WRF/NMM-CMAQ derived planetary boundary layer heights and vertical diffusivity for transport of trace species

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1. INTRODUCTION

During 2003, NOAA and the U.S. EPA signed a Memorandum of Agreement to work together to develop a National air quality forecasting capability. To meet this goal, NOAA's National Weather Service (NWS), the Office of Atmospheric Research (OAR) and the U.S. EPA developed and evaluated a prototype ozone forecast capability for the North Eastern U.S. (Davidson et al. 2004). Subsequently, a national Air Quality Forecast System (AQFS) was constructed comprising the NWS/National Centers for Environmental Prediction (NCEP) North American Model (NAM) model at 12 km (Janic 2003) to provide meteorological predictions for the EPA Community Multi-scale Air Quality (CMAQ) model (Byun and Schere 2007). The capability of AQFS has been expanded to cover the eastern half of U.S. and the 48 contiguous states (CONUS) in September of 2005, and 2007, respectively (McQueen et al. 2007).

It is advantageous to have a common dynamical package to drive both the meteorological and the air quality models. Among other advantages of such an ideal coupling between the models is a good confidence in mass consistency of the atmospheric constituents (e.g. Lee et al. 2004).

In the interim of the 2007 upgrade of AQFS and the end of the 2006 ozone season, a thorough investigation on the commonality of the vertical mixing schemes within the Planetary Boundary Height (PBL), *h*, between the models has been conducted. Two alternative schemes have been tested besides the default scheme of using NAM-forecasted PBL to derive CMAQ's vertical eddy diffusivity for tracer species, *Kz*, for vertical mixing parameterization for both stable and unstable atmospheric conditions. The alternative vertical mixing schemes have been incorporated into the air quality modeling part of the AQFS aiming to strengthen the commonality between the vertical mixing processes of the meteorological and air quality models below the free troposphere.

Sensitivity studies of these schemes basing on a selected period of elevated surface O_3 concentration of last August have been carried out. The following sections describe the parameterization, characteristic, and rankings of these schemes in the context of an AQFS-like air quality forecast of this period, respectively.

2. VECTICAL MIXING SCHEMES IN AQFS

In 2006, AQFS uses a version of CMAQ closely abided to CMAQ-4.5. It is configured with Asymmetric Convective Model for in-cloud convective mixing (Pleim 2007), NAM derived radiative field for photolysis attenuation calculation, and static boundary conditions for all chemical constituents.

a. RADM scheme with TKE-based PBL height

The vertical mixing scheme used was the default parameterization methodology applied to RADM and CMAQ (Pleim and Chang, 1992; Byun and Dennis, 1995). It is a similarity parameterization of the mixing in the surface and convective boundary layer. For the sake of completeness, the equations for *Kz* for the two stability regimes for the surface layer and layers above that and below PBL are repeated below (Byun and Ching, 1999):

$$K_z = \begin{cases} \dfrac{ku_* z}{\phi_H(z/h)} & \text{for surface layer} \quad (1a) \\ \dfrac{ku_* z(1-z/h)^{3/2}}{\phi_H(z/L)} & \text{for stable PBL above surface layer when } z/L > 0 \quad (1b) \\ kw_* z(1-\dfrac{z}{h}) & \text{for unstable PBL above surface layer when } z/L < 0 \quad (1c) \end{cases}$$

where k is the von Karman constant, u_*, friction velocity, z is height, w_* is convective velocity, and L is the Monin-Obukhov length. The non-dimensional profile functions of the vertical gradient of potential temperature, Φ_H, were also given (Byun and Ching, 1999):

$$\phi_H = \begin{cases} \Pr_0\left(\beta_H + \dfrac{z}{L}\right) & \text{for very stable conditions } (z/L \ge 1) \quad (2a) \\ \Pr_0\left(1+\beta_H \dfrac{z}{L}\right) & \text{for moderately stable conditions } (1 \ge z/L \ge 0) \quad (2b) \\ \left(1-\gamma_H \dfrac{z}{L}\right)^{-1/2} & \text{for unstable conditions } (z/L < 1) \quad (2c) \end{cases}$$

where $\Pr_o$ is the Prandle number for neutral stability, and β_h and γ_h are coefficients of the profile functions determined through field experiments.

The determination of h is defined in NAM as the first vertical height at which the Turbulent Kinetic Energy (TKE) value drops below 0.1 J Kg^{-1} during an upward search from the surface along an atmospheric column.

b. RADM scheme but MIXHT as PBL height

There is an opinion that the TKE-based PBL height overshoots the height within which atmospheric mixing of the tracer species actually take place. There are weak shallow convection and horizontal advection processes that entrain TKE into layers above the actual mixing depth of the atmospheric column. Therefore it is observed that NAM often predicts the TKE-based PBL height more than one to two layers above that of mixed layer depth.

In light of this, it has been proposed that the mixed layer height (MIXHT), which in essence represents the capping of turbulence production due to the diminishing buoyancy of a convective plume at that height, should be used as h in Equations 1 and 2. In NAM, MIXHT has been quantified by a cut-off value 0.505 of the local bulk Richardson number, Ri_{bk}, when exercising an upward search from the surface along an atmospheric column.

$$Ri_{bk} = \frac{gz[\theta_v(z)-\theta_v(1)]}{\theta_v(1)[(u(z)-u(1))^2+(v(z)-v(1))^2+\beta u_*^2]} \quad (3)$$

where g is gravitational acceleration, θ_v is virtual potential temperature, u and v are the latitudinal and longitudinal components of wind, respectively; and β is a field experiment determined coefficient.

c. Use NAM predicted Kz for vertical mixing

Due to the geometrical and package differences between NAM and CMAQ (Otte el al. 2005) of the AQFS, it can be a challenge to maintain high precision of mass consistency as discussion in the introductive section. However, there has been an important vertical grid alignment improvement between NAM and CMAQ since 2005 (Lin et al. 2006). Both models are now using a hybrid sigma-*P* vertical coordinate; namely, NAM uses 61 interface levels, and CMAQ in AQFS selects from them a 23 interface levels with finer spacing near the surface. In NAM, *Kz* is defined at these interface surfaces basing on the Mellor-Yamada Level 2.5 turbulence closure scheme (Janjic 1996).

