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Air Quality forecast using WRF/NMM-CMAQ during the TexAQS

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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 (AQF) 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 O_3 forecast capability for Northeastern U.S. (Davidson et al, 2004). The NWS/ National Centers for Environmental Prediction (NCEP) North American Meso-scale (NAM) model (Rogers et al, 1996; Janjic 2003) at 12 km was used to drive the EPA Community Multi-scale Air Quality (CMAQ) model (Bynn et al, 1999) to produce up to 48 hour O_3 predictions.

From the outset, plans have called for the AQF capability to include particulate matter forecast guidance also. The importance of such a capability is obvious. High volume of particulate matter suspended in the atmosphere posts hazard to health and impairment to visibility. Several regions in the country have recently reported haze and degraded visibility for prolonged period of time (e.g., Taubman et al, 2004). Moreover, every year, upwards of 40,000 premature deaths in the US are attributed to exposure to airborne particulate matter (Kaiser, 2005).

A developmental version of the AQF capability (Lee et al, 2006), hereafter dubbed as AQF-β, that includes the predictions of airborne fine particulate matter (PM2.5) has been tested during the summer of 2006. It covers the CONtinental US (CONUS) with daily 48 h predictions.

The Texas Air Quality Study (TexAQS) 2006 is an intensive field campaign aimed to better understand the sources and processes responsible for the formation and distribution of tropospheric O_3 and aerosols (TCEQ, 2006). The campaign was conducted between early August and mid October 2006. Data collected during TexAQS by multiple air and land based stations provided a unique opportunity to verify the forecast quality of AQF-β.

2. Model CONFIGURATIONS

The NAM meteorological model is also known as the Weather Research and Forecasting/ Non-hydrostatic Meso-scale Model (WRF/NMM). It provides met and hydrometeor fields to CMAQ to derive the transport, and transformation, as well as the meteorological dependent emission strengths, of the various atmospheric gaseous and aerosol species and their precursors.

a. WRF/NMM Model

The model is the successor of the NCEP Eta model. The three major improvements of WRF/NMM from its predecessor are: (1) non-hydrostatic approach, (2) adoption of a 60 levels, upper-levels pressure-surfaces, and lower-levels terrain following σ-p hybrid coordinate, and (3) conform to the WRF data interface infrastructure. Otherwise the horizontal griding and physics packages are rather similar to those used in the Eta model (Rogers et al, 2005, Ferrier et al, 2005); namely, they both use Arakawa E-grid horizontal stencil; Noah unified 5-layer land and surface model; Mellor-Yamada-Janjic planetary boundary layer closure scheme; Ferrier cloud microphysics; and Betts-Miller-Janjic convective mixing scheme.

b. CMAQ Model

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CMAQ version 4.5 has been adapted for this testing (Pleim et al, 2005). To take advantage of the generalized co-ordinate system in CMAQ, the 22 layered vertical grid structure used in the model is a subset of the 60 hybrid layers used in WRF/NMM (Lin et al, 2006). Therefore there is no need for vertical interpolation of the met fields as was done previously (Otte et al, 2005). Table 1 below shows the main parameterization features configured for AQF-β.

Table 1. CMAQ configuration for AQF-β

Phyical Processes	Scheme used in CMAQ
Vertical diffusivity	NMM PBL height to derive Pleim-Xiu 1^o Kz (2001)
Subgrid In-cloud convective mixing	Asymmetric Convective Scheme (Pleim & Chang, 1992) constraint by NMM given convective precip
Photolysis attenuation due to cloud	Scale J-table to reflect the ratio of NMM given actual and clear sky radiation fields
Aerosol processes	Modal model (Binkoski and Roselle, 2003)
Dry deposition	Pleim Xiu scheme (2001) using NMM given canopy conductance
Concentrations boundary conditions	Static condition with a single representative profile for each lateral boundary

3. The August 2-4, 2006 O_3 Episode

During the five days between August 1st and 5th, 2006, there were many O_3 exceedances in the U.S. A heat wave started from central U.S. on July 31st, 2006 eventually affected most of country within the following few days. Figure 1 shows daily maximum temperature between August 2nd and 4th noting the continue expansion of the affected area despite of its ebbing intensity during the shown period. Figure 2 shows that AQF-β was able to capture the magnitude and distribution of surface O_3 for those three days considerably well as the predicted values of daily 1 h maximum concentration largely lie within ±10 ppb of the observed values. The model tended to have a high bias in Florida, New England Up-states; yet a low bias in the lower Central Valley in California. The observations used for verification of the current testing are provided by EPA's AIRNOW network (EPA, 2006). Over the CONUS in the period of interest it compiled observation data from 1103 stations for surface O_3 and 466 stations for surface PM2.5. Figure 3 is similar to Fig. 2 but shows the PM2.5 forecast quality of AQF-β. There is a general low bias for the prediction of the daily averaged surface PM2.5 particle mass concentration. It is interesting to note that the localities with elevated surface O_3 concentration do not necessarily co-locate with those with high surface PM2.5 concentration. For areas near Houston, TX, there was O_3 exceedance on August 4th, but rather low surface O_3 concentrations for the 2nd and 3rd. On the contrary, surface 24 h averaged PM2.5 concentration for the area is consistently in the high end of between 20 and 30 μg m^{-3} during those 3 days.

