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Final Technical Report

Understanding Processes Controlling the Temporal and Spatial Variations of PBL Structures Over the ARM SGP Site

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Executive summary

The surface heat, moisture, and momentum fluxes are transferred to the atmosphere above through the planetary boundary layer (PBL), where vertical mixing due to turbulent eddies of different sizes plays critical roles. Therefore, reliably representing PBL processes in numerical models is critical for weather, climate, and air quality prediction. Currently, there are over ten PBL schemes that are selectable within the advanced research version of the Weather Research and Forecasting (WRF) model, indicative of the challenges in capturing the impacts of turbulence within the PBL in models. Further improvements in PBL parameterizations are needed for both weather and climate models, as emphasized in many recent national reports, but require an advanced understanding of the underlying boundary layer processes from observations. This project takes advantage of Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) investments in the atmospheric boundary layer observations and Large-Eddy Simulation (LES) ARM Symbiotic Simulation and Observation (LASSO) simulations to characterize PBL structures, understand key physical processes controlling the mixed layer development, and to evaluate PBL parameterization. Our key accomplishments are:

1. **Improved PBL Characterizations**: PBL has a strong diurnal cycle, including daytime convective mixing layer (ML) and nighttime residual layer. Therefore, for PBL characterization, a PBL height (PBLH) is not enough. We developed improved algorithms to combine ARM Raman lidar (RL) and Doppler lidar (DL) measurements to determine temporal variations of PBLH and ML height (MLH) at the ARM SGP central site. RL water vapor structures provide consistent day and night signatures for PBL height characterizations. DL vertical velocity measurements offer direct information for vertical mixing associated with daytime convective ML or nighttime wind shear. The algorithms were applied to multi-year ARM observations at the SGP site to support PBL processes study and PBL parameterization evaluations.

2. ***Understand processes controlling PBL variations:*** Multi-year observation results showed significant spatial ML heterogeneities among the five SGP sites. Although the differences are smaller before ML reaches the PBL top, the observed local lower tropospheric stability (LTS) and sensible and latent heat fluxes can only explain less than 60% of observed ML variabilities, highlighting a significant role of advection. When ML deepens near the PBL top, there are over 500 m peak height differences and reaching different times amount the sites, indicating an essential role of PBL top entrainment and different entrainment strengths at these sites. The multi-scale LASSO analysis focused on identifying key meteorological conditions that control the development of shallow cumulus (ShCu), therefore are critical to skillful predictions of ShCu. The case composite of multi-scale LES revealed that the development of ShCu, under the same surface forcing constraints, is highly correlated with large-scale conditions near or right above the PBL top, such as the strength of the capping inversion and relative humidity right above the PBL.

3. **Evaluation and comparison of various PBL parameterization schemes used in different modeling systems in a single column model (SCM) framework**: The Common Community Physics Package (CCPP) SCM was used, and both case study and case composite analysis were performed for well-developed ShCu over the SGP site driving by LASSO input and forcing datasets and evaluated with observations. The PBL schemes include the scale-aware turbulence kinetic energy (TKE)-based moist eddy-diffusion mass-

flux (EDMF) (SATMEDMF) PBL in the operational NCEP Global Forecast System (GFS); the Mellor-Yamada-Nakanishi-Niino (MYNN)-EDMF (MYNN EDMF) PBL in the NOAA Rapid Refresh (RAP) and High-Resolution Rapid Refresh (HRRR) models; the Yonsei University (YSU) PBL and the Asymmetric Convective Model version 2 (ACM2) PBL in the Weather Research and Forecasting (WRF) model. The two WRF PBL schemes — YSU and ACM2 — were implemented into the CCPP-SCM by the NSF NCAR team during this project. The CCPP-SCM with these PBL parameterizations was archived and available for others. The case composite of CCPP-SCM simulations showed that the four PBL schemes produce similar multi-year mean PBL height (PBLH) evolutions but different ShCu, and the differences in simulated clouds are mainly associated with vertical flux distributions and PBL top entrainment. The LES results indicated the critical role played by the PBL top processes, which was consistent with observations. The SCM results showed considerable uncertainty in modeling these processes in existing PBL schemes, stressing the need to improve model representations of the PBL top processes.

4. The project provided a great training opportunity for graduate students and young scientists and promoted close interactions between observation and modeling teams.

1. **Project Objectives:**

The study has three primary goals:

1) **Characterize PBL structure and variations**: Long-term ARM observations of fine-scale temperature, water vapor, and wind profiles from Raman lidar and Doppler lidar, together with other measurements used to characterize planetary boundary layer (PBL) structure, including PBL height (PBLH), mixed layer (ML) height (MLH), vertical turbulent mixing and water vapor flux profile at the SGP site. The spatial and temporal variations of the PBL structure are documented under different meteorological and thermodynamic conditions.