3. SENSITIVITY CASES: AUGUST 2-3, 2006

There were a few elevated surface O_3 concentration scenarios in many cities in continental U.S. between August 2 and 4, 2006. Figure 1 shows the 1 h daily maximum surface O3 concentration on August 3: Fig. 1a shows that compiled by the AIRNOW observation network (EPA 2006), and Fig. 1b shows that forecasted by AQFS and overlaid by the AIRNOW data. It can be noted that there were areas with 1 h daily max value in excess of 100 ppb.

This study aims to investigate the spatial and temporal characteristics of the various vertical mixing schemes discussed in section 2. Pertinent to the context of maximum surface level O_3 concentration prediction, the distributions of O_3 and its precursors, the temporal evolutions of PBL height, and the vertical profiles of *Kz* will be examined where and when the surface O_3 concentration is at its peaks.

Table 1 Run cases included in the sensitivity study

Case	Vertical mixing scheme
Base	Use *Kz* derived in Eq. 1 & 2 basing on NAM TKE-based *h*
MIXHT	Use *Kz* derived in Eq. 1 & 2 using NAM Predicted MIXHT as *h*
NAM-Kz	Use NAM predicted *Kz*

Three sites of interest has been selected in accordance with the aforementioned rationales, and restrained by the availability of ozone-sonde and RAOBS data for verification purposes for chemistry and meteorological fields, respectively. They are the Beltsville, MD; Huntsville, AL, and Table-mount, CA sites. The Table-mount site represents an interesting location down wind of the LA basin often subjected to polluted outflow from the city. It is an elevated site at 2250 m, its reading in late afternoon and at night can reveal the lofted O_3 and precursor plumes transported from LA.

Investigations focused on the afternoon hours on August 2 and 3, 2006. However regional verification is based on runs of the three cases between July 21 and August 4, 2006.

4. DISTRIBUTION OF O_3

Figure 1b depicted the Base-case forecasted daily maximum hourly surface O_3 over continental U.S. on August 3, 2006, overlaid with that compiled by AIRNOW. The state of California represents a challenging area for AQFS. Patterns of low and high biases closely co-located in relative small regions in around central San Joaquin Valley and immediately downwind of LA are often registered by verification records. Figure 2a shows the mean bias of daily maximum 8 h averaged surface O_3 forecasted by the Base-case verified with AIRNOW. This reinforces the impression that this intricate pattern occurs rather often. Figure 2b shows the topology of the state. Figure 3 shows a verification diagram for NAM predicted 10 m wind from 15Z August 1st to 12Z August 3rd, 2006 for the western half of continental U.S. Figure 4 shows the definition of regions for the meteorological and chemical concentration verification statistics.

Figures 5a and b show the temporal evolution of *h* in both the Base and MIXHT cases over LA, CA; and Table-mount, CA, respectively. It also shows evolution of the vertical structures of the O_3 concentration predicted by the Base-case, and wind and temperature fields given by the NAM model at the locations.

It is evident from Fig. 5a and b that the lower level O_3 concentration over the city of LA is considerably lower than that over the outskirt site at Table-mount. It is particularly truth for the lowest level, where emitted NO_2 titrates out O_3 at a rapid rate during both day and night hours. The predicted low level wind below 4000 m is largely south-south-westerly. Therefore it can be postulated that Table-mount can be subjected to the downwind transport of pollution plumes from LA.

Figure 5c shows the profiles of predicted and observed O_3 taken at 20:45Z on 2 August (Thompson et al. 2006). The large spike of O_3 concentration between 2000 and 4000 m registered by the ozone-sonde was not reconstructed by the model.

Figures 6a and b show a difference map by subtracting from Fig. 4b by the predicted O_3 concentration by case MIXHT and NAM-Kz, respectively. The two difference maps looked similar with the ground level difference stronger in the former than the latter. This becomes the most obvious at around 21 to 22Z August 3, 2006, when the difference between the NAM TKE-based *h* and MIXHT is large when predicted surface O_3 concentration was at its temporal peak.

Figures 7a and b are similar to those of Fig. 5b and c but for Huntsville, AL; and Beltsville, MD, respectively. The two sites are in relatively flat terrains at elevations of 24 m and 196 m, respectively. The daily hourly maximum surface O_3 concentration prediction of these sites verified quite well basing on the AIRNOW data. In contrary with the gradual collapsing of PBL in LA and Table-mount, CA, as shown in Figs. 5a and b, respectively; it collapsed rather abruptly in Huntsville, AL; and Beltsville, MD on 2 August, 2006, as shown in Figs. 7a and b. However, this timing behavior is different between the two different schemes at these two sites: namely; at Huntsville, PBL collapsed at 22Z and 23Z basing on the MIXHT and NAM TKE-based scheme, respectively. On the other hand, the collapses of PBL at Beltsville in accordance with the two schemes were both at 23Z. In Beltsville, AQFS predicts that a significant amount of O_3 has been lofted above the mixing layer just after sun set.