4. Concentrations at two TexAQS sites

In concert with the large data set that will soon be available from the TexAQS 2006 campaign, there is interest to study some of the characteristics of the studied area. One of those areas is the coastal region near the Galveston ship channel. The complex irregularities of the coast represent a highly variable forcing of the land and sea flow pattern. Given that there are major point sources of VOC from local petro-chemical plants and NOx from the channel traffic, narrow plumes of air pollutants can constitute sharp gradients of concentrations in the area (e.g., Darby, 2005). Across the ship channel two stations, one on each side, both are AIRNOW stations as well as TexAQS stations, have been chosen to provide insights into the temporal and spatial variations of the various chemical species. Figure 4 shows the locations of these stations: (A) Channel View Station (CVS), near downtown Houston, is a typical urban site; and (B) Beaumont Port Arthur Station (BPAS), near the Texas-Louisiana border, is situated at the interface of urban and rural environments.

a. Surface Concentration Time Series

Figure 4 also showed the sharp horizontal gradient of surface O_3 concentration around the city center of Houston, where CVS is roughly situated. These gradients are evident of large amount of emission, such as surface level NOx emission from automobiles that depletes O_3 formed from photochemical reactions. In the surrounding suburbs, there were elevated surface O_3 concentrations. There were a couple

of exceedances in the western suburb of the city. At both CVS and BPAS the daily diurnal pattern of surface O_3 concentration is appropriately captured by AQF-β between 6 UTC August 4 to 6UTC August 6, 2006, as shown in the time series plots of Fig. 5a and b, respectively.

Figure 5a also shows that the model failed to reproduce the early afternoon peaks on August 4th and 5th at CVS. Apparently the effect of O_3 titration as postulated in the previous paragraph has a stronger impact near the city center rendering the low bias during most the day, especially in the night hours when photolytic production of O_3 is not active. AQF-β does a better job in reproducing the daily peaks at BPAS as shown in Fig. 5b.

Figures 6a and b show the surface level PM2.5 concentration for the CVS, and BPAS sites, respectively. There is a persistent low bias for both sites, particularly during the mid afternoon hours. It is not sure that AQF-β exhibited any skill in reproducing the somewhat un-pronounced diurnal pattern of concentration variations of having daily peaks around noon to mid-afternoons.

b. Vertical O_3 Profile & a refined structure

INTEX Ozonesonde Network Study (IONS) data were available at CVS on August 2nd and 4th during the period of interest in this study. Figure 7 shows predicted concentration profiles of O_3 at CVS. Also displayed in the same diagram are: (1) those obtained from the ozone-sonde, and (2) AQF-β predicted yet with a refined vertical grid configuration of 40 hybrid model levels with most of the additional 18 layers inserted in the lower 3 km. This 40 layer configuration run has been conducted exactly like that for the 22 layer run. The ozone-sondes were launched at 18:04 UTC on both days. The red and green lines depict forecast results from the 22 vertical layers, and 40 vertical layers, respectively. Figure 7a shows that both AQF-β runs with 22 and 40 vertical-layer configurations over-estimated O_3 for the entire Planetary Boundary Layer (PBL). The predicted O_3 concentration profile in the free troposphere is much better. There is no obvious advantage of improved forecast quality by the refined structure of 40 layers over that with 22 layers. Figure 7b shows the same profiles for August 4th. In contrast to that shown on August 2nd, in Fig. 7a, the model prediction showed large low bias for the O_3 concentrations within the PBL. The same argument about the strong local influence of NOx induced O_3 titration may offer some account of the large low bias.

