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**IMPLEMENTATION OF A TWO-EQUATION VERTICAL TURBULENT MIXING  
SCHEME IN A MESOSCALE ATMOSPHERIC MODEL**

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August 2008

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NATIONAL OCEANIC AND  
ATMOSPHERIC ADMINISTRATION



Office of Oceanic and  
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## ABSTRACT

A two-equation vertical turbulent mixing scheme is implemented in the National Center for Atmospheric Research and the Pennsylvania State University mesoscale model (MM5-V3). This scheme is based on the Mellor-Yamada level 2.5 second-moment closure (MY closure), and consists of two prognostic equations: one for the turbulent kinetic energy (TKE) and the other for the length scale multiplied by twice the TKE. In this first effort to apply the scheme to simulating vertical turbulent mixing in the atmospheric boundary layer (ABL), it is found that the physical meaning of the length scale is of fundamental importance in the determination of the closure constants in the length-scale equation for simulating vertical turbulent mixing in the ABL. If the length scale is defined as the characteristic length scale of the largest energy-containing eddies and is related to the distance that these eddies travel in the vertical direction before losing their initial TKE due to turbulent mixing and buoyancy effects, it is concluded that the closure constants in the length-scale equation should be different than those proposed previously for oceanic applications. To ensure physically sensible performance of the scheme, the technique developed by Janjić (2002) is applied for deriving necessary constraints on the length scale and for numerically integrating the scheme. The constraints on the length scale are derived by requiring that the TKE equation be nonsingular under different stability regimes in terms of the gradient Richardson number. The numerical integration is performed using an innovative splitting algorithm to control the computational modes encountered when using conventional numerical schemes. The results from a series of numerical experiments indicate that when properly choosing these constants, the evolution of the ABL structure simulated by the scheme is similar to the original scheme of the MY closure in MM5-V3 where the length scale is diagnosed. Despite the theoretical appeal and the successful implementation of this two-equation scheme, future effort will be required to use comprehensive turbulence observations to further evaluate its performance.



## 1. Introduction

One of the popular methods to simulate vertical turbulent mixing in the atmospheric boundary layer (ABL) is to use the Mellor-Yamada level 2.5 second-moment closure (MY closure) turbulence model (Mellor and Yamada 1974, 1982), which is centered on the prognostic equation for the turbulent kinetic energy (TKE, denoted as  $q^2/2$ ). An important closure parameter in the turbulence model is the so-called length scale (denoted as  $l$ ). Although the length scale is essential to the level 2.5 second-moment closure, there is no unique approach to its specification. The simplest approach to specifying the length scale is to assume that  $l$  is proportional to the distance from the surface within the ABL (see, e.g., Blackadar 1962, Mellor and Yamada 1982, and Janjić 1994). While this method works well in many applications, it is diagnostic and its treatment of the length scale far above the surface has a rather empirical nature (Holtslag 2003). Therefore, it is more desirable to use a prognostic equation with minimum empiricism to predict the length scale. A vertical turbulent mixing scheme of the MY closure uses a prognostic equation for specifying  $l$  is often called a two-equation scheme, in contrast with a one-equation scheme in which  $l$  is diagnosed.

Various approaches to deriving the prognostic equation for  $l$  have been proposed. Unlike the TKE equation that is derived from the Reynolds-averaged Navier-Stokes equations, the equation for  $l$  cannot be derived systematically from the governing laws of fluid motion. Essentially, it is cast as a transport equation for a quantity involving  $l$  that is analogous to the TKE equation with a different set of closure constants. In general, the equation for  $l$  can be written as a transport equation for a quantity involving  $q$  and  $l$ :  $c^p q^m l^n$ , where  $c$  is a constant, and  $p$ ,  $m$  and  $n$  are integers (see, e.g., Burchard 2002 and Kantha 2004). It has been suggested that for a homogeneous shear layer all the approaches to deriving the equation for  $l$  are equivalent (Burchard 2002, Umlauf and Burchard 2003, and Kantha 2004), and thus no one approach is fundamentally superior to another. It should be noted, however, that the ABL is not a homogeneous shear layer, and the non-uniform thermal stratification in the ABL plays an important role in controlling vertical turbulent mixing. Therefore, various length-scale equations may perform differently for the ABL.

In this paper, we present the implementation of a two-equation vertical turbulent mixing scheme in the National Center for Atmospheric Research and the Pennsylvania State University mesoscale model (MM5-V3). The prognostic equation for  $l$  in this scheme is formulated in

terms of the turbulence transport of twice the TKE. This two-equation scheme was first proposed by Mellor and Yamada (1974, 1982) for general applications in geophysical flows, and later revised by Kantha and Clayson (1994) and Burchard (2001) to simulate the vertical turbulent mixing in the ocean. Although this scheme has been applied extensively in simulating oceanic mixed layer, this is the first effort to implement it in an atmospheric mesoscale model.

Three major issues are encountered during the implementation. The first issue is related to the closure constants in the length-scale equation. The values of the closure constants in the length-scale equation are determined *a priori* according to turbulence measurements or direct turbulence simulations. In oceanic applications, measurements of simple turbulent flows generated in laboratories are commonly used to determine these closure constants (see, e.g., Mellor and Yamada 1982, Umlauf and Burchard 2003). It has been recently recognized that there exist constraining relationships among the closure constants that can be utilized to determine the closure constants according to comprehensive turbulence measurements, (see, e.g., Burchard 2002). Although in many oceanic applications the closure constants determined from the laboratory measurements have appeared to work well, uncertainties remain in the constants' values and continuing efforts are still being made to refine them. It is also not clear whether the closure constants that have worked well in oceanic applications are well suitable for simulating vertical turbulent mixing in the ABL. Therefore, how to properly determine the closure constants that are suitable for applications in the ABL needs to be investigated.

The second issue is related how to ensure physically sensible performance of the scheme. Vertical turbulent mixing schemes based on the MY closure have been known to require the use of the so-called realizability constraints on the shear and stability parameters as well as on the length scale to perform reasonably and robustly (see, e.g., Mellor and Yamada 1982, Galperin *et al.* 1988, Helfand and Labraga 1988, and Burchard 2002). The equation for the length scale itself does not provide a guarantee that the predicted  $l$  is always in agreement with the realizability constraints such that the modeled turbulent mixing is physically meaningful for a given flow situation. Therefore, properly established constraints are required to limit the solution of the length-scale equation. Although various approaches to imposing the constraints on the length scale have been proposed for oceanic applications, they are not as theoretically appealing as that proposed by Janjić (2002). Janjić's approach is innovatively different than the others in that the constraints on the length scale are derived based on requiring that the analytical

solution of the TKE equation be nonsingular, and thus there is no need to constrain the shear and stability parameters like the other approaches. However, this approach has not been applied to a two-equation scheme.

The third issue is concerned with numerical integration of the scheme. In oceanic applications, the scheme is discretized implicitly in time with centered in space differencing for numerical integration. It is found that the numerical solution of the equations for both the TKE and the length scale are apparently contaminated with computational modes. To make the results from the two-equation scheme physically meaningful, the computational modes need to be eliminated or significantly reduced. The numerical scheme proposed by Janjić (2002) is found to be effective to that end.

The rest of the paper is organized as follows. The two-equation vertical turbulent mixing scheme is described in section 2. Section 3 presents results from the investigation on how to determine the closure constants in the length-scale equation. How to apply Janjić's approach to establishing the constraints on the length scale and to numerical integrating the two-equation scheme is presented respectively in sections 4 and 5. Results from a series of numerical experiments are shown in section 6 to illustrate the sensitivity of the scheme to different values of the closure constants within their admissible ranges, which is followed by summary and final remarks (section 7).

## 2. The Vertical Turbulent Mixing Scheme

The vertical turbulent mixing scheme consists of two equations: the equation for the TKE and the equation for  $l$ . The TKE equation is written as

$$\frac{\partial \left( \frac{q^2}{2} \right)}{\partial t} - \left( \frac{\partial}{\partial z} \right) \left[ l q S_q \left( \frac{\partial}{\partial z} \right) \left( \frac{q^2}{2} \right) \right] = P_s + P_b - \varepsilon, \quad (1)$$

where

$$P_s = -\overline{wu} \left( \frac{\partial U}{\partial z} \right) - \overline{wv} \left( \frac{\partial V}{\partial z} \right), \quad P_b = \beta g \overline{w\theta_v}, \quad (2)$$

$$\varepsilon = \frac{q^3}{B_1 l}, \quad (3)$$

$$-\overline{wu} = K_m \frac{\partial U}{\partial z}, \quad -\overline{wv} = K_m \frac{\partial V}{\partial z}, \quad -\overline{w\theta_v} = K_H \frac{\partial \Theta_v}{\partial z}, \quad (4)$$

$$K_m = lqS_M, \quad K_H = lqS_H, \quad (5)$$

$$S_M (6A_1 A_2 G_M) + S_H (1 - 3A_2 B_2 G_H - 12A_1 A_2 G_H) = A_2 \quad (6a)$$

$$S_M (1 + 6A_1^2 G_M - 9A_1 A_2 G_H) - S_H (12A_1^2 G_H + 9A_1 A_2 G_H) = A_1 (1 - 3C_1) \quad (6b)$$

$$G_M = \left( \frac{l^2}{q^2} \right) \left[ \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{\partial V}{\partial z} \right)^2 \right], \quad G_H = - \left( \frac{l^2}{q^2} \right) \beta g \frac{\partial \Theta_v}{\partial z}, \quad (7)$$

where  $U$ ,  $V$  and  $\Theta_v$  are the velocity components and virtual potential temperature of the mean flow, and the rest of symbols are of the same meaning as in Mellor and Yamada (1982).