5. *KZ* PROFILES ON 2 AUGUST, 2006

Figures 8a-d shows the *Kz* profile over Table-mount, CA, with respect to the three runs stipulated in Table 1 at 18Z, and 21Z, August 2, and 00Z, and 02Z, August 3, 2006, respectively. The NAM TKE-based *Kz* and MIXHT-based *Kz* are both parabolic in shape as governed by Eq. 1c. However, as explained in Section 2c, the peak value and extent of the latter is smaller than those of the former. The NAM predicted *Kz* profile is usually non-parabolic in shape, and has maximum values in lower in attitude than those of the first two schemes. As the figures show, PBL Height rose gradually between noon and 6 pm local time, and collapsed completely by 8 pm, as depicted in Fig. 8a,b,c, and d, respectively.

Figures 9 and 10 are similar to Fig. 8 but for Huntsville, AL, and Beltsville, MD, respectively. Another difference is the timing of the sub-figures a-d. They are for 15Z, 18Z, 21Z, August 2, and 00Z, August 3, 2006, respectively. The observations in the above paragraph also apply to Fig. 9 and 10, for in these two eastern sites. The NAM predicted *Kz* has rather large values over Huntsville, AL.

6. REGIONAL MEAN BIAS

Figure 11 shows the regionalized mean bias of the 2 week forecast by the three runs described in Table 1. The definitions of the regions are illustrated in Fig. 4.

The NAM-predicted *Kz* case has the tendency to have the largest high biases among all regions except for the Pacific Coast (PC). On 2 August, this high bias dominance is the most noticeable in the Northeastern U.S. (NE). The Base-case and the MIXHT-case usually track one another closely over all the regions.

There is no episode specific trend of bias increase in the western regions of Rocky Mountain (RM) and PC. For instance there were 14, 17, and 13, O_3 officially declared exceedance episodes in Western U.S. on July 24, 25 and 26, respectively. On record, these three days stood out from the rest of the two week period between 21 July and 4 August, where there were at most 4 declared exceedances per day, except for the 9-exceedance day of 3 August, 2006. However, Fig. 11a and b do not show any characteristic bias change for those high exceedance days for any of the Kz scheme.

For the eastern regions of Upper Midwest (UM), Northeastern (NE), Lower Midwest (LM), and Southeastern (SE) U.S., there is no clear episode specific bias change characteristics either, especially for LM and SE. During the aforementioned two week period there was a cluster of consecutive high O_3 declared exceedance days with 8, 24, 14, and 9 exceedances on 31 July, and 1, 2, and 3 August, 2006, respectively. The NE and UM regions do have their high biases increased for those high exceedance days for all three Kz schemes tested.

The sample sizes for the various regions are: LM has 135, NE has 161, PC has 156, RM has 108, SE has 216, and UM has 231 observation stations, respectively.

All the three Kz schemes tested have high biases for most of the days of the two week period considered. The NAM-predicted Kz scheme did best for PC, but it has the largest high bias for all the other regions. The MIXHT and Base schemes are similar in their performance for the period, having a slight edge over that forecasted by the NAM-predicted Kz scheme overall, when all the regions were taken into consideration.

7. SUMMARY

Three vertical mixing schemes have been tested in a recent version of the national Air Quality Forecast System (AQFS). They are namely: (1) the Base-case of using the default AQFS scheme of supplying NCEP's NAM predicted Planetary Boundary Layer Height, *h*, to CMAQ-4.5's default RADM mixing scheme (Chang et al, 1987), (2) same as the previous configuration but uses NAM predicted Mixed Layer Height (MIXHT) as *h*, and (3) directly use NAM predicted vertical eddy diffusivity, *Kz*, to parameterize the mixing process. The schemes are tested for a 2 week period with high O_3 exceedance episodes between 21 July and 4 August, 2006.

The *Kz* profiles derived in the schemes have characteristics pertinent to geographical and temporal variations. The first two schemes show profiles of parabolic distribution. During full blown PBL growths in late afternoons, *Kz* peaks are often hundreds of J Kg^{-1}. They collapsed rather abruptly around sunset.

The MIXHT and NAM-predicted *Kz* approaches may be aligning the vertical mixing processes better between the methodologies used in NAM and CMAQ. However, they are not doing convincingly better as shown in the runs done in the test period. It may be said that the MIXHT approach is showing promise as it is as good as the Base case approach and it does best in the challenging region of the Pacific Coast.

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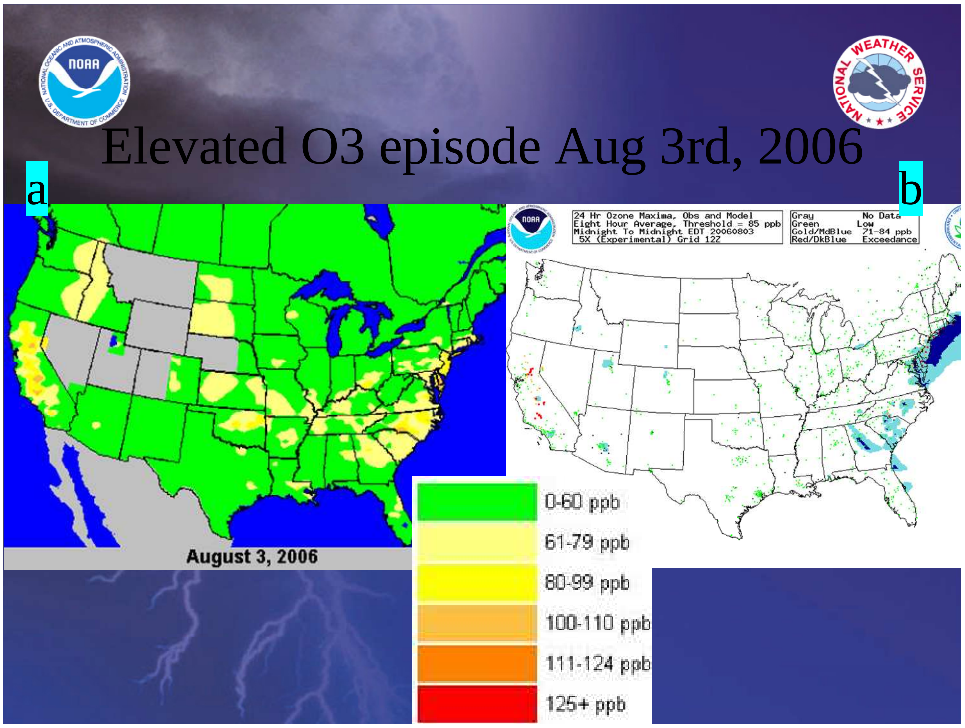