On the interface of the PBL and the free troposphere, the 40 layer configuration offers a better agreement in terms of capturing the multiple inflexion points of the observed profile. This maybe explained by ability of the finer vertical structure to preserve sharper vertical concentration gradients of the chemical species. Figures 8a and b show the cross section for O_3 concentration for the 22 layers configuration run along points A and B as depicted in Fig. 4, for 18 UTC August 4, and 6 UTC August 5, respectively. They correspond to noon and mid-night hours local time, respectively. Figures 8c and d are similar plots but for the 40 layers run. The local minimum of Fig. 8d during the mid-night hour is confined to a shallower vertical extent than that in Fig. 8b. There is also shown evidence of less dispersed O_3 plume above the nocturnal inversion layer. This preservation of sharper concentration gradients can contribute to the capturing of multiple inflexion points in the observed profile. Figures 9a-d show that the same phenomenon is also in play for one of the O_3 precursors, NOx. Noting that Figs. 9d shows that for the 40 layers run there is a more ground-hugging elevated concentration distribution of NOx in the vicinity of CVS when compared to that shown in Fig. 9b of the 22 layers run. This can explain in part the lowest level difference of the profiles of these two runs within the PBL as shown in Fig. 7b.

5. Summary

A developmental version of the NOAA/EPA AQF capability with 22 and 40 layer configurations had been tested during the TexAQS 2006 field experiment. Preliminary results have been verified with the AIRNOW network. Both the 22 and 40 layer configurations showed reasonable skill in predicting the magnitude and the diurnal peak characteristics of surface ozone in an urban and an urban-rural interface sites. The model does not exhibit a similar degree of skill in forecasting surface PM 2.5. In lieu of the fact that the vast amount of the observation data is currently under processing, some ozone-sonde data collected during the experiment has been utilized to verify the model results. Analyses of two vertical profiles suggest that the 40 layer configuration better captures multiple inflexion points of vertical O_3 concentration profiles.

6. Acknowledgement and disclaimer

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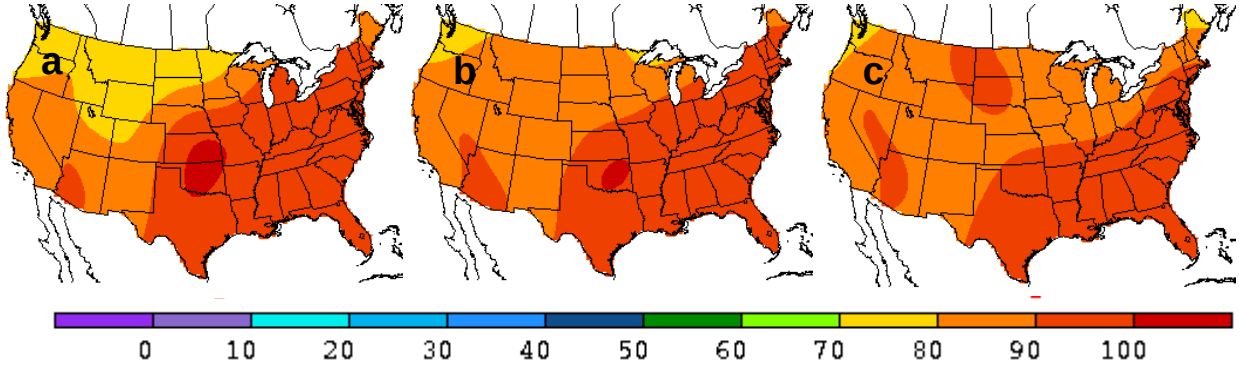

Fig 1. Maximum daily surface temperature in ^{o}F measured on August (a) 2nd, (b) 3rd, and (c) 4th, 2006, respectively.

