

# The Influence of PBL parameterizations on the distributions of chemical species in a mesoscale chemical transport model, WRF-Chem

Si-Wan Kim\*, S. A. McKeen\*, E.-Y. Hsie\*, M. K. Trainer, G. J. Frost\*, G. A. Grell\*, and S. E. Peckham\*

NOAA ESRL, Boulder, Colorado, USA

\*Also CIRES, University of Colorado, Boulder, Colorado, USA

## 1. INTRODUCTION

The turbulent mixing and chemical transformation in the planetary boundary layer (PBL) play a crucial role in the distribution of chemical species. Thus, the reasonable representation of the PBL processes in a mesoscale chemical transport model is a key to the accurate prediction of concentrations of chemical species, e.g., ozone. In this study, we utilize WRF-Chem model (Weather Research and Forecasting – Chemistry model) to examine the effects of the PBL modeling on the distribution of the chemical species, such as carbon monoxide (CO), ozone (O<sub>3</sub>), nitrogen dioxide (NO<sub>2</sub>), odd nitrogen species (NO<sub>y</sub>), and isoprene (C<sub>5</sub>H<sub>8</sub>). WRF-Chem simulations are evaluated with the NOAA P3 aircraft observation during 7/15/04–8/15/04 ICARTT (International Consortium for Atmospheric Research on Transport and Transformation) field campaign ([www.noaa.gov/ICARTT](http://www.noaa.gov/ICARTT)). Two PBL models are tested: YSU (K-profile method, Hong, 2005) and MY (2.5 turbulence closure, Mellor and Yamada, 1982) PBL models.

## 2. MODEL DESCRIPTION

The Weather Research and Forecasting (WRF) Chemical model has foundation on the non-hydrostatic mesoscale numerical weather prediction model, WRF community model developed at National Center for Atmospheric Research by collaboration of several research institutes. WRF provides operational forecasting model that is flexible and efficient computationally, while offering the advances in physics, numerics, and data assimilation contributed by the research community (<http://www.wrf-model.org>). WRF Chemical model (WRF-Chem, Grell et al., 2005) is an extension of the earlier MM5-Chem regional scale chemical transport model (Grell et al.,

2000) to the WRF architecture. This model system is “online” in the sense that the all processes affecting the gas phase and aerosol species are calculated in lock step with the meteorological dynamics (McKeen et al., 2005). Meteorological initial conditions are taken from the National Centers for Environmental Prediction (NCEP) Global Forecast System model analysis fields, and lateral boundary conditions are derived from the NCEP Eta model forecast. Gas phase chemistry is based upon the Regional Acid Deposition Model version 2 (RADM2) (Stockwell et al., 1990) with updates to the original mechanism (Stockwell et al., 1997). Lateral boundary conditions for ozone and its precursors are the same as in McKeen et al. (2002) and are based on averages of mid latitude aircraft profiles from several field studies over the eastern Pacific. Biogenic emissions are calculated at each time step using the Biogenic Emissions Inventory System (BEIS3.11) algorithm

(<http://www.epa.gov/asmdnerl/biogen.html>).

WRF-Chem retrospective simulations are WRF-Chem 24-hour forecasts starting at 0000 UTC each day between 15 July and 15 August 2004. The horizontal domain of 134 × 110 grid points has a grid spacing of 27 km and is centered at 86.3 °W and 38.0 °N. The spacing of the model's 35 vertical levels is about 16m near the surface and increases to about 1.5 km at the top of the domain (at ~18 km). We use the emission, in which the Environmental Protection Agency National Emission Inventory 1999 NO<sub>x</sub> and SO<sub>2</sub> emissions for about 1000 power plants were updated using ratio of the 2004/1999 Continuous Emission Monitoring System (CEMS) emission rate data similar to Frost et al. (2006). Two WRF-Chem retrospective cases are performed. One used YSU PBL option, and the other adopts Mellor-Yamada Eta PBL option. We use NOAA land surface model for the both simulations.