2) **Understand processes controlling PBL variations**: PBL evolutions are controlled by multi-scale processes, including surface fluxes, radiation, dynamics, and turbulence, as well as cloud and precipitation systems. ARM offers the necessary complement of measurements at the SGP site for process-oriented study together with the DOE ARM's LES ARM Symbiotic Simulation and Observation (LASSO) LES simulations. We focus on processes important for mixed layer development and vertical water vapor transport because of their importance for cloud/precipitation development. The impact of land-atmosphere interactions on PBL developments is constrained by observed surface latent and sensible heat fluxes. Analyses are performed to understand the roles of multi-scale dynamics interactions in controlling the mixed layer development and PBL spatial heterogeneity at the SGP site.

3) **Improve PBL modeling in WRF**: We combine the validated the LASSO simulations and observational results to explore ways to improve the PBL parameterizations. The SCM framework provides an observation-constrained setup to better isolate the PBL parameterized physics from a dynamics-physics coupled system. Large-scale forcings from validated LASSO simulations are used to drive SCM simulations under observational constraints to discover the consistent deficiencies of selected WRF PBL schemes using observations and test potential improvements for the selected schemes.

2. **Key Accomplishments**

1) Characterize PBL structure and variations:

PBL has a strong diurnal cycle, including a daytime convective mixing layer and a nighttime residual layer. Therefore, for PBL characterization, a PBL height (PBLH) is not enough. We developed improved algorithms to combine ARM Raman lidar (RL) and Doppler lidar measurements to determine temporal variations of PBLH and ML height (MLH) at the ARM SGP central site (Chu et al., 2022). RL water vapor structures provide consistent day and night signatures for PBL height characterizations. DL vertical velocity measurements offer direct information for vertical mixing associated with daytime convective ML or nighttime wind shear. For ML height determinations, we focused on challenges related to different size eddies, gravity wave interference, and different data quality data from five Doppler lidars at the SGP supersite.

An example of PBL and ML height determination results is presented in Fig. 1. The algorithms are applied to multi-year ARM observations at the SGP site to support PBL processes study and PBL parameterization evaluations. Figure 2 shows the warm season PBLH and MLH diurnal evolution.

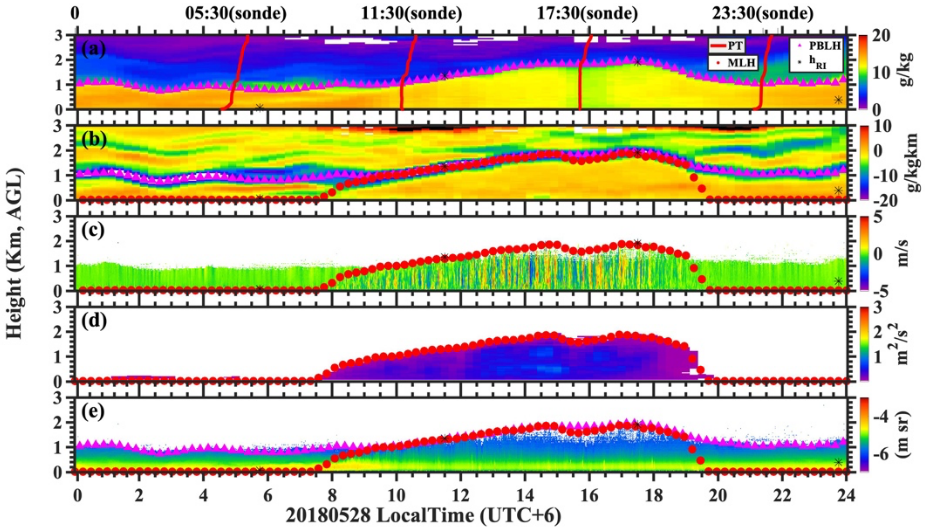

Figure 1. PBLH and MLH on May 28, 2018 derived from the developed new approaches. (a) RL water vapor mixing ratio (WVMR) with determined PBLHs (purple triangles) with radiosonde potential temperature profiles; (b) WVMR vertical gradients; (c) wavelet derived high-frequency wave energy from vertical velocity measurements given in (d); DL aerosol profiles over-plotted with PBLHs and MLHs (red dots).

