^{-1} {C_S}^2 (\Delta)} \left| \widehat{\widetilde{S}} \right| \frac{\partial \widehat{\widetilde{\theta}}}{\partial x_i} \right). \tag{11}$$

Again minimizing the error as in Section 2 yields, besides Eq. (8), another equation for $Sc_{sgs}^{-1} {C_S}^2 (\Delta)$:

$$Sc_{sgs}^{-1} {C_S}^2 (\Delta) = \frac{\langle K_i' X_i' \rangle}{\langle X_i' X_i' \rangle}. \tag{12}$$

Setting Eq. (8) equal to Eq. (12) yields

$$\langle K_i X_i \rangle \left\langle X_i' X_i' \right\rangle - \left\langle K_i' X_i' \right\rangle \langle X_i X_i \rangle = 0, \tag{13}$$

which has two unknowns, $\beta_\theta = Sc_{sgs}^{-1} {C_S}^2 (2\Delta) / Sc_{sgs}^{-1} {C_S}^2 (\Delta)$ and $\gamma = Sc_{sgs}^{-1} {C_S}^2 (4\Delta) / Sc_{sgs}^{-1} {C_S}^2 (\Delta)$. In order to close the system, a relationship between β_θ and γ is required. Thus, a functional form of the scale dependence of the coefficient needs to be postulated. As in Porté-Agel et al (2000), we assume a power law of the form $Sc_{sgs}^{-1} {C_S}^2 (\Delta) \sim \Delta^\alpha$, or, in a dimensionally appropriate way,

$$Sc_{sgs}^{-1} {C_S}^2 (\alpha\Delta) = Sc_{sgs}^{-1} {C_S}^2 (\Delta)\, \alpha^\phi. \tag{14}$$

For such a power-law behavior, β_θ does not depend on scale and is equal to $\beta_\theta = 2^\phi$. Note that this assumption is much weaker than the standard dynamic model, which corresponds to the special case $\phi = 0$. We stress that one does not need to assume the power-law to hold over a wide range of scales, but only between scales Δ and 4Δ. A consequence of the assumed local power-law is that $Sc_{sgs}^{-1} {C_S}^2 (2\Delta) / Sc_{sgs}^{-1} {C_S}^2 (\Delta) = Sc_{sgs}^{-1} {C_S}^2 (4\Delta) / Sc_{sgs}^{-1} {C_S}^2 (2\Delta) = \beta_\theta$, and thus $\gamma = Sc_{sgs}^{-1} {C_S}^2 (4\Delta) / Sc_{sgs}^{-1} {C_S}^2 (\Delta) = \beta_\theta^2$. With this substitution Eq. (13) only contains the unknown β_θ, and can be rewritten as a fifth order polynomial on β_θ. One can show that only the largest root is physically viable. A Newton-Raphson method is used to find that root. Once β_θ has been computed, it is used in Eq. (6) to compute X_i which in turn is used in Eq. (8) to obtain $Sc_{sgs}^{-1} {C_S}^2 (\Delta)$.

3.2 Numerical simulations

The scale dependent dynamic model is applied to compute C_S and $Sc_{sgs}^{-1} {C_S}^2$ in simulations of the same neutral atmospheric boundary layer with a constant scalar flux presented in section 2. The scale-dependent coefficients are computed every 10 time steps. We found that the scale-dependent dynamic models take only about 4% more CPU time than the traditional dynamic models.

Figure 3 shows the time averaged values of $\beta_\theta = Sc_{sgs}^{-1} {C_S}^2 (2\Delta) / Sc_{sgs}^{-1} {C_S}^2 (\Delta)$ as a function of the normalized height z/H for a resolution of $54 \times 54 \times 54$ nodes. In the interior of the flow $\beta_\theta \approx 0.8$, indicating that for that resolution $Sc_{sgs}^{-1} {C_S}^2$ remains scale dependent even far from the surface. This is consistent with the results presented in Fig. 2, and it agrees with the fact that anisotropy in turbulent flows is stronger for scalars than for the velocity field (Warhaft, 2000; Kang and Meneveau, 2001).