### 3. RESULTS

The comparisons of temperature, water vapor mixing ratio, wind speed, and wind direction between aircraft observation and two PBL simulations are shown in Fig. 1. It demonstrates that WRF-Chem model simulates PBL meteorological variables reasonably. Overall, PBL temperature from YSU and MY PBLs are lower than the observations. Below 500 m, MY PBL produces colder PBL than YSU PBL (Fig. 1a). Water vapor values from model simulations are higher than the observations for most of height (Fig. 1b). Relative humidity from MY PBL (YSU PBL) below 1000m is about 10 % (5 %)

higher than the aircraft measurement. Modeled wind speed and directions agree reasonably with the observations (Figs. 1c and 1d). Close to the surface, MY PBL shows weaker wind than YSU PBL. In summary, below 500m, boundary layer from MY PBL is wetter and colder. Wind speed from MY PBL is lower than those from YSU PBL near the surface. It implies that MY PBL has less turbulent kinetic energy near surface than YSU PBL, which suppress turbulent exchange in the boundary layer.

Fig. 2 demonstrates the vertical distributions of chemical species from aircraft measurement and two PBL simulations. All model results

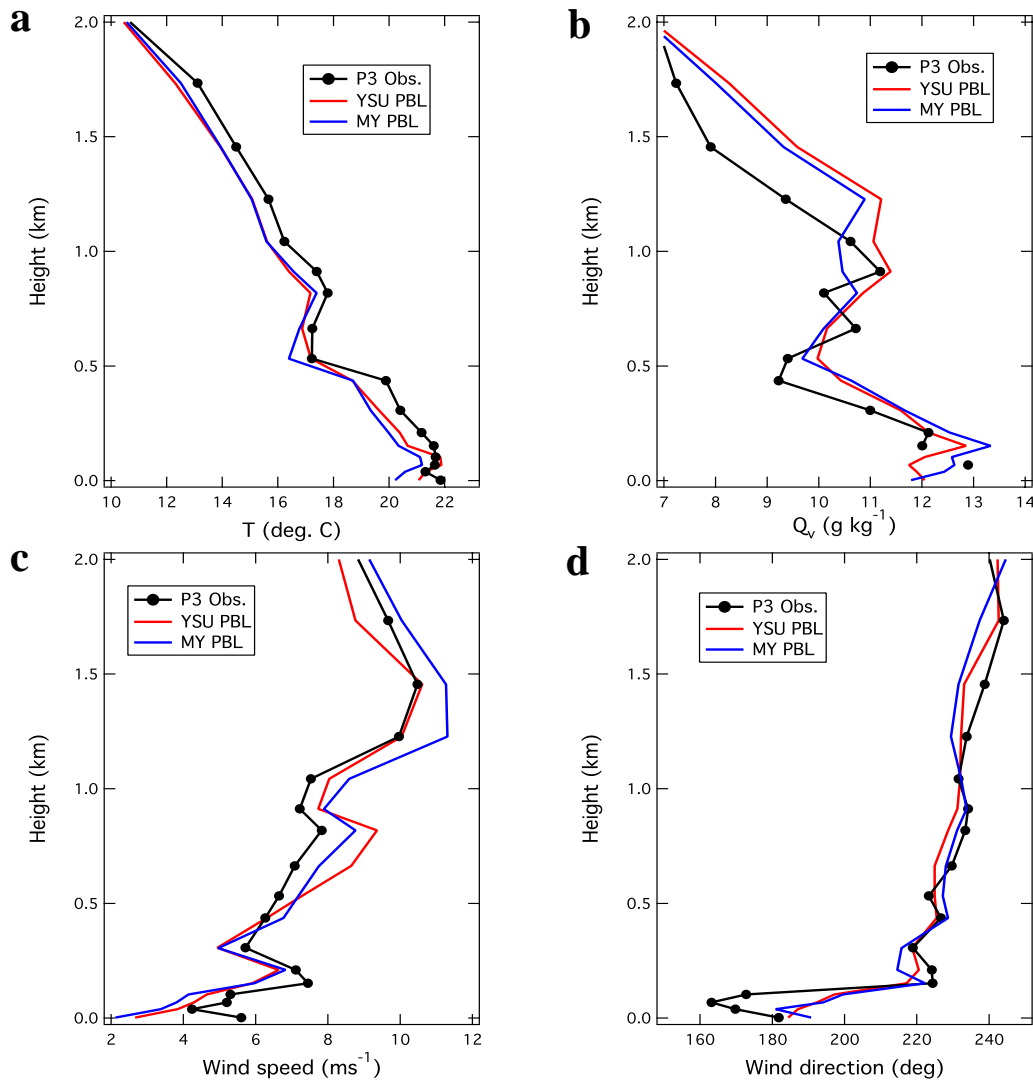


Fig. 1. Profiles of medians of meteorological variables from NOAA P3 aircraft (black line with circle), YSU PBL (red line), and MY PBL (blue line) using all data during 7/15/04–8/15/05: (a) Temperature ( $^{\circ}C$ ), (b) water vapor mixing ratio ( $g\ kg^{-1}$ ), (c) wind speed ( $ms^{-1}$ ), and (d) wind direction ( $^{\circ}$ ).

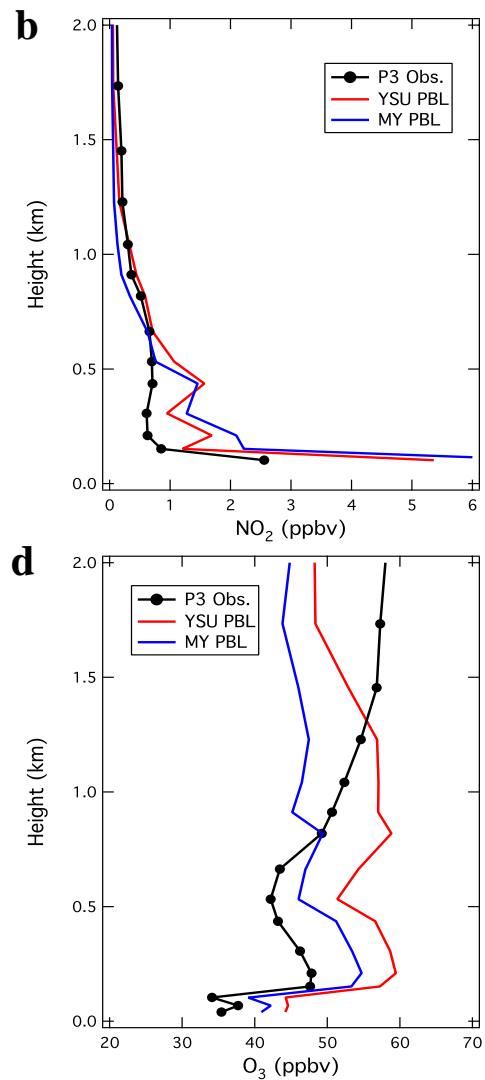
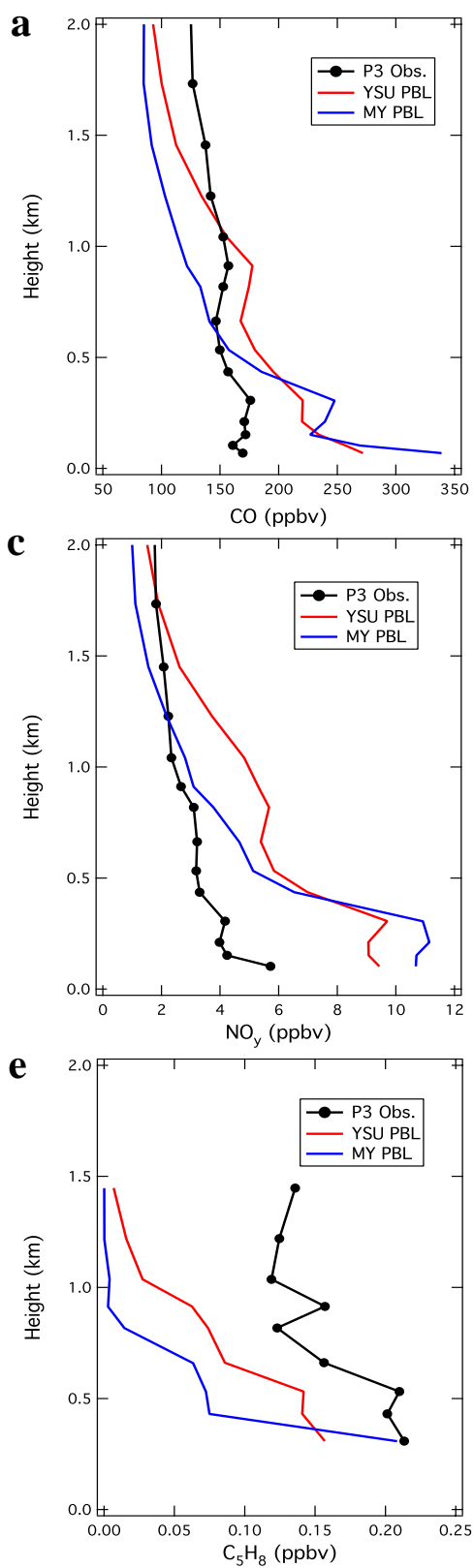