The success of (1)-(7) in the simulation of vertical turbulent mixing is critically dependent on well-calibrated closure constants ( $A_1, A_2, B_1, B_2, C_1, S_q$ ) and an appropriate specification of the length scale. The values of the constants in (1)-(6) are chosen as those by Janjić (2002), i.e.,

$$(A_1, A_2, B_1, B_2, C_1, S_q, \beta) = (0.65988838, 0.65742096, 11.877992, 7.226971, 0.00083092297, 0.2, 1./270).$$

Note that they are different than those proposed in Mellor and Yamada (1982) that are also used in Kantha and Clayson (1994). They are chosen here because they are used in the original vertical turbulent mixing scheme (hereafter referred to as the ETA scheme) in the mesoscale model in which this two-equation scheme is implemented. This original scheme, developed by Janjić (1990, 2002) for the National Centers for Environmental Prediction's (NCEP) operational limited area model, is the same as this two-equation scheme except that the length scale is diagnosed. Using these values will make it convenient and fair to compare the results from this

two-equation scheme and those from the original one-equation scheme (see the detail of the comparison later in section 6).

Following Mellor and Yamada (1982) and Kantha and Clayson (1994), the equation for  $l$  is expressed as a transport equation of  $q^2l$ , i.e.,

$$\frac{\partial}{\partial t}(q^2l) - \frac{\partial}{\partial z} \left[ q l S_l \frac{\partial}{\partial z}(q^2l) \right] = P_{sl} + P_{bl} - \varepsilon_l, \quad (8)$$

where

$$P_{sl} = lE_1P_s, \quad P_{bl} = lE_2P_b, \quad \varepsilon_l = F \frac{q^3}{B_1 l}.$$

In the above equation,  $E_1$ ,  $E_2$ , and  $F$  are the closure constants. Note that in both Mellor and Yamada (1982) and Kantha and Clayson (1994),  $F$  is not a constant, but a wall function that approaches a constant far from the surface. It seems that the inclusion of the wall function is not absolutely necessary if  $E_1$  is chosen properly. As discussed later in section 4, if  $E_1$  and  $E_2$  are chosen to be constants,  $F$  should be a constant according to the validity of (8) in a neutral surface layer. Rotta (1951) was first to propose an equation of transport form like (8) to describe the evolution of  $q^2l$  according to the two-point correlation equations derived from the Navier-Stokes equations (see also Kantha 2004).

The determination of the closure constants in (8), like that for the TKE equation, is empirical. We recommend that the following set of values be used for the results that are in the best agreement with those from the ETA scheme:

$$(E_1, E_2, F, S_l) = (2.75, 3, 3.0, 0.2) .$$

As discussed later, they are determined based on the close analogy between the TKE equation and the length-scale equation and the properties of the turbulent flow in the neutral surface layer. This analogy is regarded as physically appropriate if the length scale is defined as the characteristic length scale of the largest energy-containing eddies and is related to the distance that these eddies travel in the vertical direction before losing their initial TKE due to turbulent mixing and buoyancy effects.

It should be pointed out that the values of the constants in both Mellor and Yamada (1982) and Kantha and Clayson (1994) were determined based on reliable measurements of decaying grid-generated homogeneous turbulence or turbulence near a wall without thermal stratification. The values that they recommended are

$$(E_1, E_2, S_l) = (1.8, 1.8, 0.2) \text{ and } F = E_3 \left[ 1 + E_4 \left( \frac{l}{\kappa L} \right)^2 \right],$$

where  $(E_3, E_4) = (1.0, 1.33)$ ,  $L$  is the distance from the boundary and  $\kappa$  is the von Karman constant. It is assumed that the applicability of the constants obtained in such a way can be extrapolated to other flow situations of more complexity with thermal stratification such as in the ABL where reliable and comprehensive measurements are relatively difficult to make. However, the validity of this assumption has not been theoretically and experimentally well established, leading to the uncertainties in the determination of the closure constants. Recently, Umlauf and Burchard (2003) proposed an analytical approach in which the properties of the two equations for the TKE and the length scale are used as extra constraints to calibrate the constants. To include the buoyancy effects for stably-stratified flows, Freedman and Jacobson (2003) proposed how to modify the constants in the length scale equation that are calibrated with measurements of flows without thermal stratification. Despite the extensive effort to optimize the values of these closure constants for flow situations of different complexity, consensus has not been reached on the possibility of seeking a set of universal values suitable for the simulation of vertical turbulent mixing in geophysical flows, reflecting the fact that it is still an ongoing research how to properly specify the length scale as an essential part of parameterized turbulence modeling.

Boundary conditions are required to solve (1) and (8). In our implementation of the scheme in MM5-V3, the lower boundary condition for the TKE equation is provided using the surface flux algorithm used in the ETA scheme (Janjić 1990, 1994). This surface flux algorithm is based on the well accepted Monin-Obukhov similarity theory with the correction for the free convective limit proposed by Beljaars (1994). The lower boundary condition for  $q^2 l$  is 0.

### 3. The Closure Constants of the $q^2l$ Equation

The physical meaning of the length scale is of fundamental importance to the simulation of vertical turbulent mixing in the ABL. In the literature on the simulation of vertical turbulent mixing in the ABL, the length scale  $l$  is most often interpreted as the characteristic length scale of the largest energy-containing eddies (see, e.g., Moeng and Wyngaard 1989 and Wyngaard 1992). It is directly related to the distance that these eddies travel in the vertical direction before they loss their initial TKE due to turbulent mixing and buoyancy effects. In some references, the length scale is also linked to the so-called integral length scale (see, e.g., Kantha and Clayson 2000, p. 16). Strictly speaking, the integral length scale is associated with unbounded isotropic turbulence and is three-dimensional. The length scale  $l$  discussed here is associated turbulence in the atmospheric boundary layer, which is much more complicated than isotropic turbulence due the existence of thermal stratification in the vertical direction. The nature of the closure as described in (1)-(5) requires that the direction of  $l$  be along the vertical wind shear and thermal gradient.

The closure constants in the length-scale equation must be determined empirically. Baumert and Peters (2000) indicate that the original values proposed by Mellor and Yamada (1982), and later adapted by Kantha and Clayson (1994), are not able to simulate the most basic properties of weakly stratified shear flows. They showed that for the well-understood near-wall flow situations without thermal stratification, there exist constraints on the determination of the values of the closure constants. Here we use a different approach to address the issues related to how to determine these constants.

The equation for the length scale, (8), can be rewritten as

$$l \frac{\partial q^2}{\partial t} + q^2 \frac{\partial l}{\partial t} = E_1 l K_m S^2 - E_2 l K_H N^2 - F \frac{q^3}{B_1} + \frac{\partial}{\partial z} \left[ ql S_l \frac{\partial}{\partial z} (q^2 l) \right], \quad (9)$$

where

$$S^2 = \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{\partial V}{\partial z} \right)^2, \quad N^2 = \beta g \frac{\partial \Theta_v}{\partial z}. \quad (10)$$

Substituting (1) into (9) and using the so-called Kolmogorov-Prandtl relationships (i.e.,  $q l S_q = K_m / \sigma_m$  and  $q l S_l = K_m / \sigma_l$  where both  $\sigma_m$  and  $\sigma_l$  are empirically determined constants) yield

$$q^2 \frac{\partial l}{\partial t} = (E_1 - 2) l K_m S^2 - (E_2 - 2) l K_H N^2 - (F - 2) \frac{q^3}{B_1} + \frac{\partial}{\partial z} \left[ K_m / \sigma_l \frac{\partial}{\partial z} (q^2 l) \right] - l \frac{\partial}{\partial z} \left[ K_m / \sigma_m \frac{\partial}{\partial z} (q^2) \right]. \quad (11)$$

Now let us now apply (11) into a steady neutral surface layer in which  $\partial l / \partial t = 0$ ,  $N^2 = 0$ ,  $S = u_* / \kappa z$ ,  $q^2 = 2 c_\mu^{-1/2} u_*^2$  and  $l = \kappa z$  (where  $u_*$  is the surface friction velocity,  $\kappa$  is the von Karman constant and  $c_\mu$  is an empirical constant). It is straightforward to verify that if  $\sigma_l = 1$ , the following relationship holds for the neutral surface layer:

$$\kappa^2 = \frac{1}{2} c_\mu^{-1/2} (F - E_1). \quad (12)$$

This equation imposes an important constraint on the relationship between  $E_1$  and  $F$ . It also implies that only the difference between  $E_1$  and  $F$  controls the balance among the production, dissipation and diffusion of the length scale,  $l$ , and therefore  $q^2 l$  in the neutral surface layer. This implication is important for the determination of both  $E_1$  and  $F$  as shown later because no matter how  $F$  is determined,  $E_1$  must be determined through (12) for it to be dynamically consistent with  $F$ . A consequence of applying (12) to the determination of  $E_1$  and  $F$  is that if  $F$  involves a wall function such that it depends on  $z$ ,  $E_1$  should also be dependent on  $z$  such that the difference between them is independent of  $z$ . On the other hand,  $F$  must be a constant according to (12) if  $E_1$  is chosen as a constant.

Baumert and Peters (2000) proposed  $E_1 = 2$  according to the hypothesis introduced by Tennekes (1989) that the *integral* length scale does not, based on dimensional grounds, depend on the homogenous shear. It should be noted that setting  $E_1 = 2$  implies that the evolution of the length scale is controlled by the buoyancy and dissipation terms. Given the fact that

turbulence grows in a stratified unstable flow as well as in a weakly stratified stable flow, one has to use a positive  $E_2$  for the unstable flow and a negative  $E_2$  for the stable flow (see, e.g., Baumert and Peters 2000). Although this may not pose great difficulty in the simulation of vertical turbulent mixing in the oceanic mixed layer where the stratification is often weakly stable, it is definitely not desirable for the ABL because with a diurnal cycle, it is common for the stratification within the ABL to vary between stable stratification and unstable stratification. Moreover, although Tennekes' hypothesis may be acceptable for idealized unbounded turbulence with homogenous shear, it is perhaps too simple to be applicable to turbulence in the ABL where the shear is hardly homogenous and the buoyancy effect on turbulence is much stronger than most of the engineering flows in laboratories (more discussion on this point is provided in Kantha *et al.* 2005).