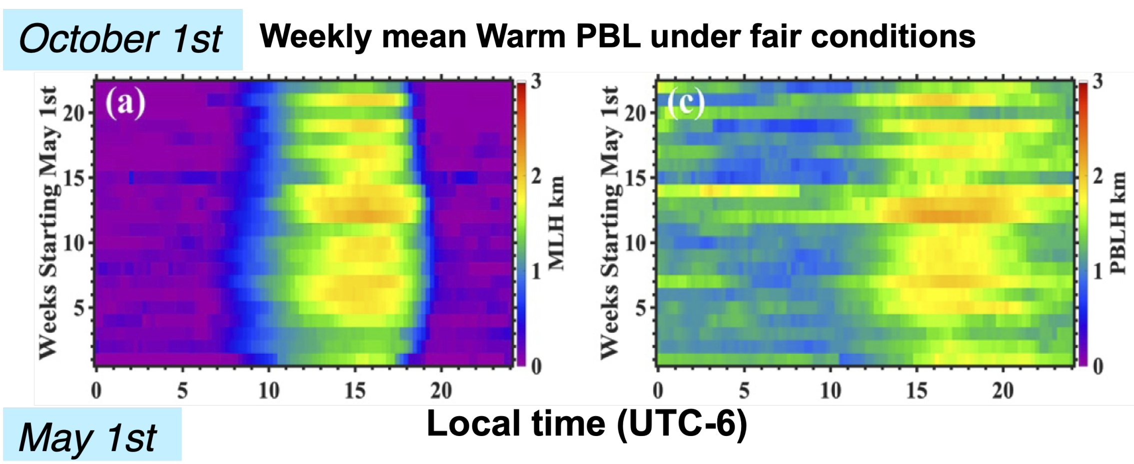

Figure 2. The diurnal cycle of MLHs (left) and PBLHs (right) at the SGP C1 site during the warm season.

2) Understand processes controlling PBL variations:

a) Seasonal-diurnal variations of warm PBL structures

The first-order PBL variations are the diurnal cycle of convective ML and seasonal variations of PBL height, as presented in Fig. 2. Driving by solar radiation, the diurnal cycle of mixing layer development is clear. With solar radiation increasing from May to July, daily maximum MLH increases, which drives PBL seasonal variations. As the daytime convective ML weakens, the nighttime residual layer develops, which leads to a slightly shallow PBLH during the night. While nighttime MLH is normally close to zero, low-level jets (LLJ) often occur at the SGP site and can maintain mechanically forced shallow ML (Chu and Wang, 2024). The significant intraday variations are driven by synoptic meteorology.

b) Mixing layer spatial variabilities at the SGP supersite

We took advantage of five Doppler lidar measurements at C1, E32, E37, E39, and E41 (see Fig. 3c) to explore the spatial variability of ML development. For a given clear day, there are noticeable differences in ML evolutions (Fig. 3c) at the five sites with distances less than 100 km from the C1 site. The mean annual-diurnal evolutions of ML at the five sites (Fig. 3a) further confirm the spatial heterogeneity of PBL development in the region.

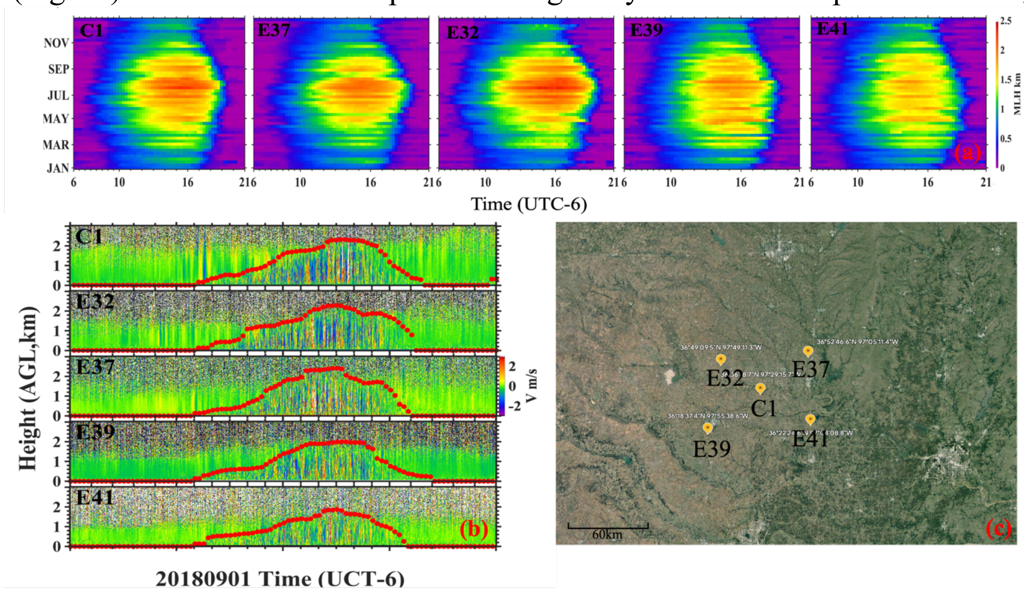

Figure 3. (a) seasonal-diurnal cycles of MLHs at the five sites based on weekly means from the four-year data, (b) MLH variations on September 1, 2018, at the five sites, and (c)

To show the site differences more clearly, warm season means are presented in Fig. 4. The maximum and minimum peak ML heights differ by more than 500 m. After using our mobile Doppler lidar to collect collocated data at multiple sites briefly, we concluded that the observed significant difference was not caused by the different data quality. The ML morning development (before noon local time) is clearly separated into two groups, with the two eastern sites (E39 and E41) developing more slowly than the other three sites.