Fig. 2. Profiles of medians of chemical species using all data from NOAA P3 aircraft (black line with circle), YSU PBL (red line), and MY PBL (blue line) during 7/15/04 – 8/15/05: (a) CO (ppbv), (b) NO<sub>2</sub> (ppbv), (c) NO<sub>y</sub> (ppbv), (d) O<sub>3</sub> (ppbv), and (e) C<sub>5</sub>H<sub>8</sub> (ppbv).

does not show enough mixing compared to the observations. Discrepancies between the model and observations is huge. The model simulated mixing ratios of CO, NO<sub>2</sub>, NO<sub>y</sub> show much higher value near the surface and lower values at the upper level than the measured values. These model values are two to three times larger than the observed ones near the surface. Although NO<sub>2</sub> mixing ratio shows maximum near the surface, O<sub>3</sub> mixing ratio shows minimum value at this height. This is due that the production rate of O<sub>3</sub> decreases as NO<sub>x</sub> increases in high NO<sub>x</sub> regimes as mentioned in Frost et al. (1998), i. e., NO<sub>x</sub> titration effect. O<sub>3</sub> is overestimated below 1 km and underestimated at the higher level. Modeled isoprene is much underestimated.

MY PBL produces higher mixing ratios near the surface and lower values at the high altitude than YSU PBL except for O<sub>3</sub>. For the reason mentioned above, higher NO<sub>2</sub> in MY PBL leads to lower O<sub>3</sub> near the surface.

The comparison between model and the aircraft observations is done at the northeastern US, limited to ICARTT field campaign domain. Next, differences between the two PBL models are examined in the full model domain. Fig. 3 shows the distribution of chemical species mixing ratios in the boundary layer from YSU PBL case and differences between YSU and MY PBL cases during daytime. Over the land, MY PBL show higher CO, NO<sub>2</sub>, and NO<sub>y</sub> than YSU PBL. However, over the lake and ocean, YSU