We wish to argue that in the simulation of vertical turbulent mixing in the ABL, if the length scale is defined as the characteristic length scale of the largest energy-containing eddies and is regarded as being related to the distance that these eddies travel in the vertical direction before they lose their initial kinetic energy due to turbulent mixing and buoyancy effects, its evolution as described by (11) should be closely analogous to that of the TKE in that the deviation from the balance between the turbulence production (by both shear and buoyancy) and the turbulence dissipation controls the change of the length scale. During the initial development of turbulence, the characteristic length scale of the largest energetic turbulent eddies increases with the intensification of turbulence. The greater the characteristic length scale is, the farther the largest energy-containing eddies are able to move in the vertical direction before they completely mix with the surrounding environment. The intensity of turbulence and therefore  $l$  cannot increase indefinitely because turbulent mixing tends to smooth out the vertical velocity shear and unstable stratification that are favorable for turbulence production. Therefore, the evolution of the characteristic length scale of the largest energy-containing eddies is governed by the same processes that control the evolution of the TKE. In order for the length-scale equation (11) to be valid for both unstable and weakly stable stratifications with the same set of closure constants, it is required that all the parameters before the turbulence production terms (i.e., the shear production and the buoyancy production) and the dissipation term be positive. With this requirement, (11) indicates that the lower bounds of the closure constants should be 2.

Requiring  $F > 2$  is not in agreement with the conventional value of  $F$  (which is close to 1.0 corresponding to the decay exponent of  $\sim 1.0$ ; see, e.g., Durbin and Pettersson-Reif 2001 and Umlauf and Burchard 2003) that is derived from the experimental data of decay exponent for homogenous, isotropic turbulence. If the behavior of the vertical turbulent mixing in the ABL is the same as in the turbulence in thermally unstratified flows, the values of all the closure constants can be determined uniquely from simple measurements in laboratories that isolate each term. However, there is no observational evidence to indicate whether or not this is indeed the case.

The simulation of vertical turbulent mixing in weather prediction models perhaps should be different than the simulation of engineering turbulence because the former emphasizes the effect of the largest energy-containing (i.e., flux carrying) eddies on vertical turbulent mixing in a thermally stratified environment. Because the two-equation turbulence model is not exact and the thermal stratification strongly affects vertical turbulent mixing in geophysical flows, it may not be practically possible to make the closure constants universally applicable to geophysical and engineering flows. Take the night-time atmospheric boundary layer for example. The largest eddies travel in the vertical direction against the restoring force caused by the stable stratification. According to the scaling argument made by Wyngaard (1992), this implies that in an equilibrium, stably stratified ABL, the distance (i.e.,  $l$ ) that the largest energy-containing eddies travel is proportional to the square root of the eddies' initial TKE. Thus, if the thermal stratification is held constant,  $l$  increases (or decreases) as  $q$  increases (or decreases). When  $F > 2$  is chosen, the behavior of our length-scale equation appears to be in agreement with this argument, but apparently contradictory to the prediction based on the data of homogeneous, isotropic turbulence. However, if  $F$  is chosen to be smaller than 2 as done conventionally for engineering-turbulence modeling, the prediction of (11) is that the decrease of  $q$  due to the turbulence dissipation will lead to the increase of  $l$ , which is contrary to the above argument.

Currently, there is no practical way to observationally/experimentally determine the decay rate of the length scale as a function of the turbulence dissipation rate in the ABL. This study suggests that it is not unreasonable to set  $F = 3.0$ . Because typically  $c_\mu = 0.09$ ,  $\kappa = 0.4$  (see, e.g., Durbin and Pettersson-Reif 2001) and  $E_1$  should be slightly smaller than  $F$ , this leads to  $E_1 \approx 2.9$ . In accordance with the consistent analogy between the length-scale equation

and the TKE equation,  $E_2$  should be close to  $E_1$ , assuming that the Prandtl number is very close to unity. Results from our numerical experiments indicate that  $E_2 = 3$  is acceptable when  $E_1$  varies between (2.5, 3.0). Hence, the set of values recommended in section 2, i.e.,  $(E_1, E_2, F, S_l) = (2.75, 3, 3.0, 0.2)$ , are obtained for the results that are in the best agreement with those from the ETA scheme.

Summarizing the above discussions, the close analogy between the evolutions of the length-scale and the TKE should be used to determine the constraints on the values of the closure constants in the length-scale equation. This is based on the interpretation that  $l$  is the characteristic length scale of the largest energy-containing eddies, which is directly related to the turbulent mixing of these eddies in the vertical direction. It is required that the values of  $E_1$ ,  $E_2$  and  $F$  be greater than 2.  $E_1$  should be slightly smaller than  $F$ , and  $E_1$  and  $E_2$  should be close to each other. The actual values of  $E_1$  and  $E_2$  are determined according to  $F$ . The ultimate validation of the value of  $F$ , and those of the closure constants, must rely on the comparison of the predictions of the scheme and the observations of the turbulence in the ABL.

#### 4. Constraints on the Length Scale

In general, the two-equation vertical turbulent mixing scheme does not ensure that the quantities of the TKE and  $l$  are both always within the physically meaningful range for a given flow situation. It does not even guarantee that both quantities are positive definite. Thus, constraints on the two quantities should be established to prevent nonphysical results. While it is straightforward to set the lower bounds for the two quantities (they should not be negative), setting the upper bounds is not straightforward.

It has been recognized for a long time that because the closure hypothesis and the specification of the length scale involve empirically determined closure constants, the MY closure has performance problems (see, e.g., Mellor and Yamada 1982, Galperin *et al.* 1988, and Burchard 2002). To alleviate the problems requires that the shear and stability parameters as well as the length scale be constrained properly. A proper specification of the limiting constraints on the shear and stability parameters as well as the length scale is very critical for the successful application of the MY closure. Various approaches to imposing the constraints on the length scale have been proposed for oceanic applications to constrain the shear and stability

parameters along with the length scale. However, these approaches are not as theoretically appealing and straight forward as that proposed by Janjić (2002). Janjić's approach is innovatively different than the others in that it only applies constraints on the length-scale by requiring that the solution of the TKE equation be nonsingular. The effectiveness of this approach was illustrated in the implementation of the ETA scheme. The essence of the approach can be summarized as the following.

When the thermal stratification is unstable corresponding to a negative gradient Richardson number ( $R_i$ ), the TKE production and dissipation, i.e., the right-hand side of (1) should be nonnegative and bounded. Following Janjić (2002) and using the definitions in (4) and (7), the contribution of the TKE production and dissipation can be written as

$$\left(\frac{\partial q^2/2}{\partial t}\right)_{prod/dissp} = [S_M G_M + S_H G_H - 1/B_1](q^3/l). \quad (13)$$

Substituting the definition of  $G_H$  and  $G_M$  along with  $S_H$  and  $S_M$  obtained by solving (6a) and (6b), (13) can be written in the following form

$$l \frac{\partial}{\partial t} \left( \frac{1}{q} \right) = - \left\{ \frac{\left[ \alpha \left( \frac{l}{q} \right)^4 + \beta \left( \frac{l}{q} \right)^2 \right]}{\left[ \gamma \left( \frac{l}{q} \right)^4 + \delta \left( \frac{l}{q} \right)^2 + 1 \right]} - \frac{1}{B_1} \right\}, \quad (14)$$

where

$$\alpha = - \left[ 9A_1 A_2^2 (\beta g)^2 g_H^2 + 3A_1 A_2 (3A_2 + 3B_2 C_1 + 18A_1 C_1 - B_2) g_M (\beta g) g_H \right]$$

$$\beta = [A_1 (1 - 3C_1) g_M - A_2 (\beta g) g_H]$$

$$\gamma = 9 \left[ A_1 A_2^2 (12A_1 + 3B_2) (\beta g)^2 g_H^2 + 2A_1^2 A_2 (B_2 - 3A_2) g_M (\beta g) g_H \right]$$

$$\delta = 3 \left[ 2A_1^2 g_M + A_2 (7A_1 + B_2) (\beta g) g_H \right]$$

$$g_h = \frac{\partial \theta_v}{\partial z}$$

$$g_M = \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{\partial V}{\partial z} \right)^2$$

In order for the right-hand side of (13) or (14) to be bounded and nonnegative when the stratification is unstable or neutral, it requires that

$$l < q(P_1)^{1/2} \quad (\text{for } R_i < 0) , \quad (15)$$

where  $P_1$  is the nonnegative root of the following equation:

$$\gamma \left( \frac{l}{q} \right)^4 + \delta \left( \frac{l}{q} \right)^2 + 1 = 0 .$$

It is known that an equilibrium solution may exist when the thermal stratification is neutral or stable (i.e.,  $G_H \leq 0$ ), but the gradient Richardson number ( $R_i$ ) is smaller than a critical value ( $R_{ic}$ ) (see, e.g., Gerrity *et al.* 1994). This critical value of the gradient Richardson number can be obtained by letting the right-hand side of (13) or (14) be zero. It is equivalent to the following:

$$\frac{\left[ \alpha \left( \frac{l}{q} \right)^4 + \beta \left( \frac{l}{q} \right)^2 \right]}{\left[ \gamma \left( \frac{l}{q} \right)^4 + \delta \left( \frac{l}{q} \right)^2 + 1 \right]} - \frac{1}{B_1} = 0, \quad (16)$$

which can be rewritten as

$$\left( \frac{q}{l} \right)^4 + \chi \left( \frac{q}{l} \right)^2 + \kappa = 0 \quad (17)$$

with

$$\chi = [3A_2(7A_1 + B_2) + A_2B_1](\beta g)g_H + [6A_1^2 - A_1B_1(1 - 3C_1)]g_M$$

$$\kappa = [9A_1A_2^2B_1 + 9A_1A_2^2(12A_1 + 3B_2)](\beta g)^2g_H^2 \\ [3A_1A_2B_1(3A_2 + 3B_2C_1 + 18A_1C_1 - B_2) + 18A_1^2A_2(B_2 - 3A_2)]g_M(\beta g)g_H$$

By definition, when  $R_i > R_{ic}$ ,  $q/l$  vanishes, and thus  $\kappa = 0$ . This implies

$$R_{ic} = \frac{3[A_1A_2^2B_1 + A_1A_2^2(12A_1 + 3B_2)]}{A_1A_2(3A_2 + 3B_2C_1 + 18A_1C_1 - B_2) + 6A_1^2A_2(B_2 - 3A_2)} \quad (18)$$

For the empirical constants listed in section 2, it is obtained that  $R_{ic} = 0.505$ .