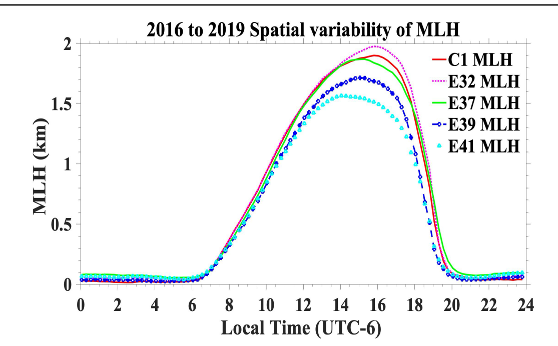

Figure 4. The mean diurnal cycles of MLHs during the warm season at the five sites from four-years measurements.

We explore the impacts of major factors on observed ML heterogeneities with additional ARM observations. Before ML reaches the top PBL, ML developments are mainly controlled by surface sensible heat fluxes, turbulence intensity, and stability and residual layer properties. With AERI retrieved temperature profiles, we estimated lower tropospheric stability (LTS) at each site, consistent with radiosonde-based estimations. Sensible and latent heat fluxes are provided by the eddy correlation flux measurement systems. As illustrated in Fig.5, MLH dependencies on LTS and fluxes vary strongly among the sites. These local properties can only explain less than 60% of observed ML variabilities. It means that local energy supplies are not enough to constrain energy supply for ML observed at a fixed site as the airmass advected through. Due to the surface heterogeneity, it is problematic to assume that local measured fluxes represent the upper wind conditions. We showed significant spatial latent heat flux variations with airborne near-surface measurements and a wavelet-based flux estimation technique (Lin et al. 2024). When ML deepens near the PBL top, PBL top entrainment could become an essential factor in determining ML developments. Reaching peak heights at different times indicates different PBL top entrainment strengths at these sites.

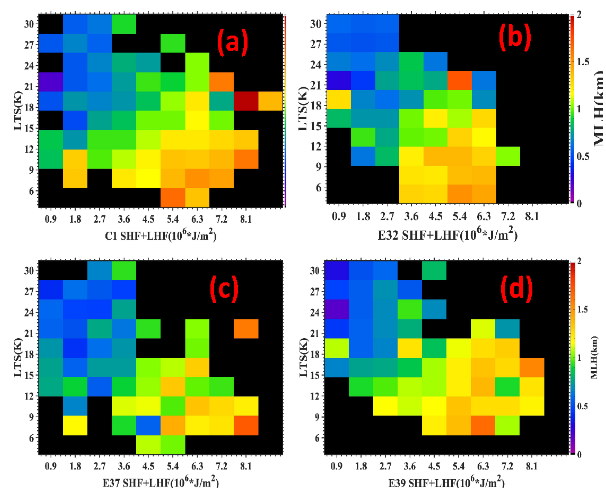

Figure 5: MLH at 11:00 (local time) as a function of integrated total heat flux (SHF+LHF) and LTS for sites C1, E32, E37, and E39 are shown in panels (a-d), respectively based on data from 2016–2019. (Site E41 does not have LTS data.)

Furthermore, terrain-locked boundary layer circulations could also impact local ML developments. However, new observations are needed to quantify entrainment and circulation impacts. A journal paper on this part of the study is close to submission.

3) Improve PBL modeling in WRF:

a) Multi-scale LES analysis

We developed a streamline for the process-level analysis of LASSO LES outputs, linking LSF, meteorological mean profiles, high-order turbulence statistics, and ShCu development (Shin et al. 2021). An example of the analysis is summarized in Figure 6. Figure 6 shows that the selected ShCu case is affected by large-scale warm and dry advection in the free troposphere (Figure 5a), which leads to a strong capping inversion indicated by the shallow layer of convective inhibition (blue shaded in Figure 6b) above LCL. Figure 6c shows that the strong capping inversion suppresses the penetration of surface-driven thermals, therefore vertical moisture transport by the thermals (Figure 6c), hindering the growth of clouds (Figure 6d). The time-height cross-section of the length scales that dominate horizontal variability of moisture fields supports the impact of larger-scale motions (e.g., horizontal advection) above the cloud top (Figure 6e).

