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1. INTRODUCTION

The evolution and structure of the planetary boundary layer (PBL) are critical to understanding the formation, transport, and fates of ozone (O₃), particulate matter (PM), regional haze, and their respective precursors. To better characterize the processes that affect these air pollutants, intensive meteorological and chemical measurements were made in the Philadelphia, PA region by a consortium of investigators in the North American Research Strategy for Tropospheric Ozone - NorthEast Oxidant and Particle Study (NARSTO-NE-OPS; Philbrick 1998), during the summers of 1998, 1999, 2001, and 2002. As part of the 1999 field campaign, vertical profiles of temperature, humidity, and trace chemical species were made from an instrumented light aircraft at several locations in the US Mid-Atlantic region during July and August. Temperature and humidity profiles were also obtained from a tethered balloon and radiosondes launched at the core surface site, the Baxter Water Treatment Plant. The meteorological observations and PBL height estimates were then compared with the results from two model simulations using the Fifth-Generation Penn State University/NCAR Mesoscale Model (MM5 Version 3.3). We focus on comparing the PBL heights and vertical profiles of temperature and specific humidity, to investigate the differences in the PBL evolution between these two schemes.

2. MODELING SYSTEM

The nonhydrostatic, primitive equation MM5 (Dudhia 1993) was used to generate the three-dimensional meteorological fields over much of the eastern US from July 1 – August 3, 1999 (Zhang et al. 2001). The model was triply nested, with the innermost domain having 12 km horizontal grid dimensions (see Figure 1). The model used 25 vertical layers to about 16 km AGL, with the lowest layer 20 m thick. We generated two sets of model simulations, differing only in the PBL scheme: the Blackadar PBL (Zhang and Anthes 1982), a hybrid local and non-local mixing scheme; and the Gayno-Seaman PBL (Gayno et al. 1994), a local, 1.5-order closure mixing scheme. These two PBL schemes have been used with MM5 in previous air quality modeling applications (e.g. Seaman

et al. 1995; Shafran et al. 2000; Zhang et al. 2001; Chandrasekar et al. 2002).

The Gayno-Seaman (GS) scheme diagnoses the PBL height based upon the vertical turbulent kinetic energy (TKE) profile. During strong convection, the PBL height is set to the level where the maximum TKE falls below the critical value of 0.1 m²s⁻¹; during weak convection, the PBL height is set to the level where the TKE is 50% of the maximum value. During periods of very weak turbulence, the PBL is set to the lowest model layer.

The Blackadar (BL) scheme determines the PBL height based upon the surface Richardson number (Ri). During stable periods, the PBL height is set to the lowest model layer, while during convective periods the PBL heights is computed from the potential temperature profile. However, surface stability is not necessarily representative of the potential of the entire PBL to support convection, and sudden changes in surface Ri can lead to abrupt hour-to-hour changes in the estimated PBL height. Therefore, we estimated the PBL heights using the method of Holtslag et al. (1990), in which the PBL height is determined where the local Ri exceeds a critical value of 0.25.

3. OBSERVATIONAL DATABASE

Forty-seven aircraft spirals over various locations in the Mid-Atlantic region were obtained by the University of Maryland (UMD) on July 4-5, July 17-19, and July 30 - August 1, 1999. Millersville University (MU) obtained high-resolution profiles of meteorological variables to ~300 m during these days as well. Also during the July 30 - August 1 period, the Pacific Northwest National Laboratory (PNNL) launched 15 radiosondes from the NE-OPS surface site in Philadelphia. None of these observations were used for MM5 data assimilation, so they represent independent measurements of temperature and specific humidity for model assessment. For each spiral/sonde, the instantaneous data were assigned to the corresponding MM5 layer (below ~2.7 km AGL) and layer averages were computed so that the observations and model predictions could be compared directly. While the MM5 results are instantaneous, each aircraft profile covered a period of about 20-30 minutes; hence, the aircraft data were compared to the MM5 profile closest to the mid-point of the spiral. Also, the instantaneous aircraft height (in m AGL) was estimated by subtracting the height of the airport location (in m MSL) from the pressure altitude. The sonde data were assigned to the hour of launch. We used the "parcel" method

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(Holzworth 1964) to estimate the PBL heights from the observed potential temperature profiles.