Fig. 1 Daily maximum hourly surface O_3 concentration on August 3, 2006 (a) Compiled by AIRNOW, and (b) Forecasted by AQFS (Base case) verified with the AIRNOW data.

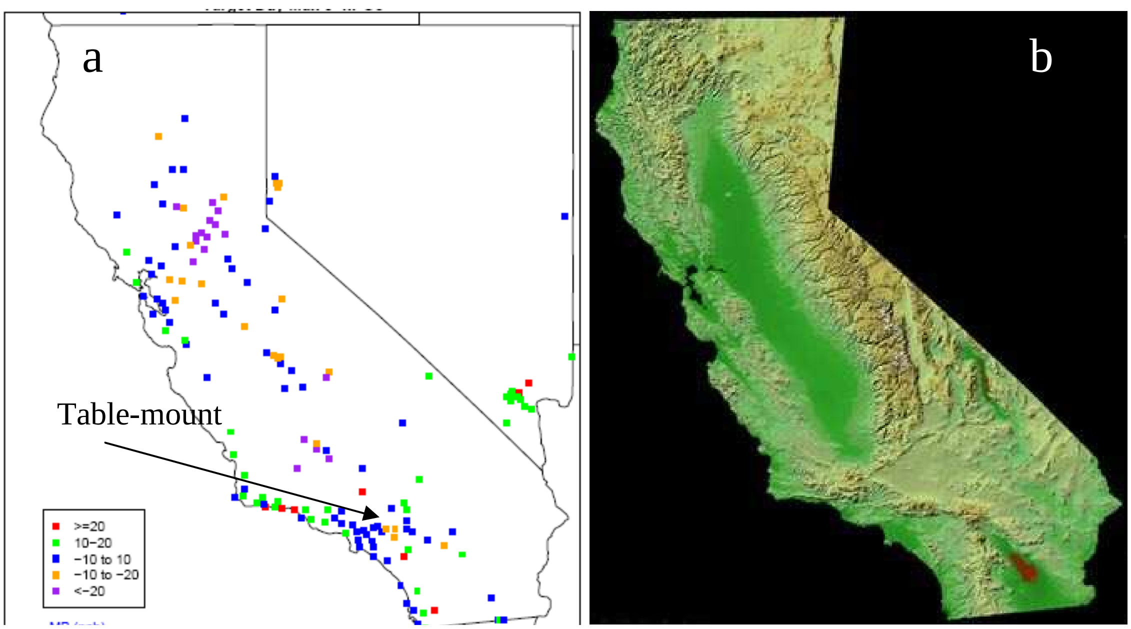

Fig. 2 Features of State of California: (a) Second day forecast of daily maximum 8 h averaged surface O_3 predicted by Base-case verified with AIRNOW for 2 August, 2006, and (b) Topology.

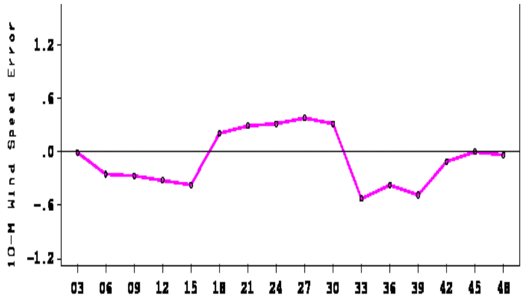

Fig. 3 10 m wind bias (m/s) over forecast hour 03 to 48 for NAM run starting at 12Z 1 August, 2006. over regions PC+RM as shown in Fig. 4.

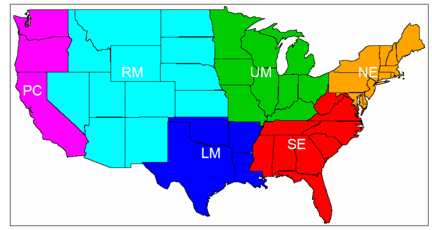

Fig. 4 Definition of regions for verification purposes.