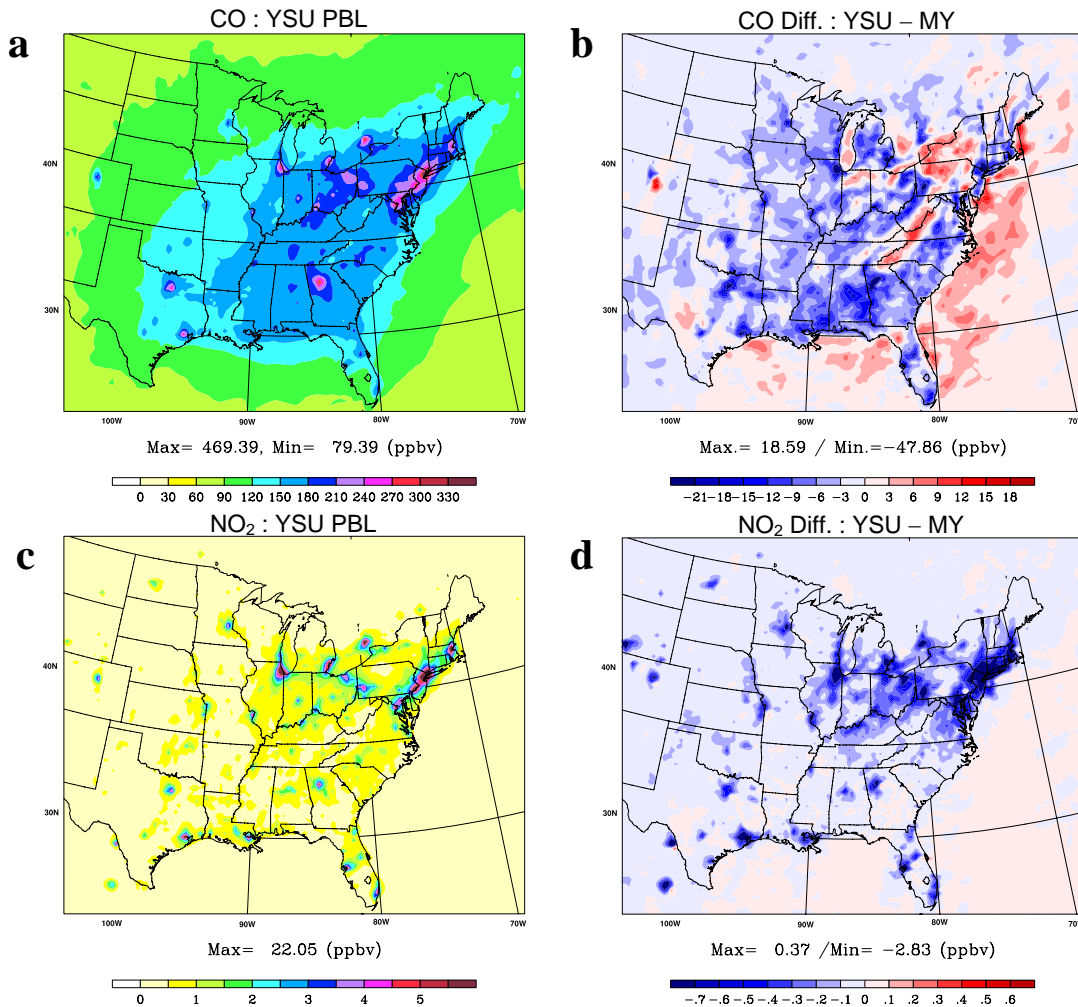


Fig. 3. Mean for YSU PBL case [(a), (c), (e), (g), (i)] and differences (= YSU - MY) between two cases [(b), (d), (f), (h), (j)] averaged from 0 to 1km using data at 20 UTC during 7/15/04-8/15/04: (a) and (b) CO, (c) and (d) NO<sub>2</sub>, (e) and (f) NO<sub>y</sub>, (g) and (h) O<sub>3</sub>, and (i) and (j) C<sub>5</sub>H<sub>8</sub>.