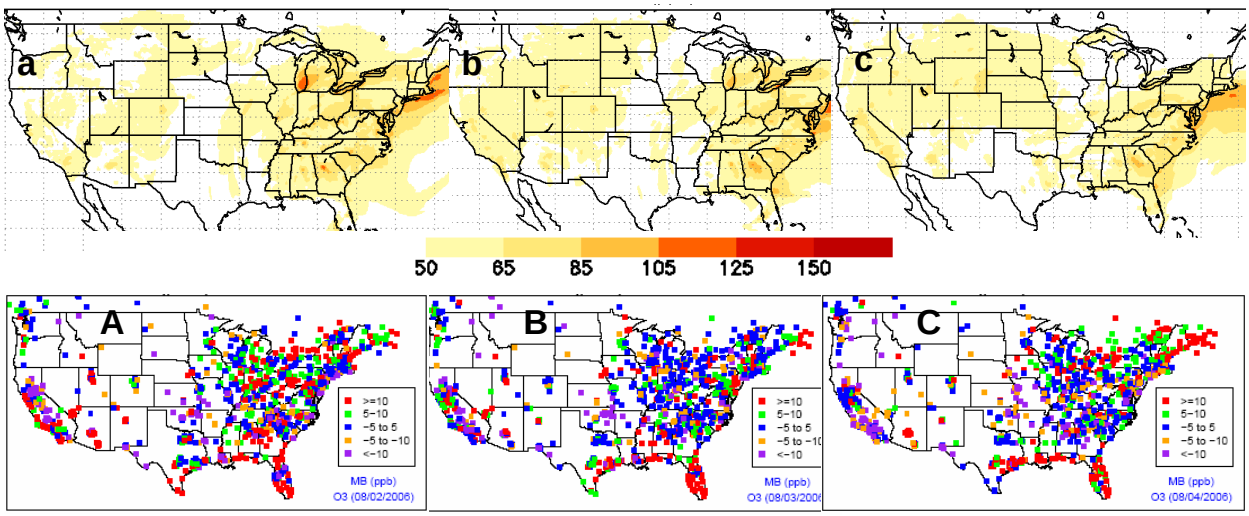

Fig. 2. Daily 1h max surface O_3 concentration in ppb: (a-c) Predicted by AQF-β with 22 layer configuration, and (A-C) their corresponding mean biases verified with the AIRNOW network, for August 2nd, 3rd, and 4th, 2006, respectively.

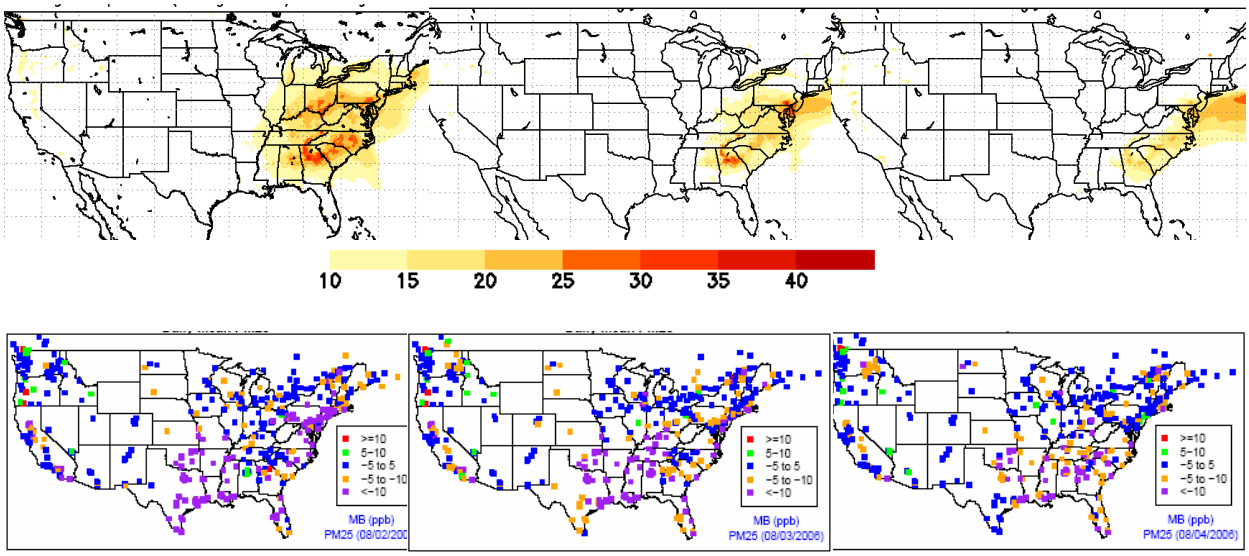

Fig. 3. Same as Fig. 2 but for daily 24h averaged PM2.5 concentration in μg m^{-3}.