We performed a statistical evaluation of the MM5 predictions of temperature and specific humidity using the combined spiral/radiosonde database within the lower troposphere. For each layer, we computed the mean and standard deviation of the difference between the observation and model predictions (defined as "observation – prediction"), as well as the normalized bias and root-mean-square (rms) error. These statistics were computed for different times of the day, nominally the morning hours (1200-1600 UTC), afternoon hours (1700-2300 UTC), and nighttime hours (0000-0400 UTC). These three periods were chosen to represent periods of PBL development, daytime mixing, and formation of the nocturnal PBL, respectively. In this analysis, we considered 25 combined morning profiles, 27 afternoon profiles, and 10 nighttime profiles. Since the tethered balloon data only covered the lowest 200-300 m of the PBL, they were not used in the statistical evaluation; rather, they were primarily used to estimate the height of the nocturnal inversion layer at the surface site. Finally, since there were so few sonde or spiral data within the lowest 20 m AGL, the statistical comparisons were only performed above the first model layer.

4. RESULTS

4.1 Temperature and specific humidity profiles

Figures 2-4 display the statistical comparison between the observed and MM5 predicted temperature and specific humidity profiles for the morning, afternoon, and nighttime periods, respectively. Note that in Figures 2a, 2d, 3a, 3d, 4a, and 4d, the BL and GS model levels are slightly offset from each other for clarity. During the morning hours (Figure 2), the BL scheme tended to overpredict temperatures below 300 m, the range where the GS scheme performed the best. At higher levels the rms error was about 1°C lower for the BL scheme than for the GS scheme. For specific humidity, the rms error was nearly identical for both PBL schemes throughout the lower troposphere. The largest differences occurred between about 700-1800 m, where the GS scheme underpredicted specific humidity and the BL scheme overpredicted specific humidity.

Figure 3 displays the statistical comparison during the afternoon hours. The GS scheme exhibited a much larger bias and rms error below about 1300 m, perhaps related to the local mixing in the GS scheme compared to the non-local mixing in the BL scheme during convective periods. For specific humidity the two PBL schemes exhibit a nearly opposite behavior from each other, alternating between underprediction and overprediction through the lower troposphere. However, the bias and rms error in the BL scheme tended to be more uniform up to about 2.7 km, suggesting that the vertical mixing of scalars such as humidity is better reproduced in the BL scheme during the afternoon hours.

Figure 4 shows the statistical comparison during the nighttime hours. Note that the behavior of each metric is very similar for the two PBL schemes. Between about 400-700 m, however, the model performance tended to be relatively weak in terms of bias, rms error, and the standard deviation of the differences between the humidity observations and model predictions. Zhang et al. (2001) suggested that MM5 may not properly simulate the structure within the lower PBL at night due to coarse vertical resolution and underprediction of nocturnal turbulence near the surface. Improvements in the model dynamics are needed if such a model is to be used to simulate nocturnal transport of O₃, PM, and their precursors and co-pollutants via low-level jets.

4.2 PBL time series

Figure 5 displays the estimated PBL time series at the NE-OPS surface site. The sonde and tethered balloon data from July 30 to August 1 were used at the surface site. Note in Figure 5 that the BL scheme appears to predict maximum afternoon PBL heights in good agreement with the observations, although the data available during this period are limited. The maximum afternoon GS-predicted PBL heights were several hundred meters lower than those predicted by the BL scheme. Also, the PBL growth and decay in the BL scheme tend to be more abrupt than in the GS scheme. Additional observational data in the late afternoon would be needed to determine which scheme better simulated the PBL decay and onset of the nocturnal PBL.

The tethered balloon system provides high-resolution meteorological data near the surface. The data from this period, as well as the data from July 17-19 (not shown here), suggest that the nocturnal PBL heights are generally in the 150-250 m range, although the inversion height could be <50 m AGL. This is in contrast with MM5, which usually diagnoses the nighttime PBL height to be within the first two model layers (<75 m).

Figure 6 displays the PBL heights estimated from MM5 and the aircraft data at PNE, about 6 km northwest of the NE-OPS surface site, from July 17-19 and July 30 to August 1. Again, it appears that the BL scheme more realistically predicts maximum afternoon PBL heights. In terms of PBL growth during the morning hours, the GS scheme predicts a slower growth rate than does the BL scheme, while the observed growth rate appears to be intermediate between the two model predictions. While the GS scheme tends to delay the onset of the nocturnal PBL compared to the BL scheme, there is evidence from Figures 5 and 6 that both schemes in MM5 overpredict the rate of PBL collapse into the evening hours. Hence, additional work is needed to optimize the model performance during the critical nighttime hours, when transport of pollutants and precursors is occurring above the surface layer, and the morning hours, when these pollutants are mixed into the surface layer.