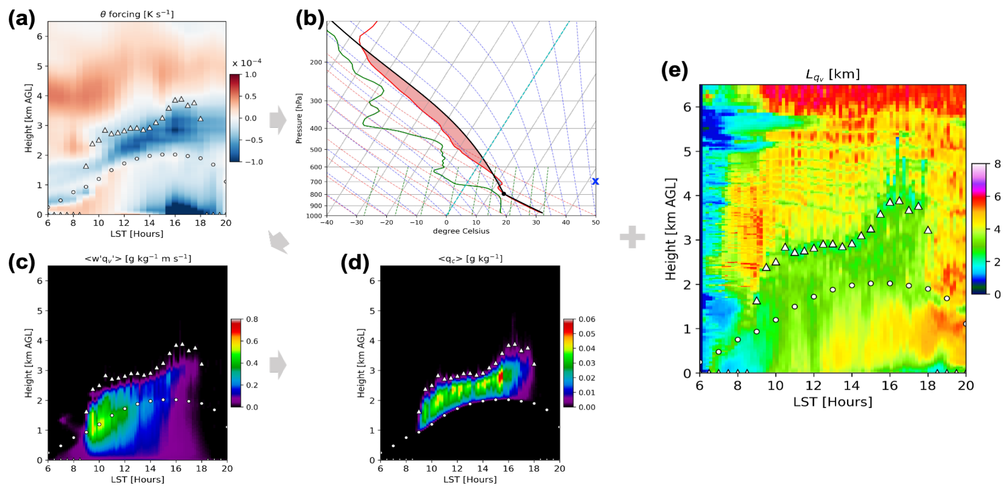

Figure 6. The time-height cross-section of horizontal temperature advection (a), skew-T log-p sounding plot at 12 LST (b), and the time-height cross-sections of vertical moisture transport (c), cloud water mixing ratio (d), and dominant length scale of moisture (e). In a and c–e, the time series of lifting condensation level and cloud-top height are shown with white dots and white triangles, respectively. The figure is adapted from Shin et al. (2021).

The multi-scale LES analysis was applied to a library of LASSO cases that consists of 82 warm-season ShCu days observed over the ARM SGP observatory for 2016–2019. Each case consists of eight LES runs driven by different LSF conditions. For each case, we selected a high (HI) skill simulation and a low (LO) skill simulation based on cloud prediction skill scores. To identify key meteorological parameters for accurate prediction of ShCu, we compared bulk cloud parameters and large-scale (LS) environmental conditions between the HI and LO groups. The LO group showed a more frequent occurrence of the transition from ShCu to deep cumulus (Deep Cu) on the days when ShCu was observed, and these “false” Deep Cu days were characterized by deeper cloud depth in the afternoon and evening hours. The analysis of relationships between the cloud depth and LS parameters showed that the cloud depth is highly correlated with LS parameters near or right above the top, i.e., positively correlated with RH right above the PBL (Fig. 7a) and negatively correlated with the strength of the capping inversion (Fig. 7b). The LO group simulations tended to have higher RH and weaker inversion (Fig. 8), leading to more frequent ShCu-to-Deep Cu transition. Therefore. PBL simulations are an integral part of cloud modeling (Morrison et al., 2020).

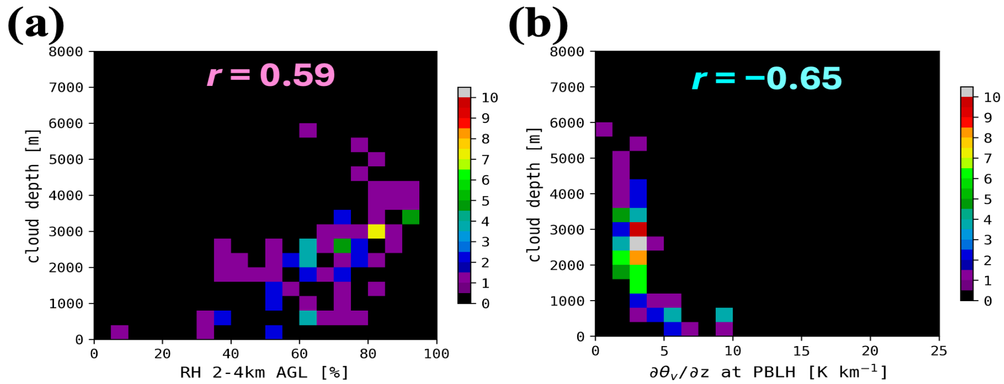

Figure 7. Correlations between simulated cloud depth and LS environmental conditions in the afternoon hours (13–14 LT): (a) RH in 2–4 km AGL and (b) strength of the capping inversion (virtual potential temperature gradient at PBLH).

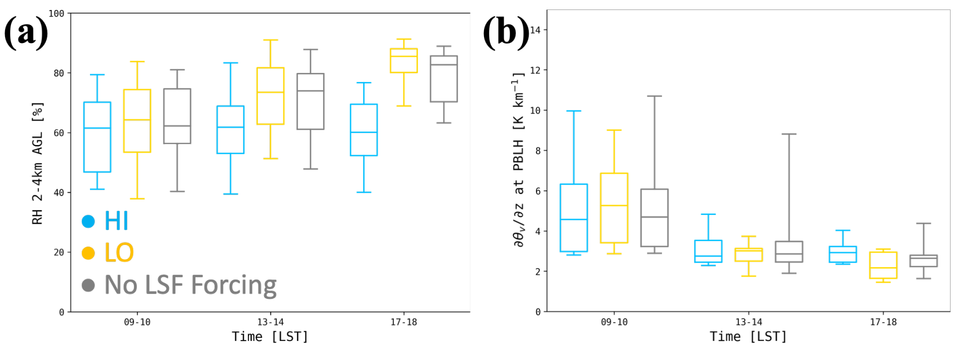

Figure 8. Box plots of (a) RH in 2–4 km AGL and (b) strength of the capping inversion (virtual potential temperature gradient at PBLH) for the HI (blue), LO (yellow), and No LSF Forcing (gray) simulations.