Since  $q$  and  $l$  may not vanish when  $G_H \leq 0$  and the gradient Richardson number  $R_i < R_{ic}$ , a constraint on  $l$  needs to be established accordingly. Again, following Janjić (2002), one can derive such a constraint by analyzing the diagnostic equation for  $\overline{w^2}/q^2$  in the MY closure. Appealing to the expression for  $\overline{w^2}/q^2$  in the Mellor and Yamada level 2.5 turbulence model (Mellor and Yamada 1982), Janjić showed that  $q/l$  depends on  $\overline{w^2}/q^2$  through the following equation:

$$\xi \left(\frac{q}{l}\right)^4 + \sigma \left(\frac{q}{l}\right)^2 + \omega = 0, \quad (19)$$

where

$$\xi = (1 - 3R_s)$$

$$\sigma = \{[18A_1^2C_1g_m + (9A_1A_2 + 3A_2B_2)(\beta g)g_H] - 3R_s\delta\}$$

$$\omega = \left\{ \left[ 27 A_1 A_2^2 B_2 (\beta g)^2 g_H^2 + 54 A_1^2 A_2 B_2 C_1 g_M (\beta g) g_H \right] - 3 R_s \gamma \right\}$$

$$R_s = \overline{w^2} / q^2$$

It can be shown then that the smallest possible value of  $\overline{w^2} / q^2$  (corresponding to  $q/l = 0$ ) for the above given closure constants is 0.144. It can also be verified that the greater  $\overline{w^2} / q^2$  is, the greater  $q/l$ . Therefore, the constraint on  $l$  is

$$l < q(P_2)^{1/2} \quad (\text{for } R_i \geq 0) , \quad (20)$$

where  $P_2$  is the nonnegative solution of (19) with  $R_s = \overline{w^2} / q^2 = 0.144$ .

It is important to emphasize that the constraints derived above are based on the TKE equation and thus irrelevant to how the length scale is specified. In other words, no matter what prognostic or diagnostic approach to obtaining the length scale, it should be limited by the same constraints as expressed by (15) and (20), so long as (1)-(7) are used for the TKE prediction.

## 5. Numerical Integration

The implicit forward in time and centered in space differencing scheme is commonly used to discretize the two-equation model, (1) and (8), for numerical integration, in which the production and dissipation terms are specified at the current time. This discretization scheme results in a set of linear algebraic equations that can be easily solved with the Thomas algorithm (see, e.g., Fletcher 1991). However, numerical experiments with this scheme often produce results that are contaminated with computational mode (see an example later in section 6). To circumvent this problem, the equations for the TKE and the length scale are solved using the numerical scheme developed by Janjić (2002), in which the TKE equation is solved first, and then the updated TKE is used in the integration of the length-scale equation. This numerical scheme solves either the TKE equation or the length-scale equation in two steps. Each equation is first integrated to obtain the intermediate solution with respect to the production and

dissipation terms using an iterative scheme derived by linearizing the production and dissipation terms. Then, with the intermediate solution as input, the final solution is obtained using the Thomas algorithm to integrate the equation with respect to the diffusion.

Because the split method is used to integrate the model, the length scale in the TKE equation can be moved into the differentiation sign on the left-hand side of (14), yielding

$$l \frac{\partial}{\partial t} \left( \frac{l}{q} \right) = - \left\{ \frac{\left[ \alpha \left( \frac{l}{q} \right)^4 + \beta \left( \frac{l}{q} \right)^2 \right]}{\left[ \gamma \left( \frac{l}{q} \right)^4 + \delta \left( \frac{l}{q} \right)^2 + 1 \right]} - \frac{1}{B_1} \right\}. \quad (21)$$

By denoting the right hand-side as  $R$ , the solution of (21) for the next time step, i.e., the intermediate solution of the TKE equation with respect to the production and dissipation terms, can be iteratively obtained using the following equation

$$\begin{aligned} \left( \frac{l}{q} \right)_{i+1} = & \left( \frac{l}{q} \right)_i - R \left[ \left( \frac{l}{q} \right)_i \right] / R' \left[ \left( \frac{l}{q} \right)_i \right] \\ & + \left\{ R \left[ \left( \frac{l}{q} \right)_i \right] / R' \left[ \left( \frac{l}{q} \right)_i \right] + \left[ \left( \frac{l}{q} \right)_0 - \left( \frac{l}{q} \right)_i \right] \right\} \exp \left\{ \Delta t R' \left[ \left( \frac{l}{q} \right)_i \right] \right\} \end{aligned}$$

where  $i$  is the index of current time step,  $(\ell/q)_i$  is the value of  $\ell/q$  around which the linearization is performed,  $(\ell/q)_0$  is the initial value of  $\ell/q$  at the beginning of the time step, and

$$R' = dR/d(l/q) = -2 \left[ (\alpha \delta - \beta \gamma) (l/q)^5 + 2\alpha (l/q)^3 + \beta (l/q) \right] / \left[ \gamma (l/q)^4 + \delta (l/q)^2 + 1 \right]^2.$$

As proposed by Janjić, the iterations are started from the equilibrium solution of the equation (21) to ensure that the solution behaves well. After the solution converges, the diffusion operation is applied to obtain the final solution of the TKE equation.

For the length-scale equation, the counterpart of (21) is

$$(1/q) \frac{\partial l}{\partial t} = - \left\{ \frac{\left[ \left( \alpha' \left( \frac{l}{q} \right)^4 + \beta' \left( \frac{l}{q} \right)^2 \right) \right]}{\left[ \gamma \left( \frac{l}{q} \right)^4 + \delta \left( \frac{l}{q} \right)^2 + 1 \right]} - \frac{F-2}{B_1} \right\}, \quad (22)$$

according to (11), where

$$\alpha' = -[9A_1 A_2^2 (E_2 - 2)(\beta g)^2 g_H^2 + 3A_1 A_2 (E_1 - 2)(3A_2 + 3B_2 C_1 + 18A_1 C_1 - B_2)g_M (\beta g)g_H]$$

and

$$\beta' = [A_1 (E_1 - 2)(1 - 3C_1)g_M - A_2 (E_2 - 2)(\beta g)g_H].$$

The procedure to solve this equation is the same as (21). As with in solving the TKE equation, after the converged solution is obtained for the intermediate  $l$  with respect to the production and dissipation terms, the corresponding diffusion operator is applied to the variable  $q^2 l$ , and thus the final solution of  $l$  is yielded.

## 6. Numerical Experiments

The mesoscale model in which the two-equation vertical turbulent mixing scheme is implemented is the National Center for Atmospheric Research and the Pennsylvania State University mesoscale model (MM5-V3) (Grell *et al.* 1994 and <http://www.mmm.ucar.edu/mm5/mm5v3.html>). The mesoscale model is run on multiple 1-way nested meshes of 36 km, 12 km, and 4 km horizontal grid spacings (Fig. 1) with 50 vertical layers in total and 20 layers within the lowest 1 km. The initial and boundary conditions for the 36-km mesh are from the NCEP's ETA Data Assimilation System (EDAS). All the simulations are started at 0000 UTC 30 July 2000. The configuration of MM5 physics for the 36-km and 12-km meshes includes the mixed-phase cloud physics, the Grell scheme for subgrid (convective) condensation (only for 36-km and 12-km meshes), the Dudhia's 5-level simple soil model, and the MM5 simple short-wave and long-wave radiation parameterization schemes. The 4-km mesh is chosen to be small (with 19 x 19 horizontal grids)

so that within the entire mesh the landuse characteristics are homogeneous. Since the synoptic forcing is weak in this case, we think that the extension of the domain is sufficient for the purpose of testing the two-equation vertical turbulent mixing scheme, and compare it with the ETA scheme that has been implemented in MM5-V3.

The differences in the length-scale distributions from the two-equation scheme and the ETA scheme are shown in Fig. 2 with an east-west cross-section cutting through the middle of the 4-km domain that is valid at 47 hours into the simulation (1700 local standard time).  $E_1 = 2.875$ ,  $E_2 = 1.0$  and  $F = 3.0$  are used in the two-equation scheme. It is seen that the two schemes yield different magnitudes and gradient of the length scale for a given location. Associated with the differences in the length scale are the differences in  $q^2$  (i.e., twice the TKE), the eddy exchange coefficients ( $K_m$  and  $K_H$ ) and virtual potential temperature ( $\Theta_v$ ) are depicted in Fig. 3. Significant differences between the two schemes are seen in the TKE and the eddy exchange coefficients fields. It can also be seen that the two-equation vertical turbulent mixing scheme produces more mixing of  $\Theta_v$  near the surface than the ETA scheme, while far above the surface the former mixes slightly less than the latter. There is no significant difference in the ABL heights (as defined as the inversion of  $\Theta_v$  at the top of ABL) simulated respectively by the two schemes, suggesting that observations of turbulence fields within ABL will be more discriminating than the ABL height for the validation of ABL models.