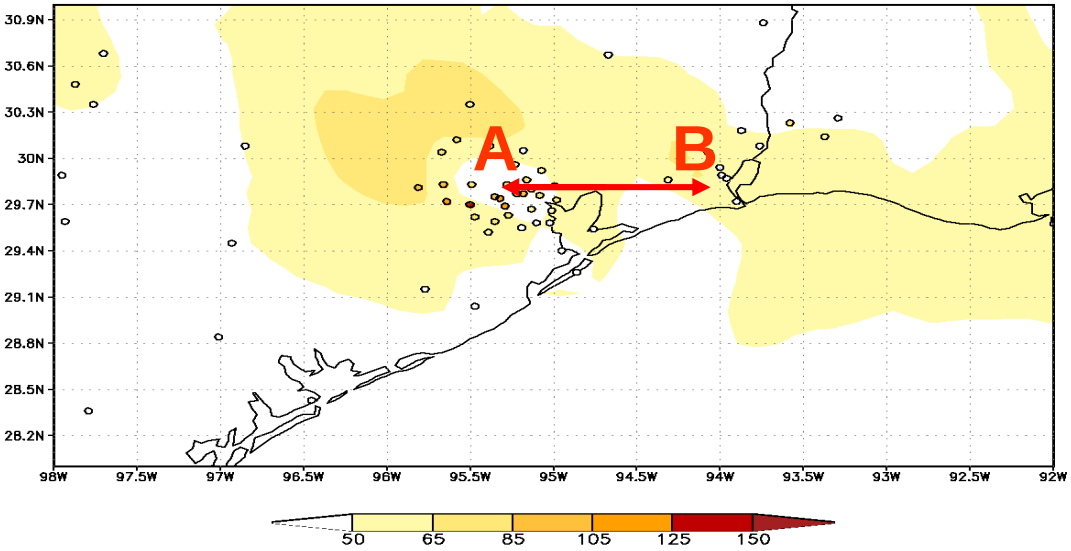

Fig. 4. A zoom in of Fig. 2.c centering around Houston, TX, with AIRNOW base verification concentrations in color-filled circles using the same accompanied color bar categorization, also shown is the location of a west to east cross-section traversing the Channel View Station (Point A) and the Beaumont Port Arthur Station (Point B).

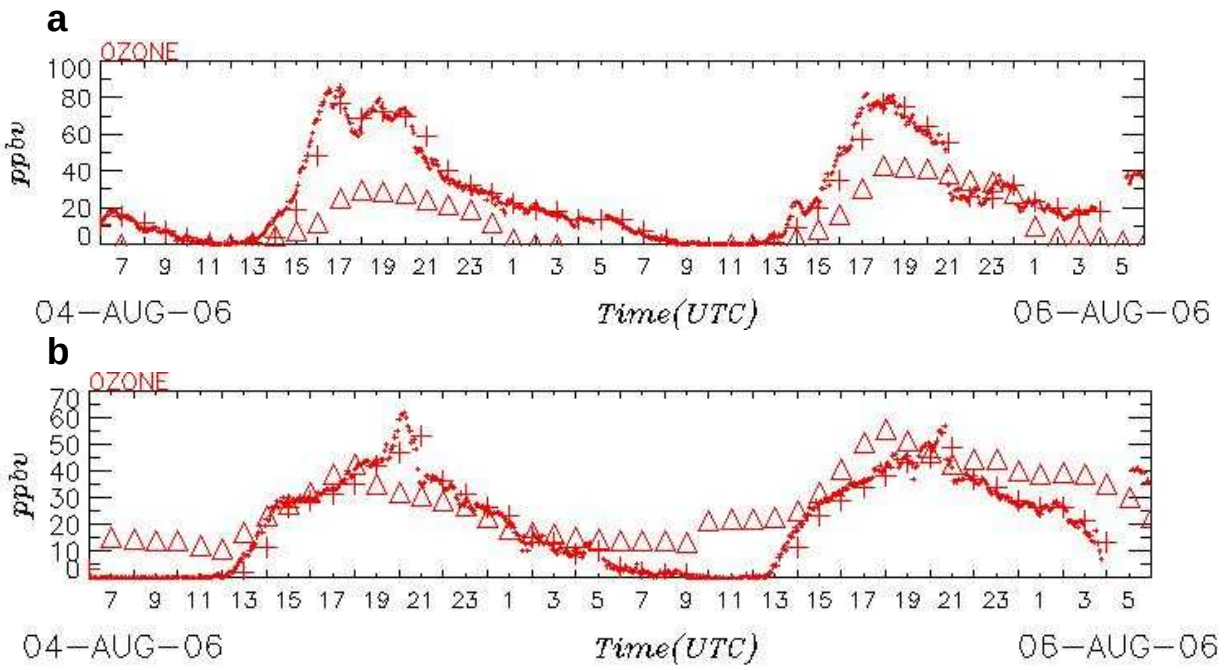

Fig. 5. Verification on the temporal evolution of surface O_3 in ppb, between 6 UTC August 4 to 6 UTC August 6, 2006 for (a) Channel View Station (Point A), and (b) Beaumont Port Arthur Station (Point B).