b) CCPP SCM modeling

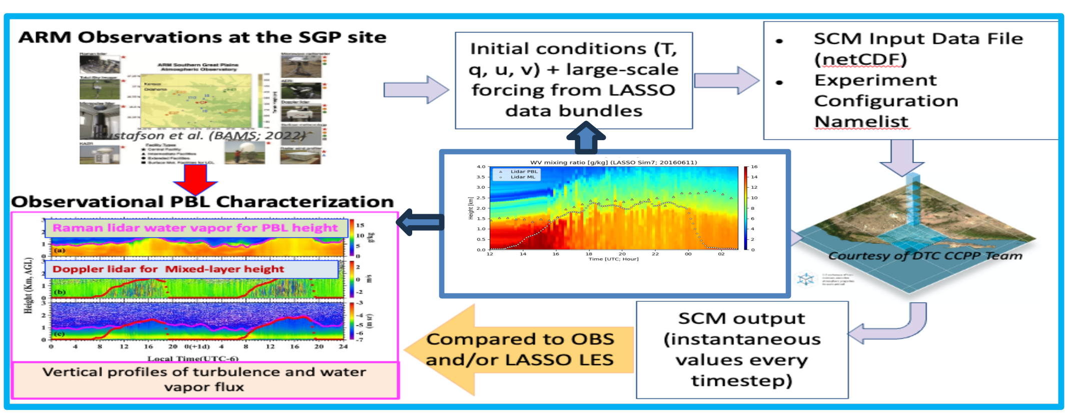

Figure 9: A schematic view of using ARM observations and LASSO analyses to drive CCPP-SCM simulation and PBL parameterization evaluations.

We developed a framework to use Common Community Physics Package (CCPP)-Single Column Model (SCM) to evaluate different PBL parameterizations with observation and LASSO results as illustrated in Fig. 9. To drive Common Community Physics Package (CCPP)-Single Column Model (SCM) using the LASSO LSF, the LASSO LSF data were converted into the CCPP-SCM LSF format (Li et al. 2024). We implemented the YSU PBL and the ACM2 PBL parameterization schemes into the CCPP SCM model to evaluate the PBL parameterization schemes in the multiple modeling systems (i.e., SATMEDMF in the GFS, MYNN EDMF in the RAP and HRRR, and YSU and ACM2 in the WRF) in the same CCPP-SCM framework using the same LASSO LSF and surface forcings.

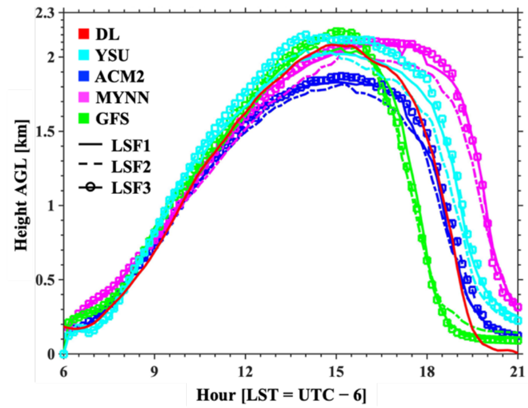

Figure 10. Comparison of CCPP-SCM simulations of MLH [km] averaged over 82 LASSO ARM SGP cases during the 2016–2019 warm seasons: YSU (cyan), ACM2 (blue), MYNN (magenta), and SATMEDNF (yellow green) PBL schemes. Mixed-layer height retrieved from Doppler lidar measurements (Chu et al. 2022) is presented in red solid line. Simulated MLH was diagnosed by searching for the lowest height where virtual potential temperature (θ_v) exceeding θ_v at the lowest model level height (LMH) by 1.5 K: i.e., $\theta_{v,PBL} = \theta_{v,LMH} + 1.5$ K. SCM simulations were performed using three different LASSO large-scale forcing (LSF) sources driven by different NWP systems: LSF1 (solid), LSF2 (dashed), and LSF3 (solid with open circle marks).

The CCPP SCM simulations were conducted for the same library of LASSO ShCu cases. Comparison of the four PBL parameterization schemes in terms of the diurnal cycles of MLH averaged over the multi-year LASSO SGP cases show relatively good agreements in the morning but significant differences in the afternoon and during the evening transition (Figure 10). For a given day, the ML differences in the morning could be substantial. As expected, these afternoon differences lead to the differences in simulated clouds. Although different LSFs have noticeable impacts on daytime convective ML developments, the differences are relatively small compared to the differences among different PBL parameterizations.