5. DISCUSSION

Vertical profiles of temperature and specific humidity from the Philadelphia, PA area were used to evaluate the performance of two MM5 simulations using different PBL schemes. The BL and GS PBL schemes differ in how they simulate the vertical profiles of temperature and specific humidity. Overall, the model predictions of temperature were better than those for humidity. In terms of the PBL development, the BL scheme tends to better reproduce maximum PBL heights, but both schemes require further evaluation during the morning growth and evening decay regimes. Also, nighttime tethered balloon data suggest that these two PBL schemes may underestimate the nocturnal inversion height by as much as 100-200 m. While these two schemes have often been applied in the past for air quality applications, there are five additional PBL modules available in MM5 that were not examined in this analysis.

We did not assess the model predictions of vertical wind profiles, since earlier work (Zhang et al. 2001; Chandrasekar et al. 2002) suggested that MM5 tends to underpredict wind speeds below ~1 km, especially at nighttime in the vicinity of the low-level jet. Also, this preliminary analysis highlights the need for additional upper-air monitoring, since it is difficult to extend the model performance from a few locations to the entire domain. Also, while individual profiles are illustrative of the model performance over selected hours throughout the day, a more complete analysis would require continuous observations. Future work will include comparisons with hourly lidar and temperature and wind profiler data from the NE-OPS surface site and other sites in the eastern US.

6. ACKNOWLEDGMENTS

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Figure 1. The MM5 108/36/12 km domain.

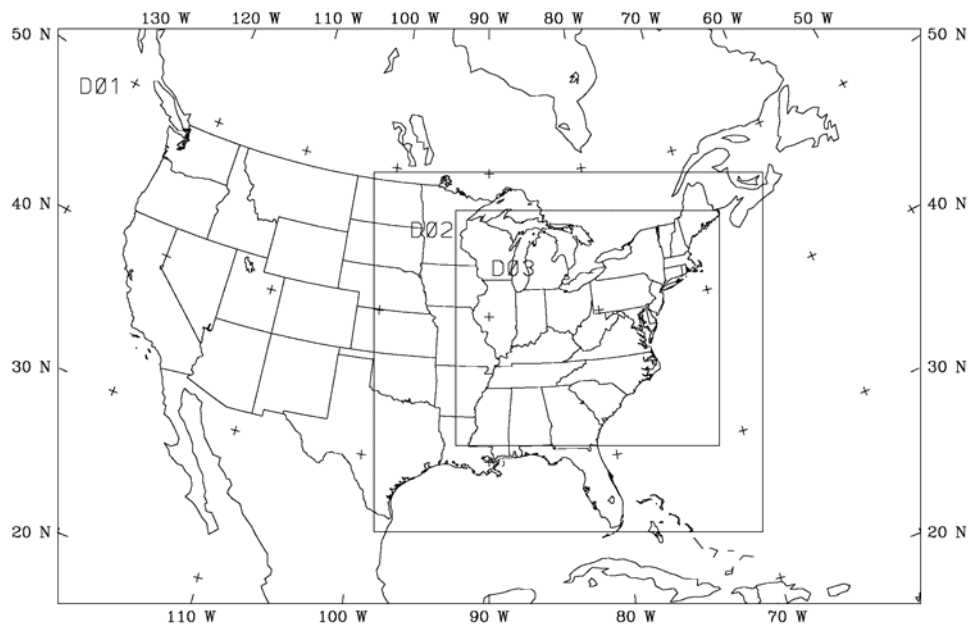


Figure 2. Basic model evaluation statistics for the Blackadar (BL; closed circles) and Gayno-Seaman (GS; \times) PBL simulations for the morning hours (1200-1600 UTC). All metrics are defined as "observation – prediction": (a) mean and standard deviation of the differences, temperature; (b) normalized bias, temperature; (c) rms error, temperature; (d) mean and standard deviation of the differences, specific humidity; (e) normalized bias, specific humidity; and (f) rms error, specific humidity.