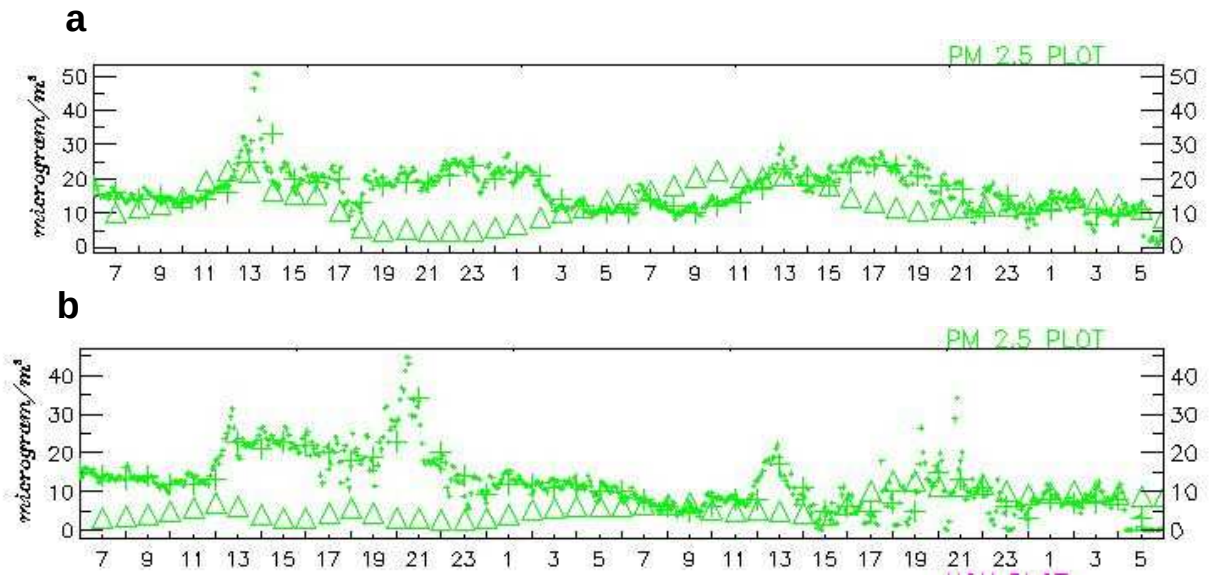

Fig. 6. Same as Fig. 5 but for PM2.5 in μg m^{-3}.