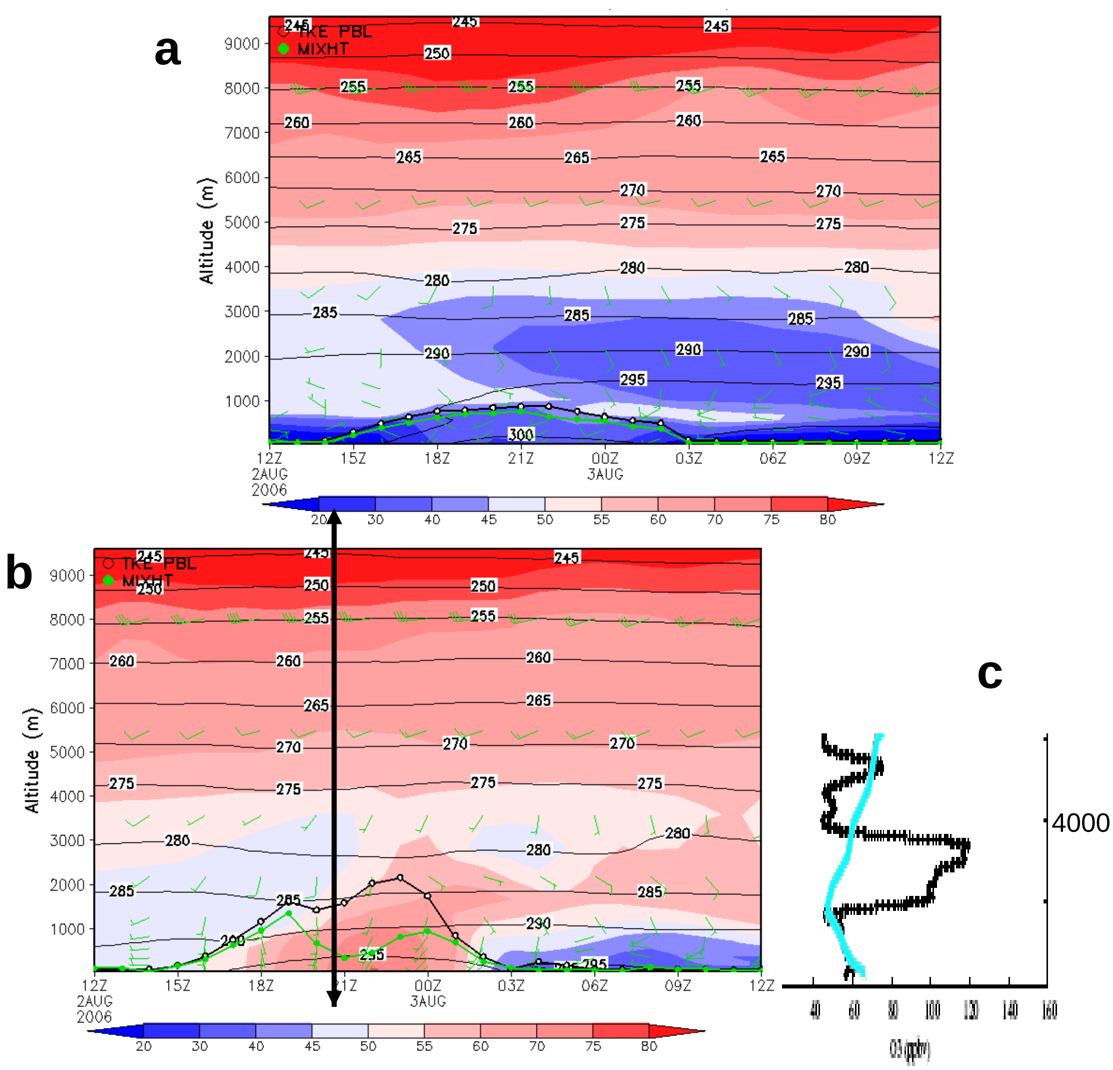

Fig. 5 Time evolution of predicted O_3 (shaded), temperature (contoured), wind (barbs), and planetary boundary height, *h*: (TKE) for Base, and (MIXHT) for MIXHT schemes over (a) LA, CA, at (118W, 34N), and (b) Table-mount, CA, at (117.7W, 34.4N) by the Base-case second day forecast valid between 12Z 2 August to 12Z 3 August, 2006. The black arrow at 20:45Z indicates the lauching time of an ozonesonde at the site whose readings (black) and modeled predicted value (blue) is depicted in (c).