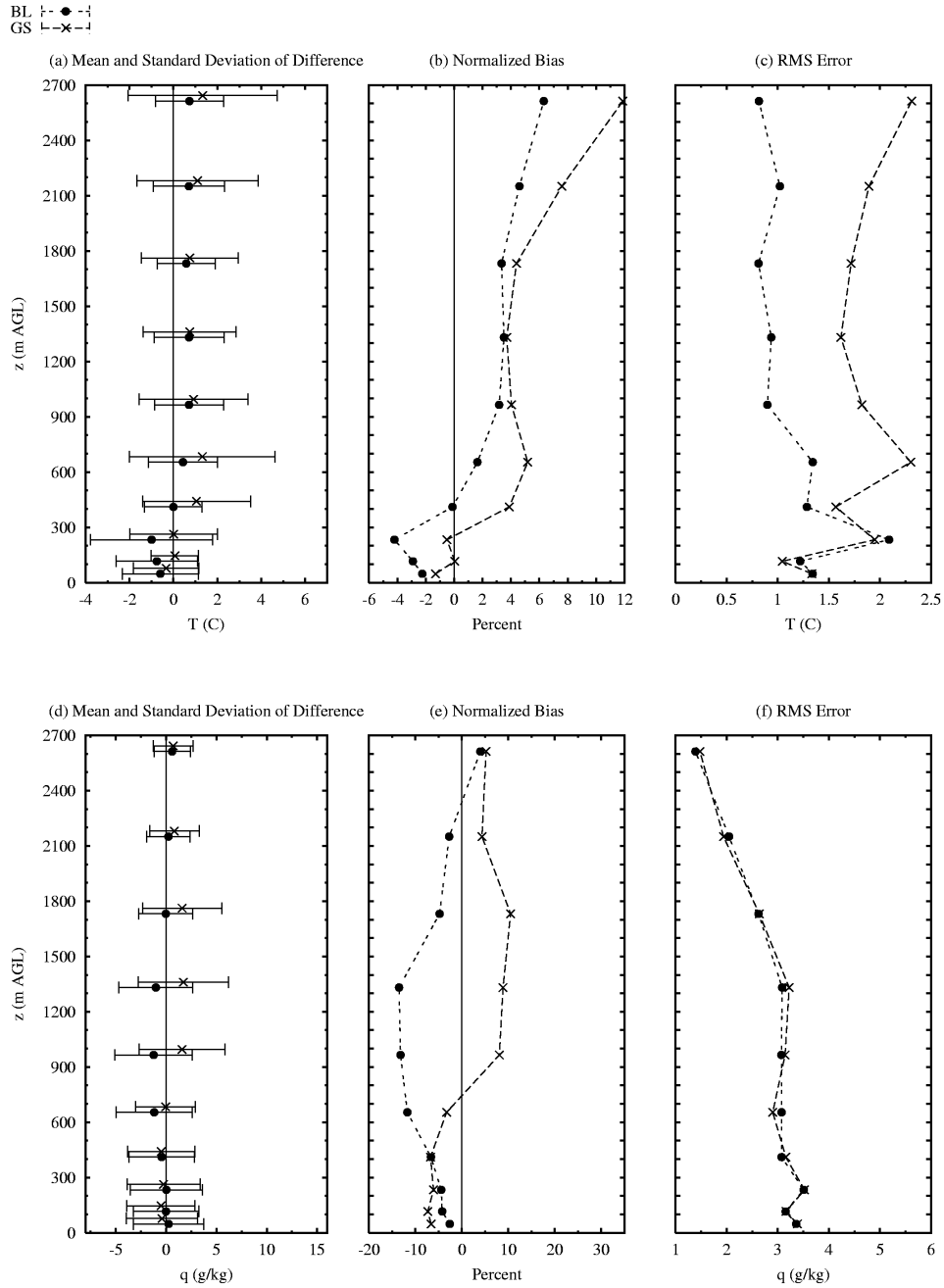


Figure 3. Same as Figure 2, except for the afternoon hours (1700-2300 UTC).