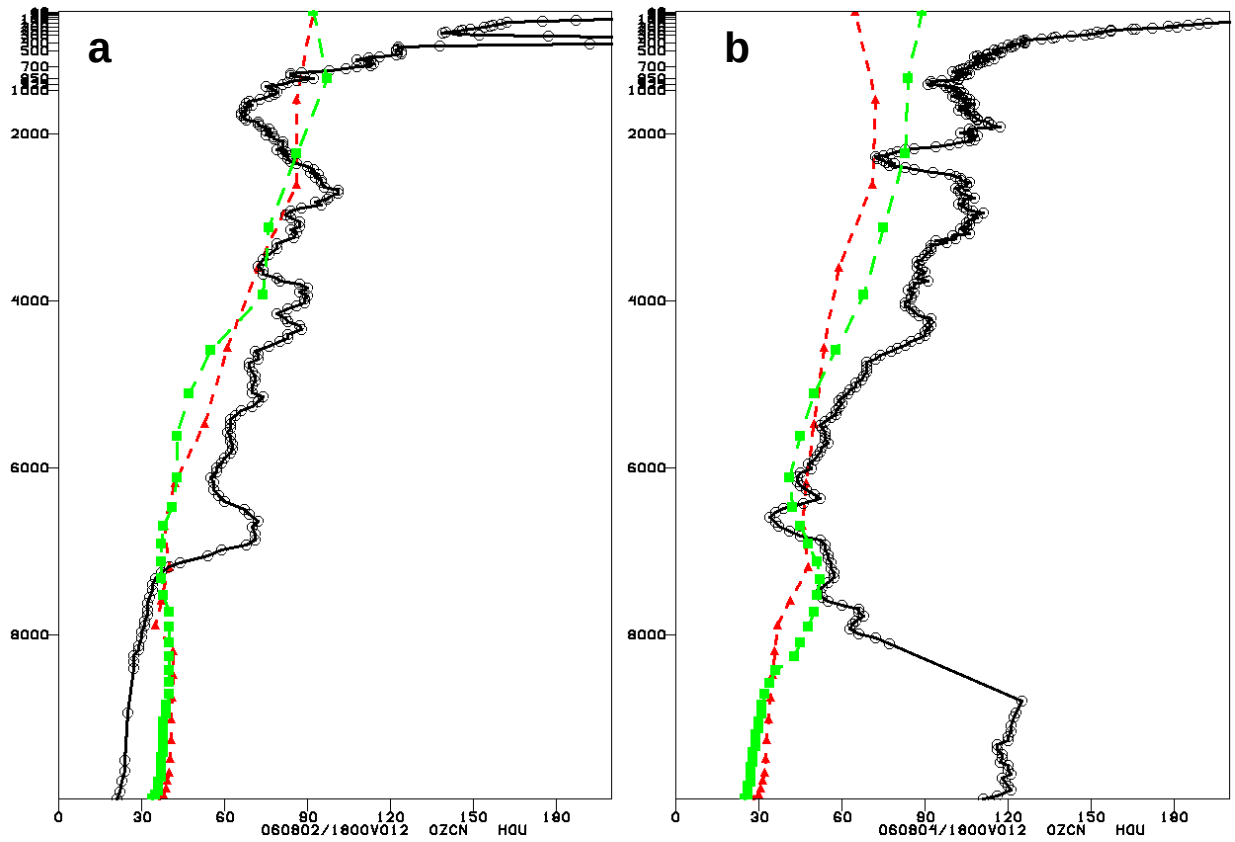

Fig. 7. Verification of O_3 profile in sigma (value has been multiplied by 10^4) ordinates for AQF-β runs with 22 layer (red), and 40 layer (green) grid-configurations using IONS data at CVS for 18 UCT on: (a) August 2nd, and (b) August 4th, 2006.

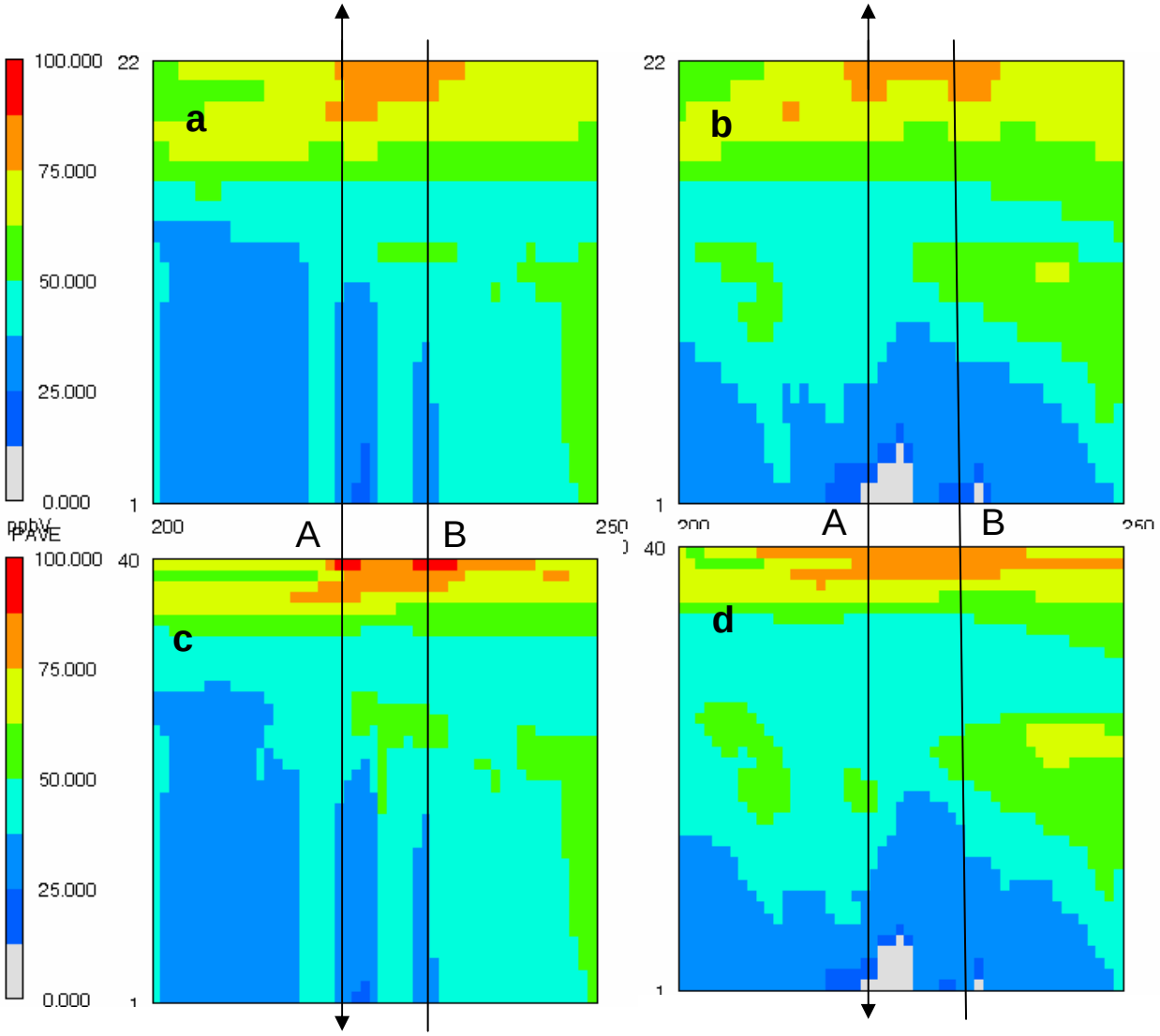

Fig. 8. Vertical cross-section of O_3 traversing points (A) and (B) --- as depicted in Fig. 4 for: (a & b) 22 layer, and (c & d) 44 layer configurations, for: (a & c) 18 UTC August 4th, and (b & d) 6 UTC August 5th, 2006.