It is desirable to have some idea of how the performance of the two-equation scheme is sensitive to the variation of  $E_1$  and  $E_2$ . Therefore, Figs. 4-7 present a sample of the results from the simulations using the two-equation scheme with different sets of values for  $E_1$  and  $E_2$ . If  $E_2$  is set to 1 and  $E_1$  varies, one can see that although the vertical distribution of the TKE with various  $E_1$  is quite similar, the maximum TKE increases only slightly as  $E_1$  decreases. On the other hand, if  $E_1$  is set to 1 and  $E_2$  varies, the vertical distribution of the TKE does not change very much with  $E_2$ , but the maximum of the TKE increases as  $E_2$  decreases, indicating that the TKE is more sensitive to variation in  $E_2$  than in  $E_1$ .

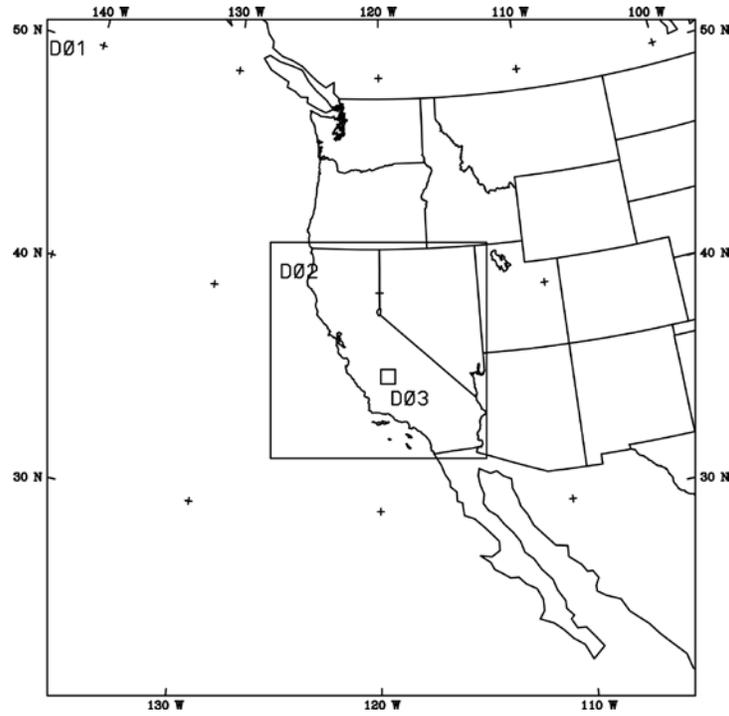


FIGURE 1. Location of the 3 nested MM5 domains.

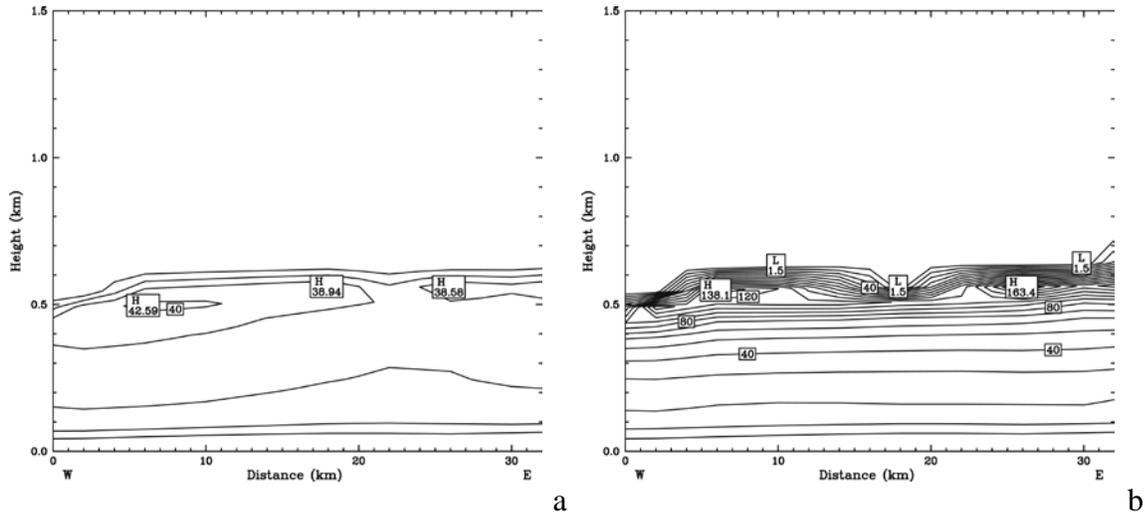
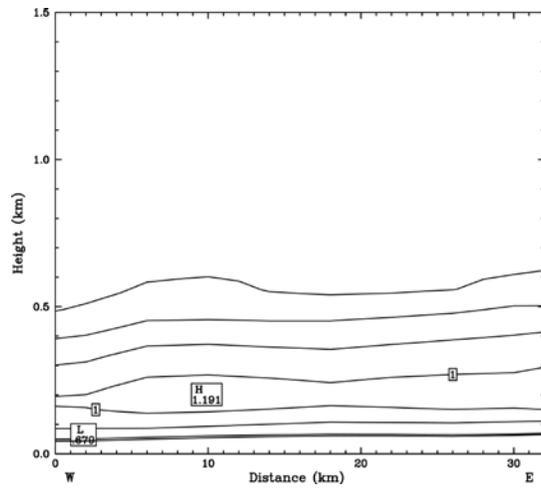
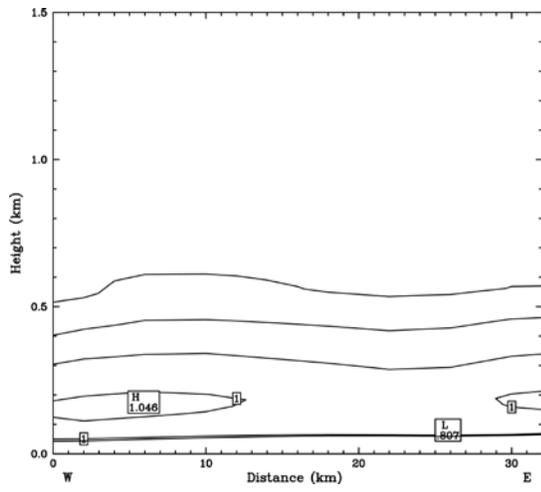
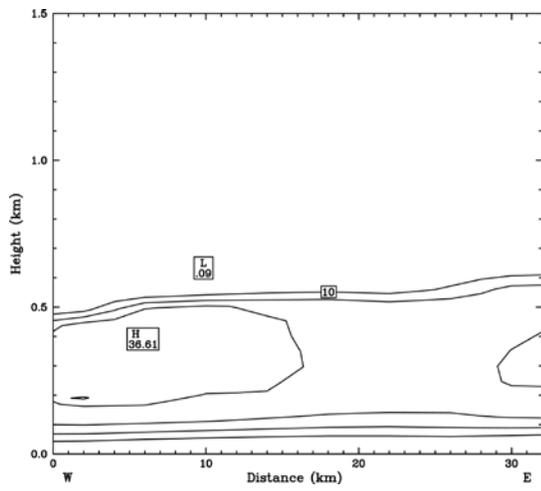


FIGURE 2. East-west cross-sections of the length scale cutting through the middle of the 4-km domain valid at 47 hours into the simulation (1700 local standard time). (a) is for the two-equation scheme with  $E_1 = 2.875$ ,  $E_2 = 1.0$  and  $F = 3.0$ , and (b) is for the ETA scheme. The contour interval is 10 m.

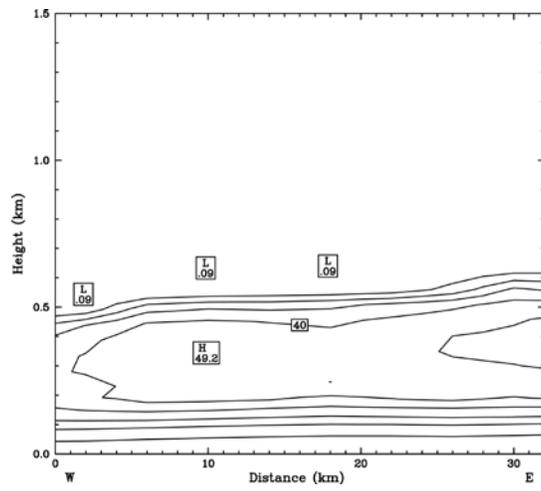


a

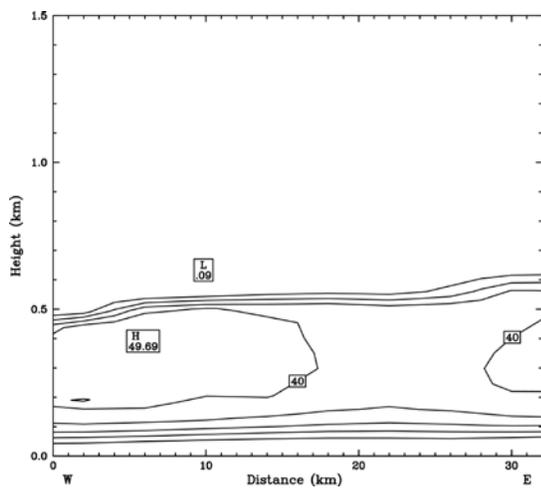
b



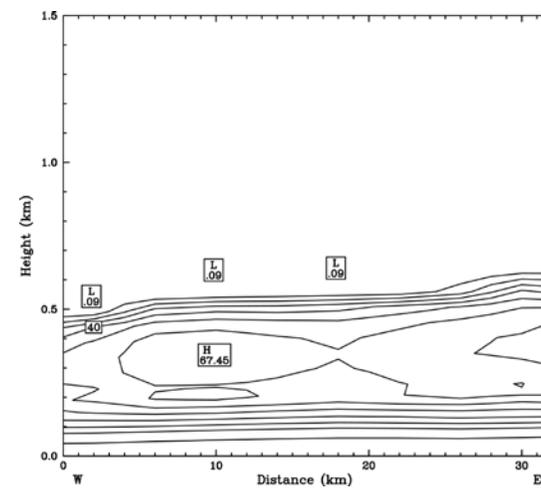
c



d



e



f

FIGURE 3. Continued on next page.