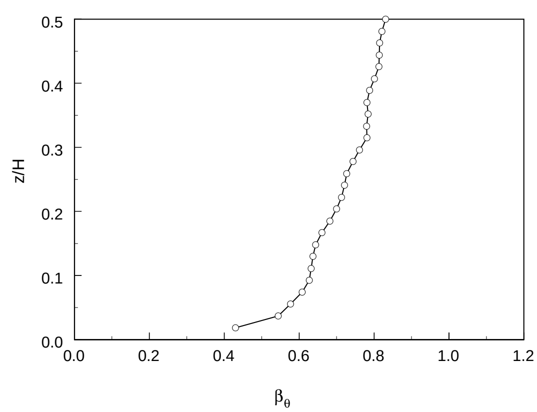

FIGURE 3. Vertical distribution of the time-averaged value of β_θ, obtained using the scale dependent dynamic model.

The averaged non-dimensional scalar concentration gradient ($\Phi_\theta = \frac{kz}{\theta_*} \frac{d\langle \widetilde{\theta} \rangle}{dz}$) from the scale-dependent dynamic model and the standard dynamic model are shown in Figure 4. The scale-dependent dynamic model yields values of Φ_θ that remain closer to 0.74, and relatively constant near the wall, indicative of the expected logarithmic profile. Also as expected, Φ_θ increase progressively as we move away from the wall into the so-called wake region.

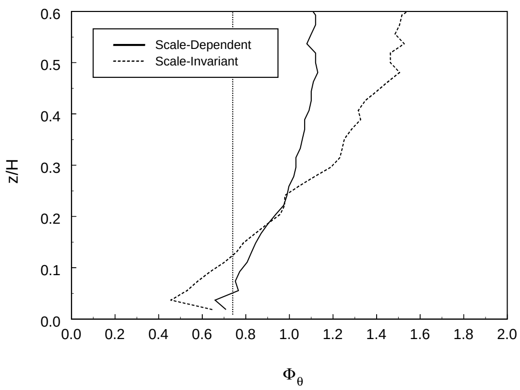

FIGURE 4. Non-dimensional vertical gradient of the mean scalar concentration ($\Phi_\theta = \frac{kz}{\theta_*}\frac{d\langle\widetilde{\theta}\rangle}{dz}$) from simulations with the traditional (scale-invariant) dynamic model and scale-dependent dynamic model.

4. SUMMARY

A modification of the dynamic model is presented that accounts for scale dependence of the lumped coefficient ($Sc_{sgs}^{-1}C_S{}^2$) in the eddy-diffusion SGS model. Motivation for including scale dependence is presented from simulations using the traditional (scale-invariant) dynamic model. Results from the simulations are consistent with previous results from an *a priori* field study (Porté-Agel et al, 2001). Scale dependence is stronger near the ground where the filter and/or test filter scales are comparable to the distance to the ground, falling near (or even outside) the upper limit of the inertial subrange.

The basic conclusions from this paper are: *(1)* The dynamic model can be generalized to allow for scale-dependence in a fully dynamic and self-consistent way. *(2)* Simulations with such a model are stable and robust, and yield expected trends of the coefficient as function of scale. *(3)* Applications to LES of the ABL show improved mean velocity and scalar concentration profiles.

Future work will extend the implementation of the scale-dependent dynamic procedure to other base models (e.g., mixed model, Lagrangian model), and to other flow conditions where scale dependence of the model coefficient is expected. In particular, the new scale-dependent procedures are expected to better capture the dynamics of the flow in boundary layers with stable stratification (e.g., nocturnal boundary layers and inversion layers) and/or high degree of surface heterogeneity (e.g., changing topography and land cover).

Acknowledgments

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