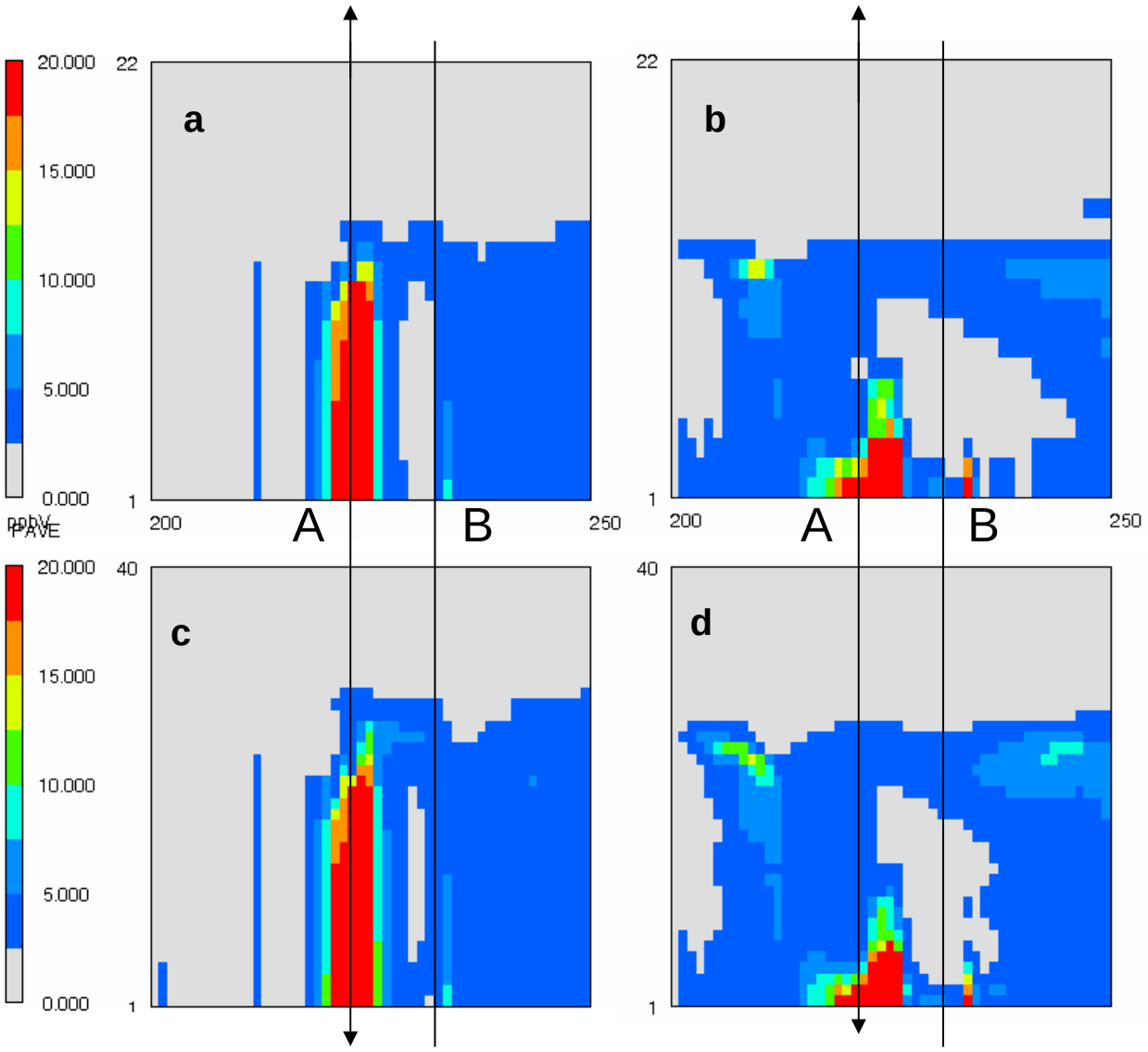

Fig. 9. Same as Fig. 8, but for NOx.