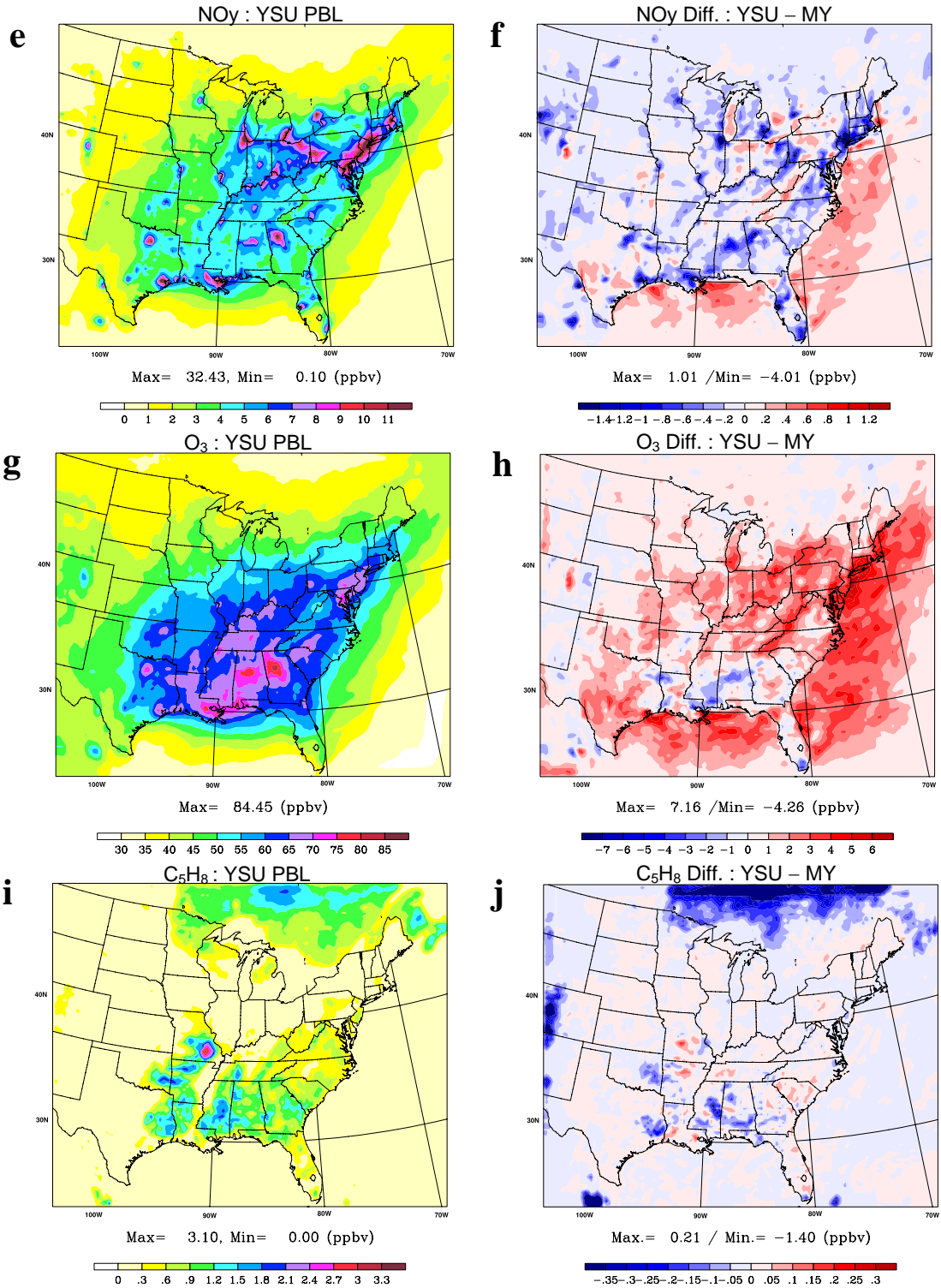


Fig. 3. Continued.

shows higher values. It indicates that the mixing in MY PBL model is suppressed over the land and that in YSU PBL model is not active over the water. PBL characteristics demonstrated in Fig. 4

support this idea. Because the PBL from YSU model is warm (Fig. 4a) and dry (Figs. 4b and 4d) over land, it has higher PBL height (more mixing) over this area. Over water, PBL height from YSU