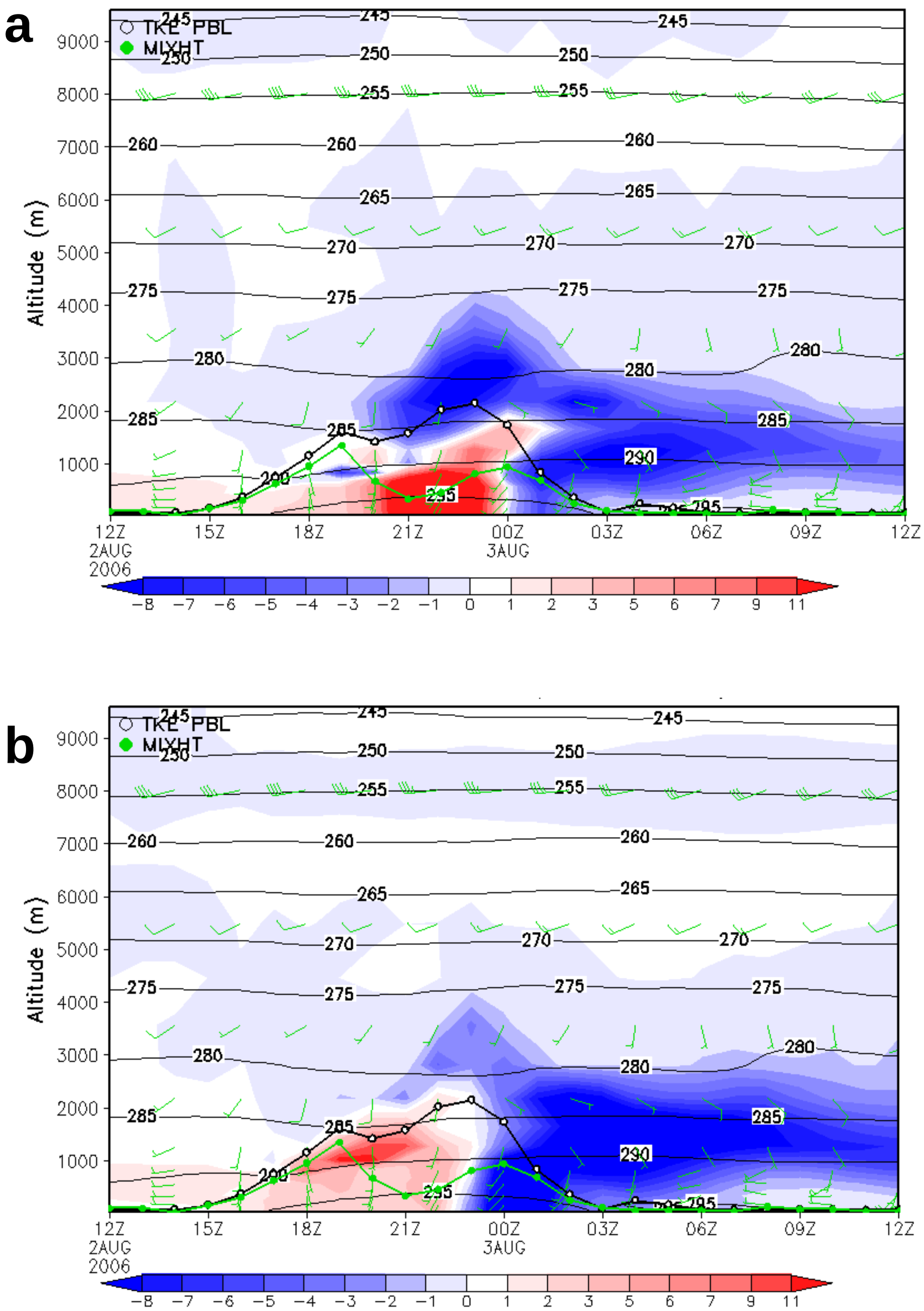

Fig. 6 Difference maps of predicted O_3 concentrations with respect to Fig. 5b by subtracting it from results based on (a) MIXHT, and (b) NAM-Kz schemes.

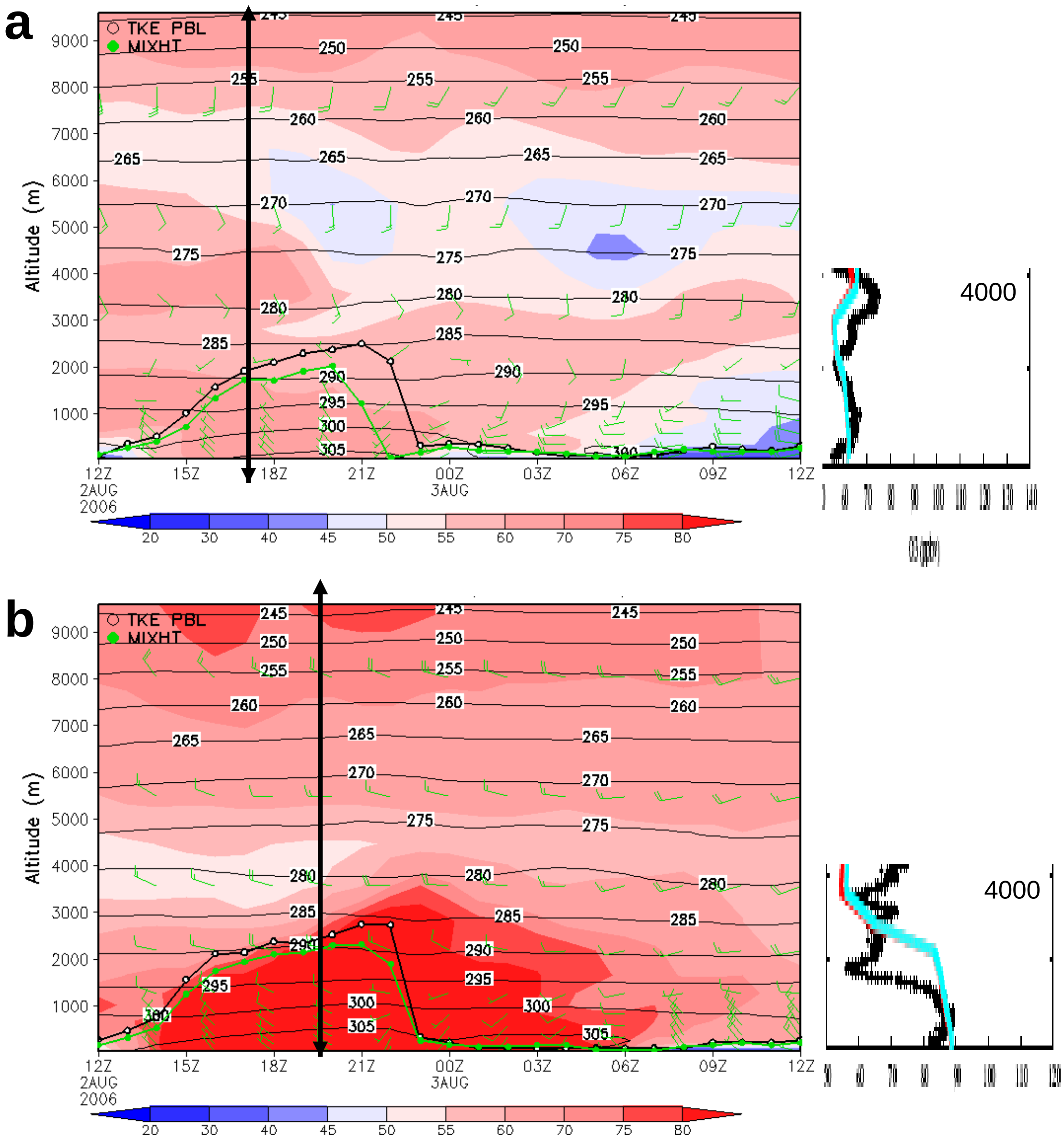

Fig. 7 Same as Figs. 5b and c but for over (a) Huntsville, AL, at (86.5W, 34.7N) with ozonesonde launched at 17:36Z 2 August, 2006, and (b) Beltsville, MD, at (76.5W, 39.0N) with ozonsonde launched at 19:18Z 2 August, 2006, respectively.