The framework allows easy testing and evaluating of the formulation details of PBL parameterizations. Sensitivity simulations of the YSU PBL scheme to the explicit parameterization of the entrainment at the PBL top confirmed that the entrainment process has a significant influence on the vertical distribution of the turbulent moisture flux (Fig. 11f), modulating RH in and above the PBL (Fig. 11g), therefore changing the simulated cloud (Fig. 11h). Our testing also led to a bug fixing in the YSU scheme to handle the calm condition. However, fully exploring the formulations of the four tested PBL parameterizations, which have significant differences, as shown in Fig. 10, requires more resources than this project has. However, we demonstrated using the CCPP-SCM framework to test and evaluate PBL parameterizations. The PBL parameterizations we added to the CCPP-SCM were based on the CCPP SCM public release Version 4 (https://github.com/NCAR/ccpp-scm/tree/release/public-v4). Thus, it could be easily accessible to others.

3. **Opportunities for training and professional development and other board impacts**

The project provided a great opportunity for graduate students and young scientist training. Yunfei Chu, who participated in the project as a visiting Ph.D. student at the CU, stayed with the project as a CU postdoc in Y2 to support observational data analysis. Through the research development, Yunfei Chu has learned to use a variety of ARM observations to characterize PBL properties and processes. CU graduate students Kang Yang, Guo Lin, and Ethan Murray supported the data analyses and trained using ARM data. An NCAR postdoc, Dan D'Amico, joined the project in Y2 to support the CCPP-SCM simulations and model-observation comparison. Dan became very familiar with the LASSO data portal, products, and data processing. NCAR young scientists Hyeyum (Hailey) Shin, Weiwei Li, and Dan D'Amico also set up accounts on the ARM cumulus cluster to further facilitate the analysis of large volumes of data.

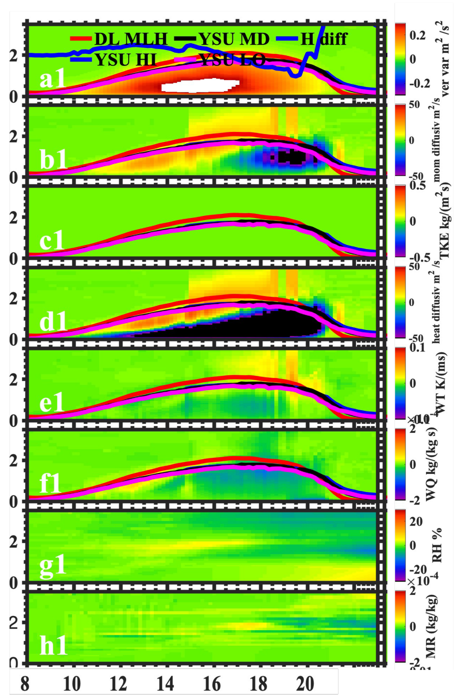

Figure 11. Differences between the YSU PBL simulations with and without the explicit entrainment parameterization.

The Xue and Wang groups have regular meetings to foster the collaborations between modeling and observation expertise in the two groups, which is critical for the success of this project and using DOE/ARM measurements to improve model simulations. This kind of activity greatly benefits young scientists and students on both the modeling and measurement sides.

The ARM instrumentation and observation data have been used in the course materials in the courses Wang was teaching. Wang is teaching "Atmospheric Remote Sensing" and "Instrumentation Lab" courses.

4. **Products**

Journal Publications:

1. Morrison, H., van Lier-Walqui, M., Fridlind, A. M., Grabowski, W. W. Harrington, J. Y., Hoose, C., et al. (2020). Confronting the challenge of modeling cloud and precipitation microphysics. Journal of Advances in Modeling Earth Systems, 12,

e2019MS001689. https://doi.org/ 10.1029/2019MS001689.

2. Shin, H. H., L. Xue, W. Li, G. Firl, D. F. D'Amico, D. Muñoz-Esparza, M. B. Ek, Y. Chu, Z. Wang, W. I. Gustafson Jr., and A. M. Vogelmann, 2021: Large-scale forcing impacts on the development of shallow convective clouds revealed from LASSO large-eddy simulations. Journal of Geophysical Research: Atmospheres, 126(20), e2021JD035208. https://doi.org/10.1029/2021JD035208.
3. Muñoz-Esparza, D., Sauer, J. A., Jensen, A. A., Xue, L., & Grabowski, W. W. (2022). The FastEddy® resident-GPU accelerated large-eddy simulation framework: Moist dynamics extension, validation and sensitivities of modeling non-precipitating shallow cumulus clouds. Journal of Advances in Modeling Earth Systems, 14, e2021MS002904. https://doi.org/10.1029/2021MS002904
4. Chu, Y., Z. Wang, L. Xue, M. Deng, G. Lin, H. Xie, H. H. Shin, W. Li, G. Firl, D. F. D'Amico, D. Liu, and Y. Wang, 2022: Characterizing Warm Atmospheric Boundary Layer Over Land by Combining Raman and Doppler Lidar Measurements, Opt. Express 30, 11892-11911, 2022. https://doi.org/10.1364/OE.451728
5. Lin, G., Wang, Z., Chu, Y., Ziegler, C. L., Hu, X.-M., Xue, M., et al. (2024). Airborne measurements of scale-dependent latent heat Flux impacted by water vapor and vertical velocity over heterogeneous land surfaces during the CHEESEHEAD19 campaign. Journal of Geophysical Research: Atmospheres, 129, e2023JD039586. https://doi.org/10.1029/2023JD039586.
6. Li, W., D. F. D'Amico, L. Bernardet, L. Xue, J. Dudhia, H. H., Shin, G. Firl, M. Harrold, L. B. Nance, M. B. Ek, and Y. Chu, 2024: Demonstration of Hierarchical System Development Using the Common Community Physics Package and Its Single-Column Model to Inform Physics Development: An Example from An ARM SGP Case on June 11, 2016. Submitted to Meteorological Applications.