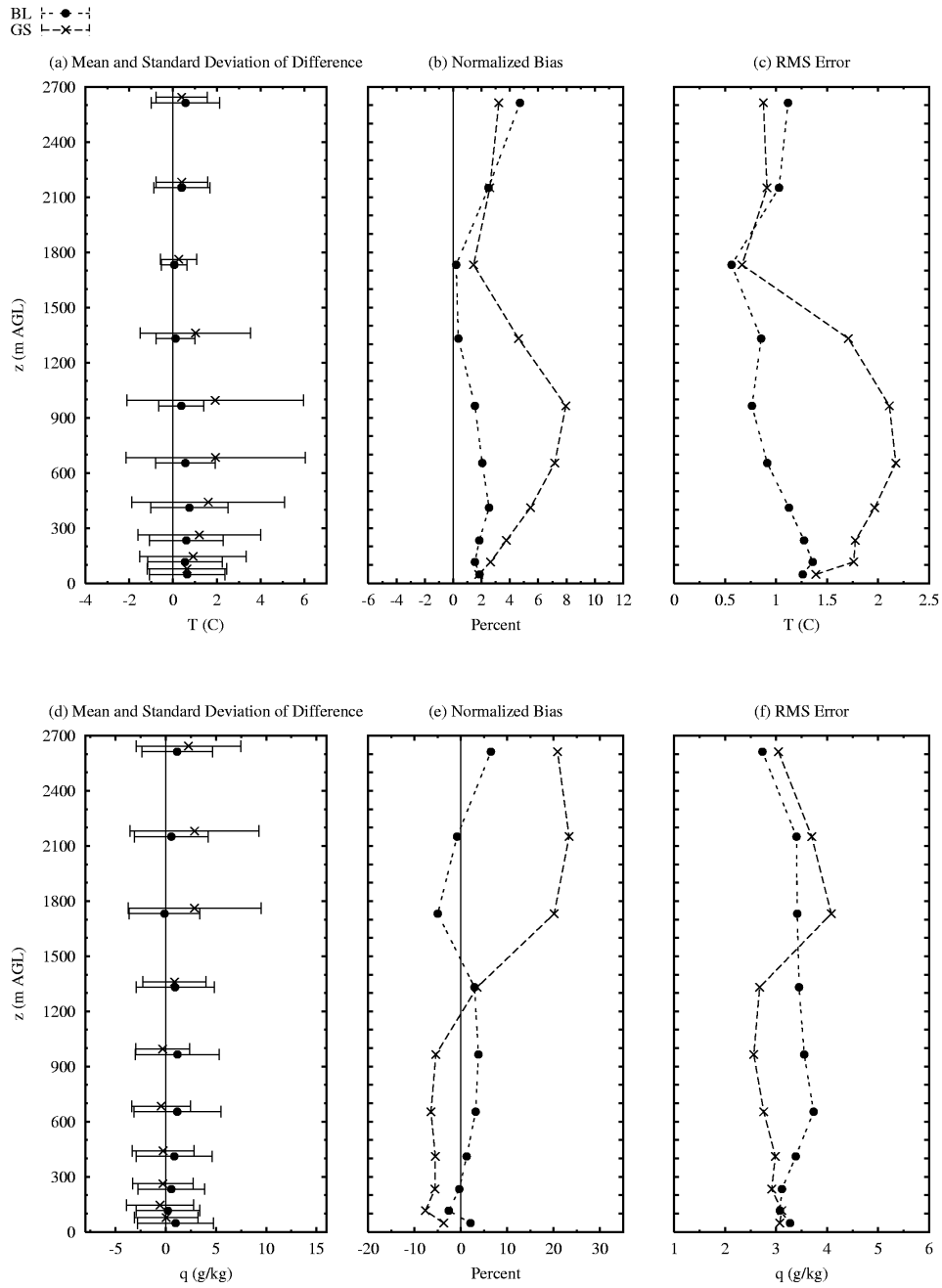


Figure 4. Same as Figure 2, except for the nighttime hours (0000-0400 UTC).