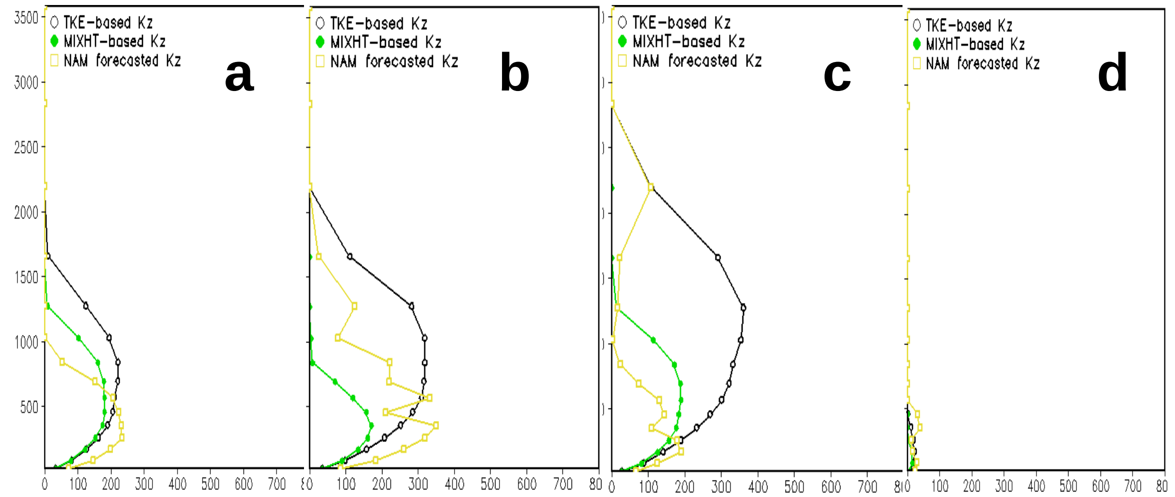

Fig. 8 Modeled vertical profiles of *Kz* (J Kg^{-1}) over attitude (m) above ground at Table-mount: TKE-based (open circle), MIXHT-based (filled circle), and NAM-forecasted (open square), at (a) 18Z, 2nd, (b) 21Z, 2nd, (c) 00Z, 3rd, and 02Z, 3rd of August, 2006.

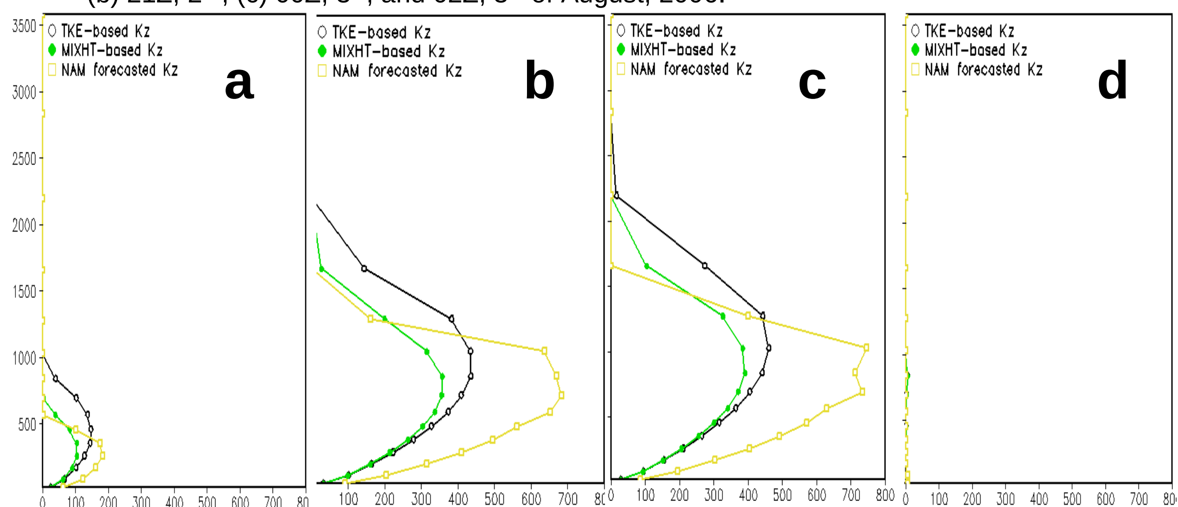

Fig. 9 Same as Fig. 8 but for over Huntsville, at (a) 15Z, 2nd, (b) 18Z, 2nd, (c) 21Z, 2nd, and (d) 00Z, 3rd of August, 2006.