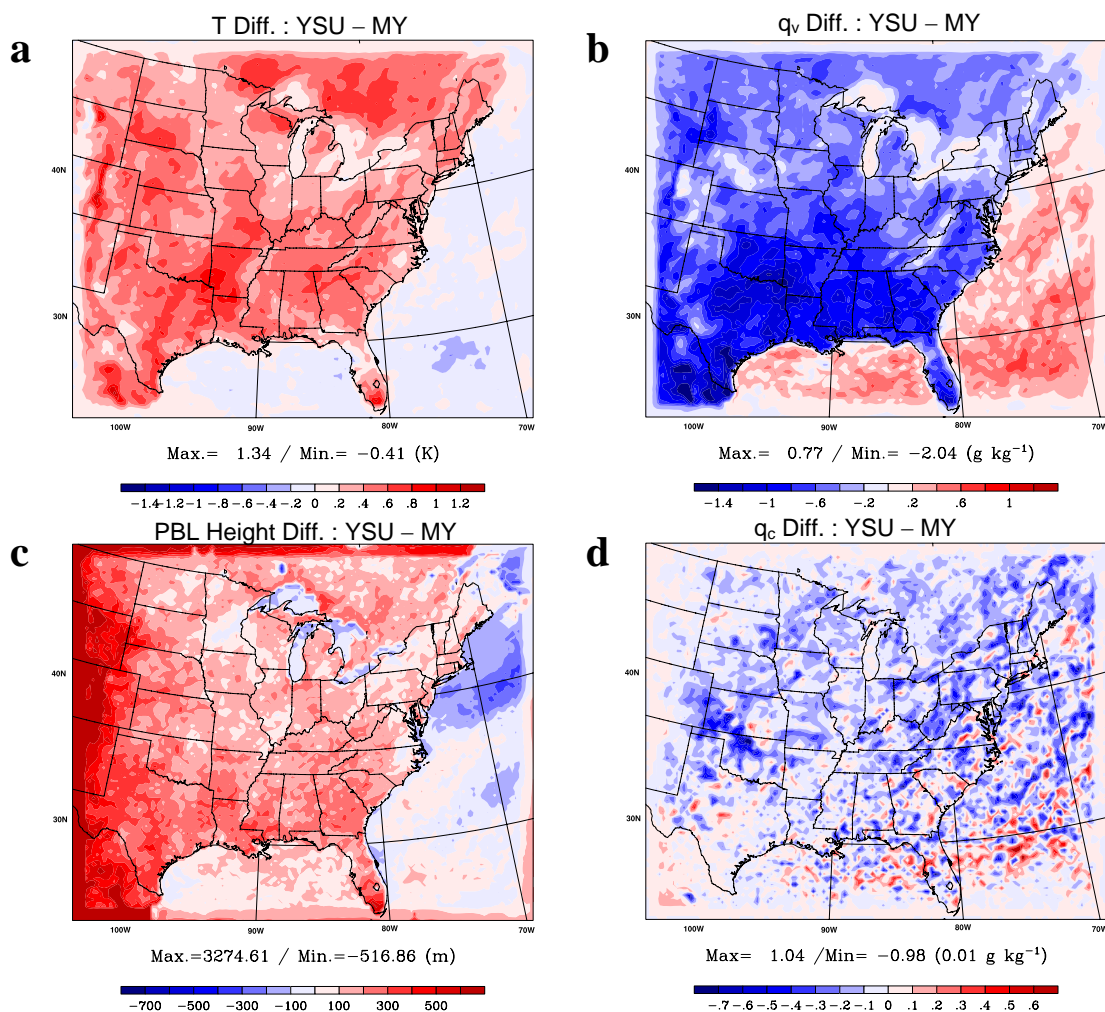


Fig. 4. Differences between YSU and MY PBL (YSU – MY) averaged during 7/15/04–8/15/04 using data at 20 UTC: (a) T (K), (b) water vapor mixing ratio ( $\text{g kg}^{-1}$ ), (c) PBL height (m), and (d) cloud water mixing ratio ( $0.01 \text{ g kg}^{-1}$ ). Every variable is averaged from 0 to 1km except for cloud water mixing ratio which is averaged to the top of the model domain.