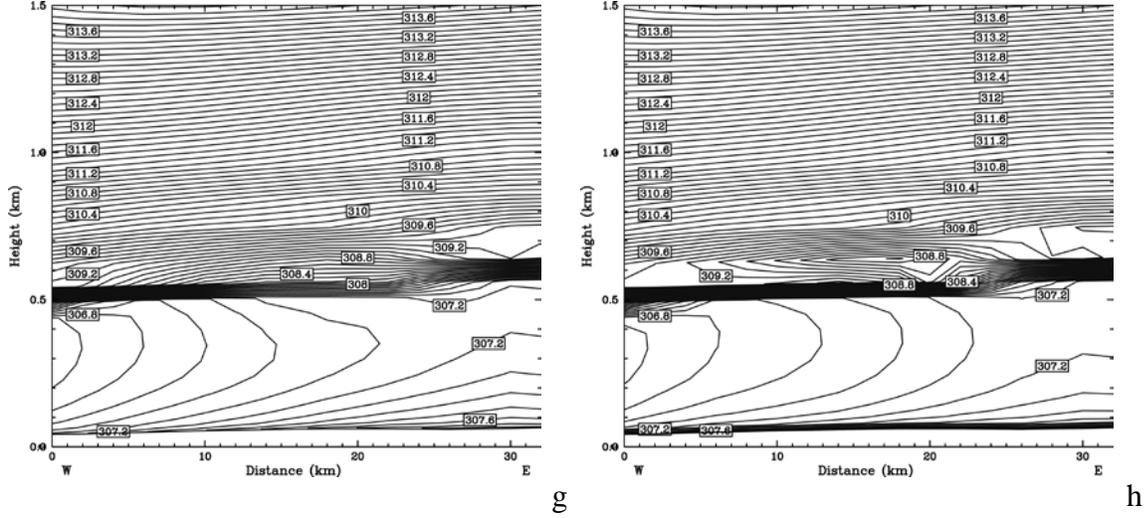


FIGURE 3. Cross-sections of  $q^2$  (a and b, contour interval of  $0.25 \text{ m}^2\text{s}^{-2}$ ),  $k_m$  (c and d, contour interval of  $10 \text{ m}^2\text{s}^{-1}$ ),  $k_H$  (e and f, contour interval of  $10 \text{ m}^2\text{s}^{-1}$ ), and  $\Theta_v$  (g and h, contour interval of  $0.1 \text{ K}$ ). The left column (i.e., a, c, e and g) are for the two-equation scheme with  $E_1 = 2.875$ ,  $E_2 = 1.0$  and  $F = 3.0$ , while the right column (b, d, f, and h) are for the ETA scheme. The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

It is mentioned in section 5 that a commonly used finite-difference scheme to discretize the two-equation model, (1) and (8), often leads to a solution that is apparently contaminated by computational modes. In this scheme, (1) and (8) are discretized using the implicit forward in time and centered in space differencing scheme except that the production and dissipation terms are specified at the current time. To illustrate the contamination of computational modes, the experiment  $E_1 = 2.875$ ,  $E_2 = 1.0$  and  $F = 3.0$  is rerun with the implicit scheme and the results are shown in Fig. 8. It is seen that there are multiple extremes in the distributions of the TKE and the eddy exchange coefficients, but not in  $\Theta_v$ . These multiple extremes cannot be explained physically given the smooth mean state, leading to the conclusion that they result from the contamination of computational modes. It is for the purpose of eliminating the computational contamination of the solution that Janjić developed his innovative numerical scheme to integrating the TKE equation (2003, personal communication).

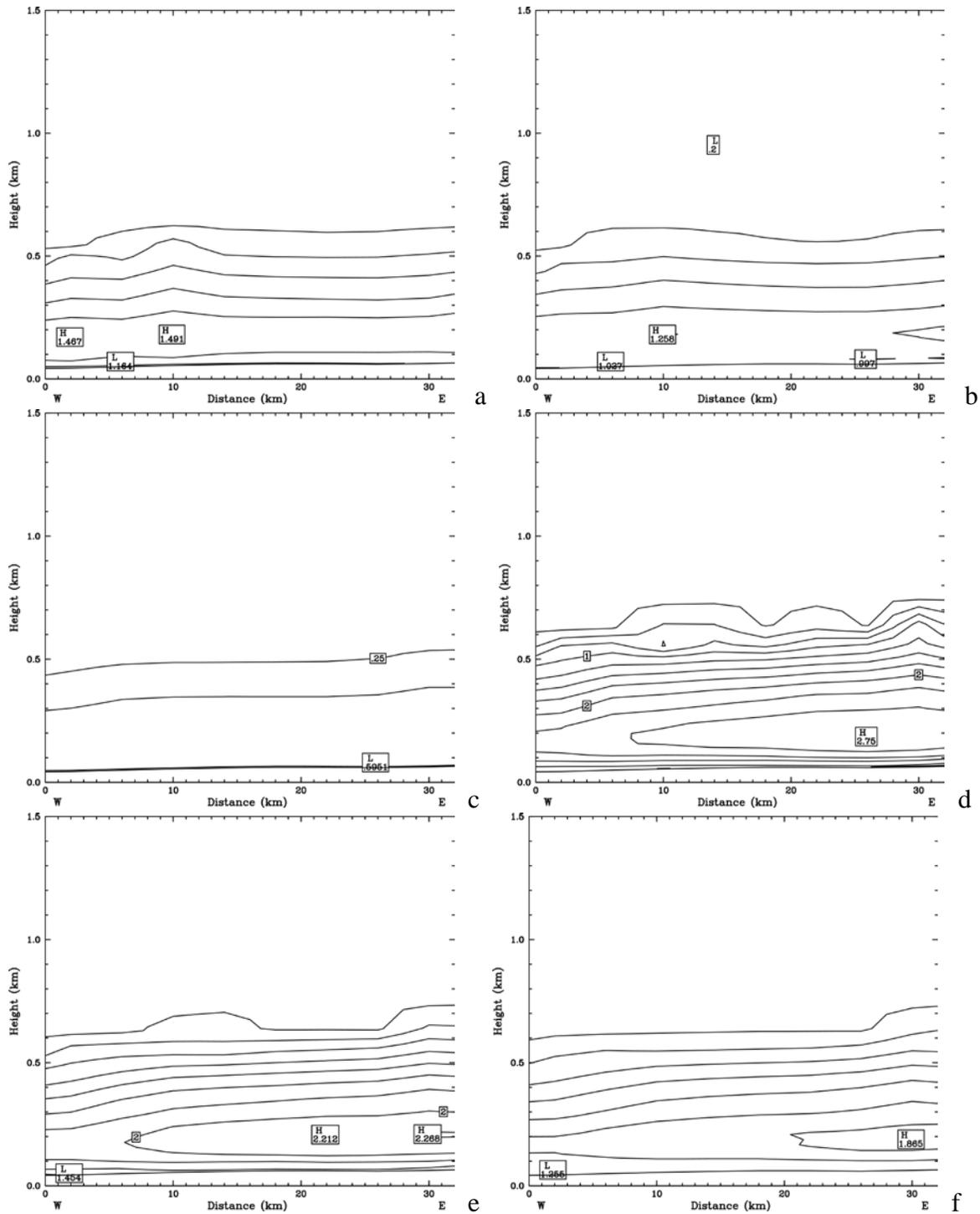


FIGURE 4. Cross-sections of  $q^2$  (contour interval of  $10 \text{ m}^2 \text{ s}^{-2}$ ) from the simulation of the 4-km domain using the two-equation scheme with (a)  $E_1 = 1.0$  and  $E_2 = 0.5$ , (b)  $E_1 = 1.0$  and  $E_2 = 0.75$ , (c)  $E_1 = 1.0$  and  $E_2 = 0.1$ , (d)  $E_1 = 0.5$  and  $E_2 = 1.0$ , (e)  $E_1 = 0.75$  and  $E_2 = 1.0$ , and (f)  $E_1 = 0.875$  and  $E_2 = 1.0$ . The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