Presentations:

1. Chu, Y., Z. Wang, H. Shin, L. Xue, W. Li, G. Firl, 2020: The Seasonal and Diurnal Variations of Planetary Boundary Layer and Convective Mixing Layer at the ARM/SGP sight Based on Raman and Doppler Lidar Measurements. *2020 AGU Fall Meeting*, Virtual, American Geophysical Union, A065-0014, https://agu.confex.com/agu/fm20/meetingapp.cgi/Paper/742552
2. Shin, H. H., L. Xue, W. Li, G. Firl, Y. Chu, and Z. Wang, 2020: Role of large-scale forcing in the development of continental shallow convection revealed from LASSO large-eddy simulations. *2020 AGU Fall Meeting*, Virtual, American Geophysical Union, A137-08, https://agu.confex.com/agu/fm20/meetingapp.cgi/Paper/718060.
3. Wang, Z., L. Xue, D. D'Amico, Y. Chu, W. Li, G. Firl, and H. H. Shin, 2021: Warm season PBL evolutions from lidar observations, LASSO and single column model simulations at the SGP site, 2021 ARM/ASR Joint User Facility and Principal Investigator Meeting, June 21 – June 24, 2021.
4. Chu, Y., Zhien Wang, Min Deng, Guo Lin, Lulin Xue, Weiwei Li and Hyeyum Hailey Shin, 2022: The Spatial and Temporal Variability of the Planetary Boundary Layer at the ARM SGP Supersite, AGU Fall Meeting, Chicago, IL, 12-16 December 2022.
5. Chu, Y., Zhien Wang, Min Ding, Guo Lin, Lulin Xue, Weiwei Li, Hyeyum Hailey

Shin, 2022: The spatial variability of the planetary boundary layer at SGP site, the 30th International Laser Radar Conference (ILRC 30), Montana, USA on June 26 – July 1, 2022.

6. Wang, Z., L. Xue, Y. Chu, H. H. Shin, and W. Li, 2022: Spatial Variability of Convective Mixing Layer at the SGP Supersite, 2022 ARM/ASR Joint User Facility and PI Meeting, October 24 – 27, 2022
7. Wang, Z., Lulin Xue, Yufei Chu, Hyeyum Hailey Shin, and Weiwei Li, 2022: The Opportunities and Challenges of Using ARM Observations and Simulations at the SGP site to Advance PBL Understanding and Parameterizations, 2022 ARM/ASR Joint User Facility and PI Meeting, October 24 – 27, 2022.
8. Xue, L., Z. Wang, Y. Chu, H. Shin, W. Li, D. F. D'Amico, and G. Firl, 2023: Using ARM Observations and the Common Community Physics Packaged Single Column Model to Advance PBL Understanding and Parameterizations, *13th Conference on Transition of Research to Operations,* January 8-12, 2023, Denver, CO.
9. Shin, H., L. Xue, Z. Wang, W. Li, Y. Chu, and W. I. Gustafson Jr., 2023: Effects of NWP-Based Large Scale Forcing on Real-Case LES: Statistical Analysis of Multi-Year LASSO LES of Shallow Convective Clouds, *24th Symposium on Boundary Layers and Turbulence*, January 8-12, 2023, Denver, CO.
10. Xue, L., Z. Wang, Y. Chu, H. Shin, W. Li, D. F. D'Amico, and G. Firl, 2023: How important is the PBL top representation to shallow cumulus simulations? 2023 ARM/ASR Joint User Facility and PI Meeting, August 7 – 10, 2023.
11. Chu, Y. and Z. Wang, 2024: Simultaneous Calculation of Turbulent Dissipation Rate and MLH Based on Doppler Lidar: A Case Study on Low-Level Jet, AGU Fall 2024, 9 - 13 December 2024 in Washington, D.C.

Software

CCPP-SCM source code used in this research is archived at https://github.com/NCAR/ccpp-scm/tree/release/public-v4.