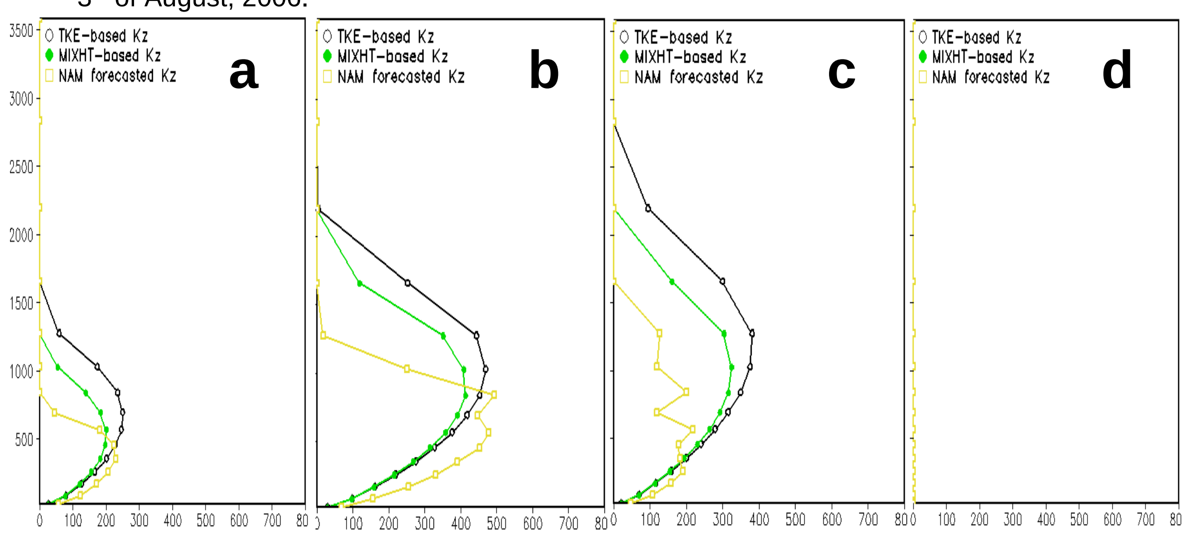

Fig. 10 Same as Fig. 9 but for over Beltsville.

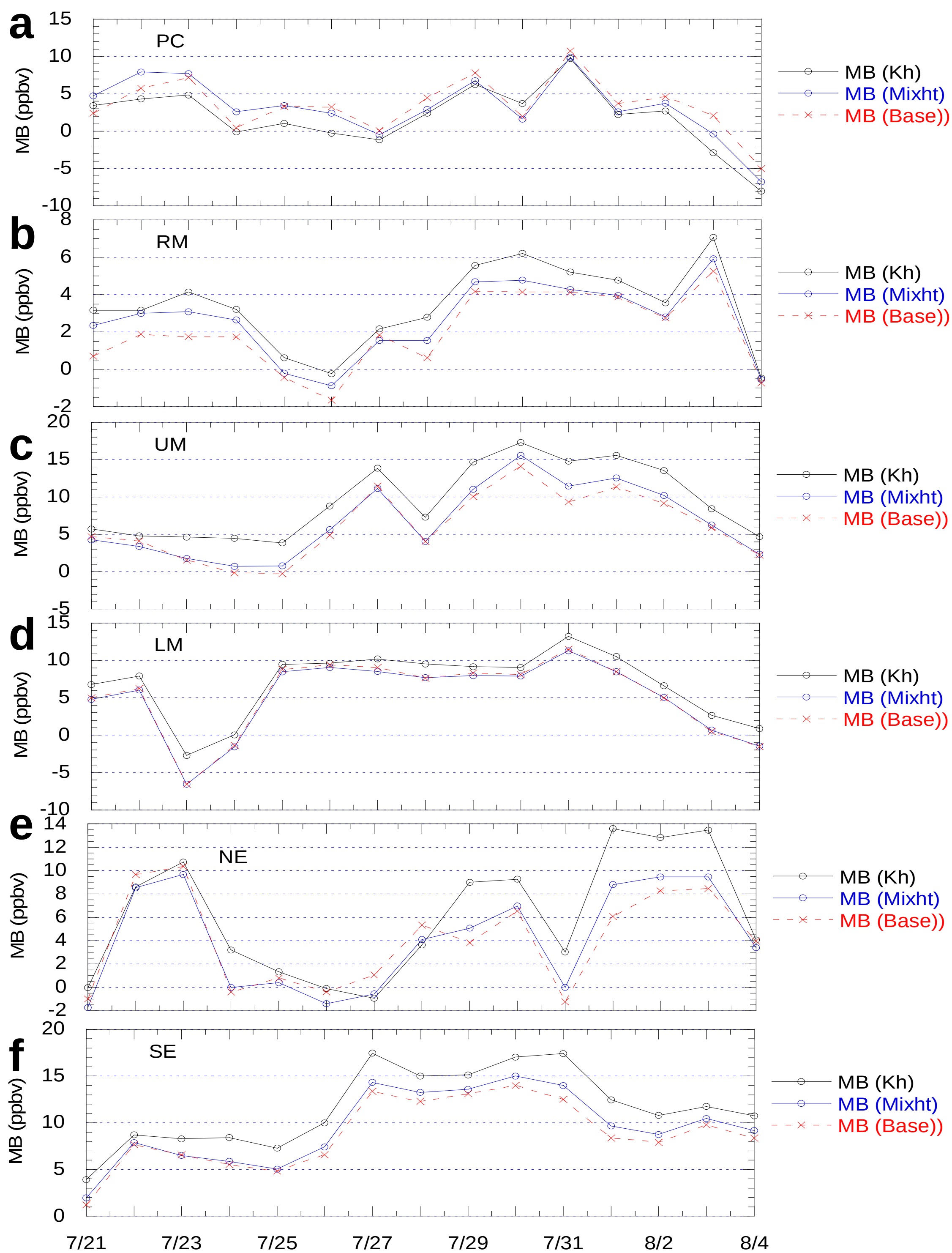

Fig. 11 Regional verification plot on mean bias based on AIRNOW data for daily maximum 8 h averaged surface O_3 for the periods between 21 July and 4 August 2006, using vertical mixing schemes described in Table 1 as: Base-case (red), MIXHT-case (Blue), and NAM-Kz case (Black) over: (a) Pacific Coast (PC) with 156, (b) Rocky Mountain (RM) with 108, (c) Upper Midwest (UM) with 231, (d) Lower Midwest (LM) with 135, (e) Northeastern (NE) with 161, and (f) Southeastern (SE) with 216 stations, respectively.