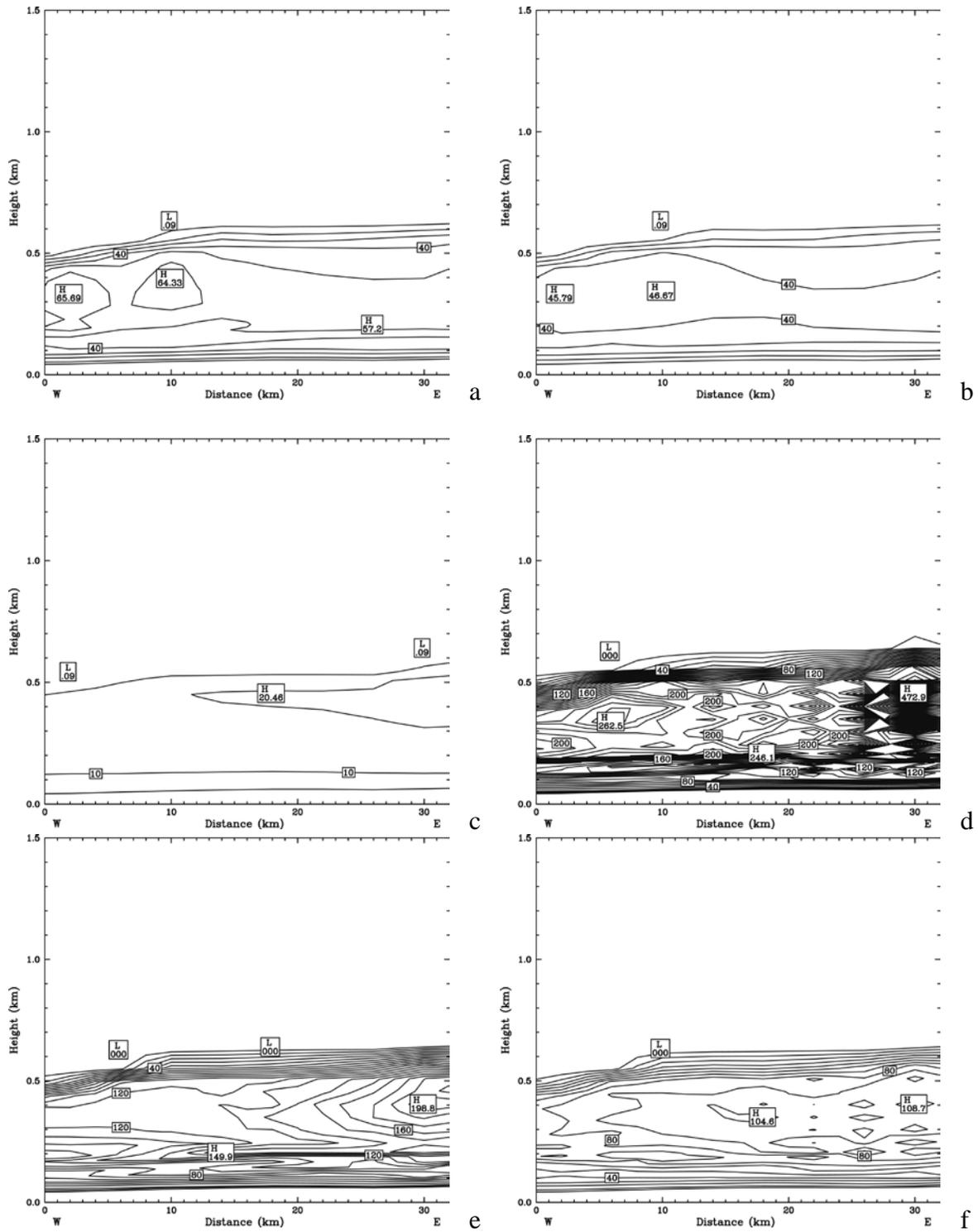


FIGURE 5. Cross-sections of  $k_m$  (contour interval of  $10 \text{ m}^2\text{s}^{-1}$ ) from the simulation of the 4-km domain using the two-equation scheme with (a)  $E_1 = 1.0$  and  $E_2 = 0.5$ , (b)  $E_1 = 1.0$  and  $E_2 = 0.75$ , (c)  $E_1 = 1.0$  and  $E_2 = 0.1$ , (d)  $E_1 = 0.5$  and  $E_2 = 1.0$ , (e)  $E_1 = 0.75$  and  $E_2 = 1.0$ , and (f)  $E_1 = 0.875$  and  $E_2 = 1.0$ . The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

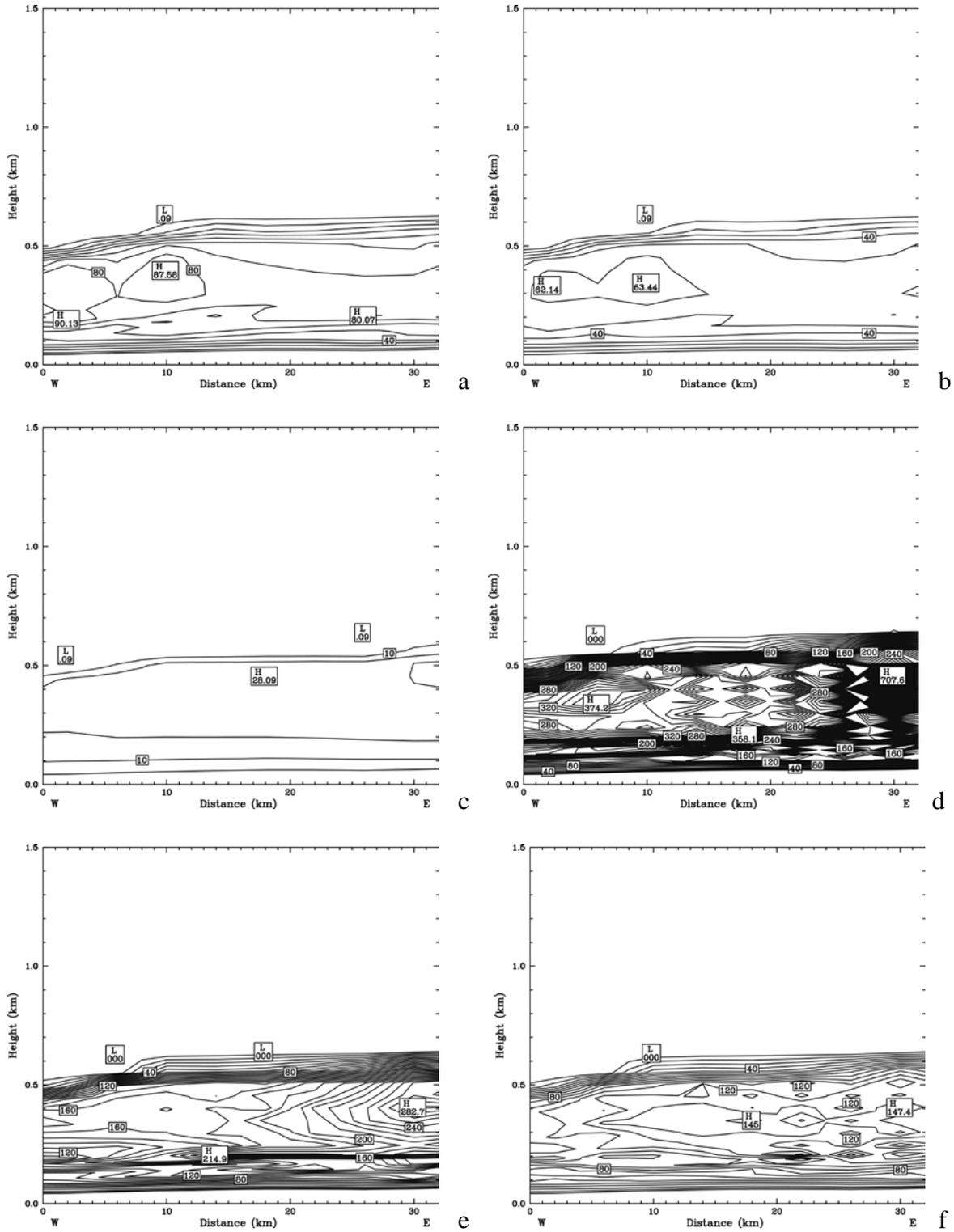


FIGURE 6. Cross-sections of  $k_H$  (contour interval of  $10 \text{ m}^2 \text{ s}^{-1}$ ) from the simulation of the 4-km domain using the two-equation scheme with (a)  $E_1 = 1.0$  and  $E_2 = 0.5$ , (b)  $E_1 = 1.0$  and  $E_2 = 0.75$ , (c)  $E_1 = 1.0$  and  $E_2 = 0.1$ , (d)  $E_1 = 0.5$  and  $E_2 = 1.0$ , (e)  $E_1 = 0.75$  and  $E_2 = 1.0$ , and (f)  $E_1 = 0.875$  and  $E_2 = 1.0$ . The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