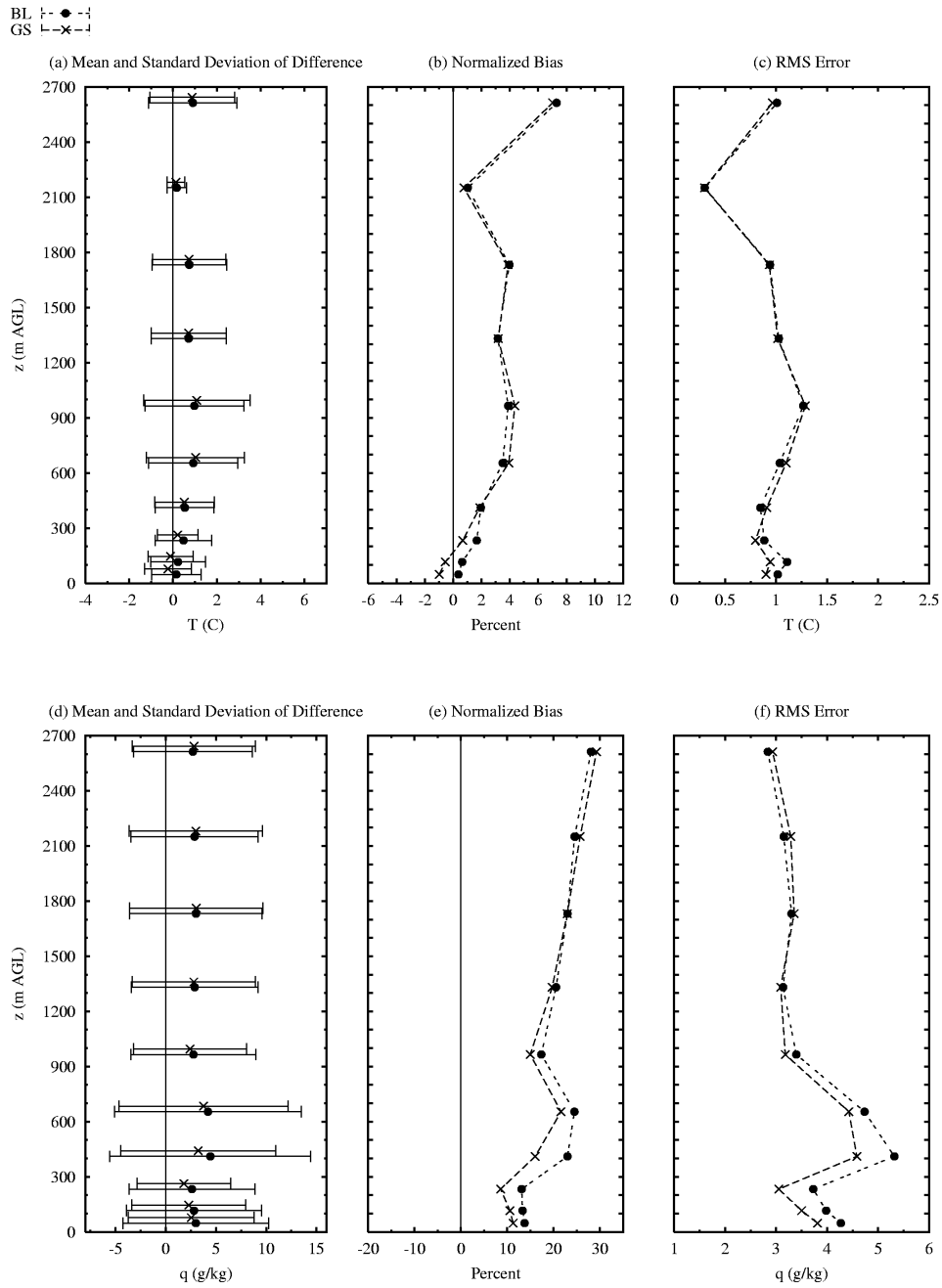


Figure 5. PBL heights at the core NE-OPS surface site, July 30 – August 1. Observed PBL heights were estimated from the PNNL radiosonde (filled squares) and MU tethered balloon data (×), and the MM5 predictions correspond to the BL (solid line) and GS (broken line) simulations.

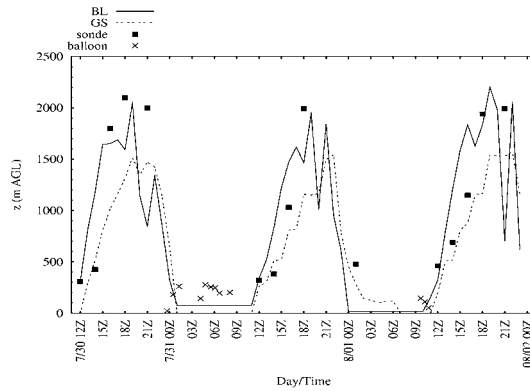


Figure 6. PBL heights at Northeast Philadelphia Airport (PNE): (a) July 17 – 19, and (b) July 30 – August 1. Observed PBL heights were estimated from the UMD aircraft spirals (open circles), and the MM5 predictions correspond to the BL (solid line) and GS (broken line) simulations.