model is lower than that in MY model with the exception of Gulf of Mexico. Thus, YSU PBL model under stable regime (daytime over cold water) needs particular attentions.  $\text{O}_3$  mixing ratio is higher in YSU PBL than MY PBL because of less  $\text{NO}_x$  titration and more isoprene emission (not shown, due to high temperature and less cloudiness) in YSU PBL. Although isoprene emission is greater in YSU model, enhanced mixing over land in YSU model leads less PBL isoprene mixing ratio than MY model for some areas.  $\text{O}_3$  fluctuations in the southeastern US (less  $\text{O}_3$  in YSU model) needs further investigations.

#### 4. SUMMARY

Both PBL models produce much higher near-surface concentrations than NOAA P3 aircraft observations. For Unstable condition, MY PBL case shows less mixed profiles: higher mixing ratio near the surface and lower mixing ratio in the upper level than YSU PBL case.  $\text{CO}$ ,  $\text{NO}_2$ ,  $\text{NO}_y$ , and  $\text{C}_5\text{H}_8$  from YSU PBL agree little bit better with aircraft observations than MY PBL. However,  $\text{O}_3$  discrepancy between model and observation is greater in YSU PBL because high  $\text{NO}_2$  values in MY PBL case suppress the production of  $\text{O}_3$  (by  $\text{NO}_x$  titration process), which in turn leads to less  $\text{O}_3$  than YSU PBL case. Under stable condition (nighttime over land, daytime over lake or ocean) boundary layer height and eddy diffusivity from YSU PBL

are too low, which traps the chemical species near the surface substantially.

In the next step, the comparison of the simulated meteorological and chemical variables with ship measurement during ICARTT field campaign and surface ozone monitoring network for the whole model domain is planned. The other aircraft measurements as well as NOAA P3 mission will be utilized for the evaluation of model simulations.

## 5. REFERENCES

Frost, G. J., et al. (2006), Effects of changing power plant NO<sub>x</sub> emissions on ozone in the eastern United States: Proof-of-Concept, *J. Geophys. Res.*, in press.

Frost, G. J., et al. (1998), Photochemical ozone production in the rural southeastern United States during the 1990 Rural Oxidants in the Southern Environment (ROSE) program, *J. Geophys. Res.*, 103, 22,491-22,508.

Grell, G. A., et al. (2005), Fully coupled "online" chemistry within the WRF model, *Atmos. Environ.*, 39, 6957-6975.

Grell, G. A., et al. (2000), Application of a multiscale, coupled MM5/chemistry model to the complex terrain of the VOTALP valley campaign, *Atmos. Environ.*, 34, 1435-1453.

Hong, Y.-S., J. Y. Noh, and J. Dudhia (2006), A new vertical diffusion package with an explicit treatment of entrainment process, *Mon. Wea. Rev.*, *In Press*.

McKeen, S. A., et al. (2005), Assessment of an ensemble of seven real-time ozone forecasts over eastern North America during the summer of 2004, *J. Geophys. Res.*, 110(D21), 307, doi:10.1029/2005JD005858.

McKeen, S. A., et al. (2002), Ozone production from Canadian wild fires during June and July of 1995, *J. Geophys. Res.*, 107(D14), 4192, doi:10.1029/2001JD000697.

Mellor, G. L., and T. Yamada (1982), Development of a turbulent closure model for geophysical fluid problems. *Reviews of Geophysics and Spacephysics*, 20, 851-875.

Stockwell, W. R., P. Middleton, J. S. Change, and X. Tang (1990), The second generation regional acid deposition model chemical mechanisms for regional air quality modelling, *J. Geophys. Res.*, 95, 16343-16367.

Stockwell, W. R., F. Kirchner, M. Kuhn, and S. Seefeld (1997), A new mechanism for regional atmospheric chemistry modelling, *J. Geophys. Res.*, 102, 25847-25879.