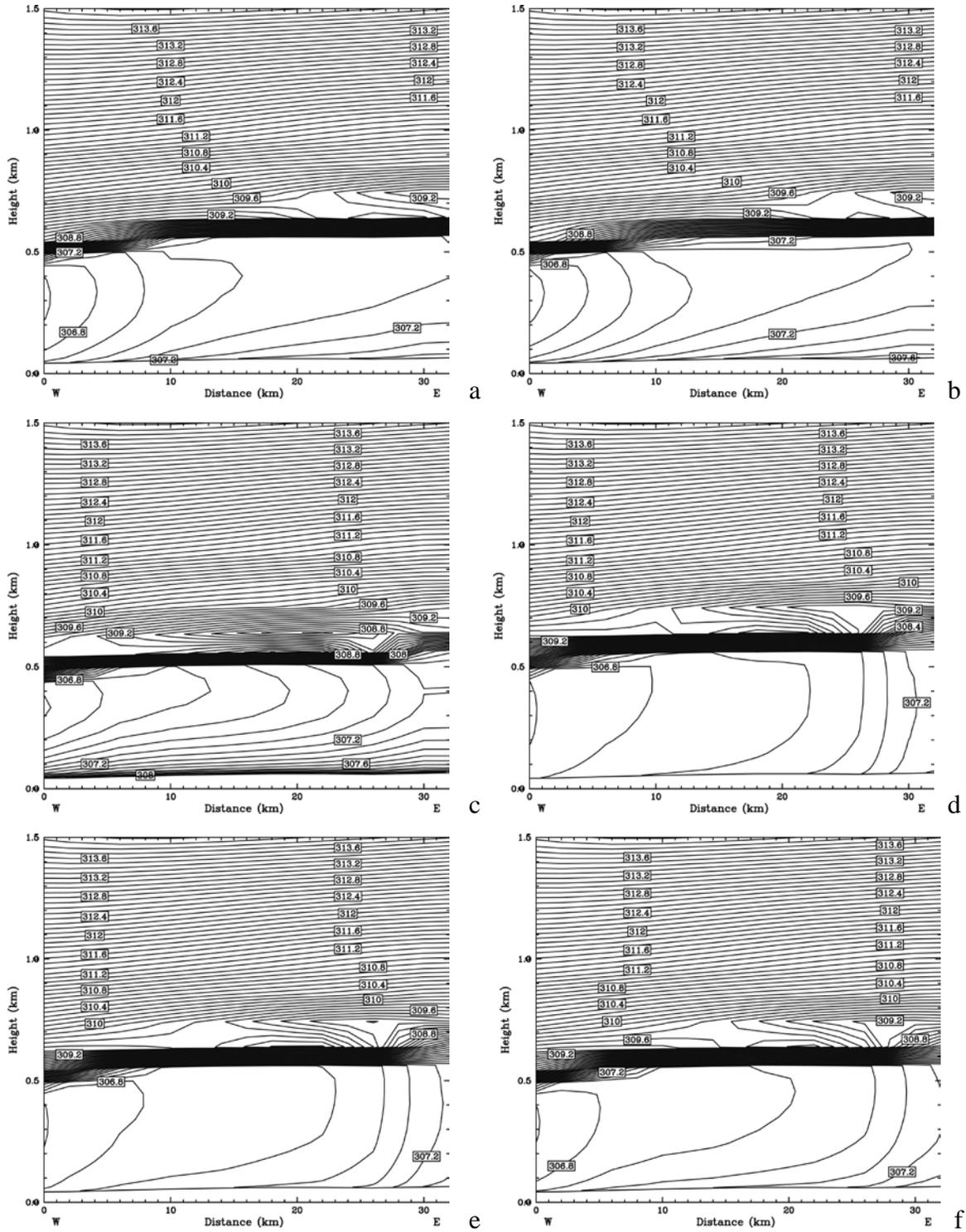


FIGURE 7. Cross-sections of  $\Theta_v$  (contour interval of 0.1 K) from the simulation of the 4-km domain using the two-equation scheme with (a)  $E_1 = 1.0$  and  $E_2 = 0.5$ , (b)  $E_1 = 1.0$  and  $E_2 = 0.75$ , (c)  $E_1 = 1.0$  and  $E_2 = 0.1$ , (d)  $E_1 = 0.5$  and  $E_2 = 1.0$ , (e)  $E_1 = 0.75$  and  $E_2 = 1.0$ , and (f)  $E_1 = 0.875$  and  $E_2 = 1.0$ . The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

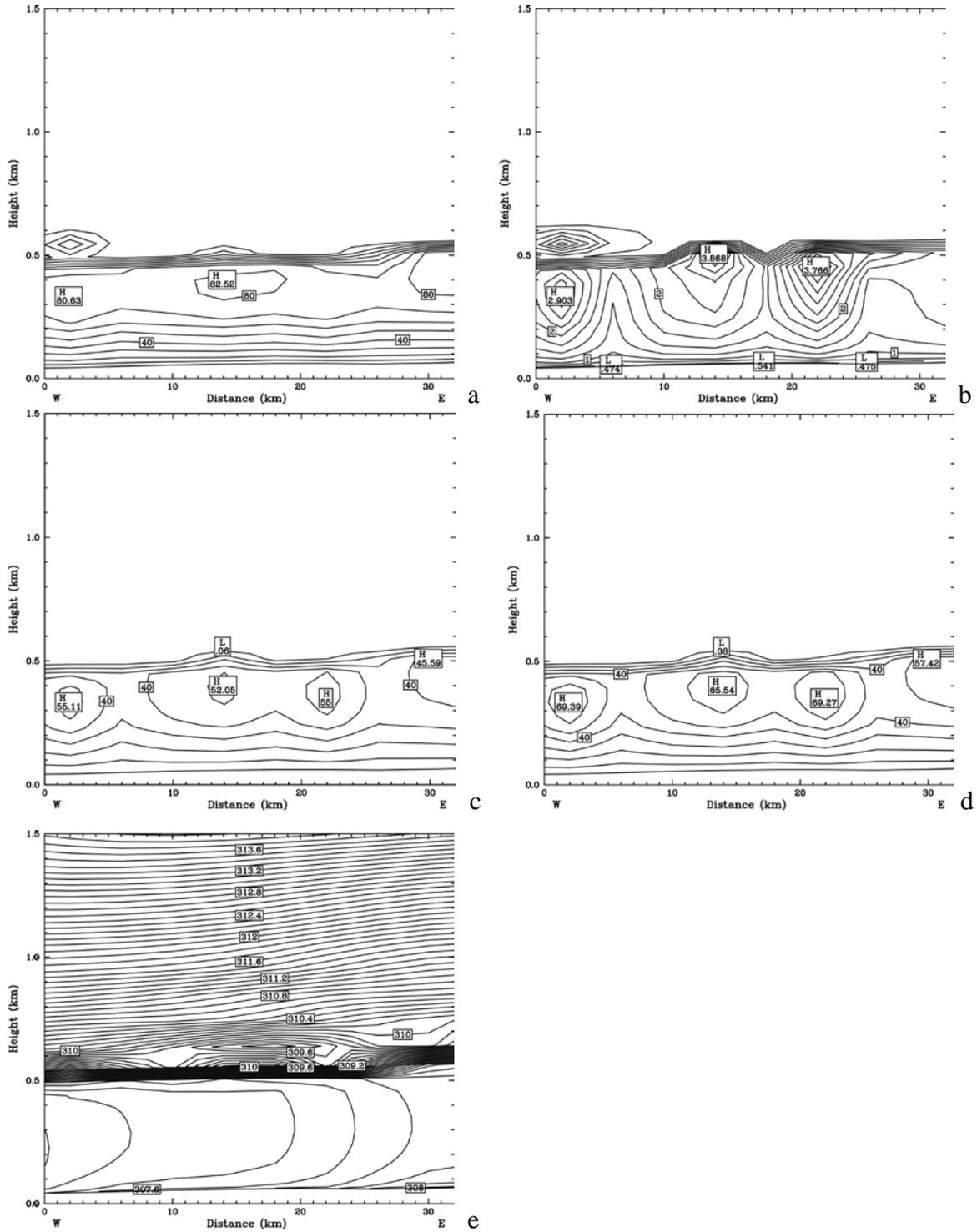


FIGURE 8. Cross-sections of (a) the length scale (contour interval of 10 m), (b)  $q^2$  (contour interval of  $0.25 \text{ m}^2 \text{ s}^{-2}$ ), (c)  $k_m$  (contour interval of  $10 \text{ m}^2 \text{ s}^{-1}$ ), (d)  $k_H$  (contour interval of  $10 \text{ m}^2 \text{ s}^{-1}$ ), and (e)  $\Theta_v$  (contour interval of 0.1 K) for the simulation using the two-equation scheme with the conventional implicit numerical scheme and  $E_1 = 2.875$ ,  $E_2 = 1.0$  and  $F = 3.0$ . The cross-sections are at the same location as in Fig. 2 and are valid at 47 hours into the simulation (1700 local standard time).

## 7. Summary and Discussion

A two-equation vertical turbulent mixing scheme is implemented in the National Center for Atmospheric Research and the Pennsylvania State University mesoscale model (MM5-V3). This scheme is based on the MY closure with two prognostic equations: one for the TKE and the other for the length scale multiplied by twice the TKE. Although the scheme has been popularly used in oceanic modeling community, the work reported here is the first effort to implement the scheme in a mesoscale atmospheric model.

The physical meaning of the length scale is of fundamental importance in the simulation of vertical turbulent mixing in the ABL. In this work, the length scale is defined as the characteristic length scale of the largest energy-containing eddies, and is related to the distance that these eddies travel in the vertical direction before losing their initial kinetic energy due to turbulent mixing and buoyancy effects. With this definition, it is concluded that the closure constants in the length-scale equation should be different than those proposed previously for oceanic applications.

In order to ensure physically sensible performance of the scheme in MM5-V3, the approach developed by Janjić (2002) is applied in the implementation of the two-equation scheme to impose the necessary constraints on the prognostic length scale. These constraints are derived by analyzing the TKE equation under different stability regimes in terms of the gradient Richardson number. They are functions of the TKE as well as the stability functions in the TKE equation, and therefore are generally applicable to limiting the length scale predicted from various versions of the prognostic equations for the length scale. The use of these constraints circumvents the need for the realizability constraints on the non-dimensional vertical gradients of mean velocity and temperature. It is also shown that the numerical scheme proposed by Janjić (2002) for integrating the TKE equation should be used to solve the prognostic equations of the two-equation scheme to control the computational modes encountered when using conventional numerical schemes to solve the equations for the TKE and the length scale.

The numerical experiments are performed using MM5-V3 to illustrate that with properly chosen closure constants in the length-scale equation, the two-equation scheme produces more (and less) mixing near the surface (and way above the surface layer within the ABL) during daytime than the original TKE based, ETA scheme in MM5-V3 where the length scale is prescribed using a diagnostic approach. The turbulence fields from the two-equation scheme are

significantly different than those from the ETA scheme, while the difference in the ABL height is almost the same. A series of sensitivity experiments indicate that the two equation scheme is more sensitive to the closure constant associated with the wind shear than to that associated with the buoyancy effect in the length-scale equation. Although the use of the prognostic equation for the length scale is more theoretically appealing than the use of the diagnostic equation, the results presented here are not enough to generalize whether or not the gain from using the two-equation scheme is proportional to the extra computational cost for the simulation of the ABL turbulent mixing in weather prediction models.

It has been known in the ABL modeling community that a successful one-dimensional test and calibration of a vertical turbulent mixing scheme does not guarantee that the same scheme will be computational robust and physical meaningful when it is used in much more complicated three-dimensional models. We would like to emphasize that a well-tested oceanic vertical turbulent mixing scheme may not automatically work well when used in simulating the vertical turbulent mixing in the atmosphere because the thermal stratification of the atmosphere varies more quickly and widely than in the ocean, and winds in the atmosphere vary more rigorously than currents in the ocean. While we do not have adequate turbulence observations to indicate which one of the available vertical turbulent mixing schemes in three-dimensional mesoscale model such as MM5-V3 is the best for a given flow situation, this two-equation scheme provides another choice in ABL parameterizations, which could contribute to the effort of effectively perturbing model physics for generating statistical ensemble forecasts.

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