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2	Deep Learning Driven Simulations of Boundary Layer Cloud over the US
3	Southern Great Plains
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5	Tianning Su ^{1*} , Yunyan Zhang ¹
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7	¹ Lawrence Livermore National Laboratory, Livermore, CA, USA
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15	*Corresponding authors: <u>su10@llnl.gov</u>
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22 Abstract. This study developed a deep learning model to simulate the complex dynamics of boundary layer clouds (BLCs) over the US Southern Great Plains. Using 23 over twenty years of extensive observations from the Atmospheric Radiation 24 Measurement program for training and validation, the model diagnoses the BLCs from 25 the perspective of cloud-land coupling. Morning meteorological profiles set as the 26 initial conditions and then identifying triggers for BLCs formation from surface 27 28 meteorology. The deep learning model offer accurate simulation of the convection initiation and cloud base of BLCs. In comparison with reanalysis data (i.e., ERA-5 and 29 30 MERRA-2), it provides a notable improvement in the vertical structure of low clouds from a climatological perspective. The deep learning model can serve as the cloud 31 parameterization and extend to analyzing stratiform and cumulus clouds within 32 33 reanalysis frameworks, offering insights into improving the simulation of BLCs. By quantifying biases due to various meteorological factors and parameterizations, this 34 deep learning-driven approach bridges the observational-modeling divide. Surface 35 humidity and parameterization emerge as key limiting factors to affect the 36 representation of BLCs in the reanalysis data. This deep learning approach holds 37 promise for improving the convection parameterization and advancing model 38 diagnostics in weather forecasting and climate modelling. 39





1 Introduction

Boundary layer clouds (BLCs), comprising primarily of stratiforms and shallow 41 cumuli, exert a profound influence on the Earth's radiative balance and climate system 42 (Betts, 2009; Teixeira and Hogan, 2002; Lu et al., 2013; Golaz et al., 2002). Their 43 44 formation and evolution within the planetary boundary layer (PBL) are critically shaped by the interactions between surface processes and atmospheric dynamics (Miao et al., 45 46 2019; Berg and Kassianov, 2008; Zhang and Klein, 2013; Guo et al., 2019; Zhang et al., 47 2017). These clouds, which frequently form in the PBL's entrainment zone, are the 48 critical part for weather prediction and climate modeling, holding the key to understanding land-atmosphere interactions (Caldwell et al., 2021; Bretherton et al., 49 2007; Wang et al., 2020, 2023; Moeng et al., 1996; Su et al. 2023; Zhang and Klein, 50 51 2010; Guo et al., 2019). Numerous studies have been dedicated to investigating the dynamics of boundary 52 layer clouds, highlighting the pivotal role of land surface in modulating cloud formation 53 and affecting the spatial and temporal distribution of low clouds (Rieck et al., 2014; 54 55 Xiao et al., 2018; Lee et al., 2019; Fast et al., 2019b; Tang et al., 2018; Tang et al., 2019; Tao et al., 2019; Tian et al., 2022; Qian et al., 2023). Despite considerable advancements 56 in observations and modeling capabilities, simulating the boundary layer clouds 57 remains a significant challenge, largely due to the complex feedback mechanisms 58 between land surface fluxes, PBL processes, and cloud microphysics (Miao et al., 2019; 59 Lareau et al., 2018; Lu et al., 2011; Fast et al., 2019a; Wang et al., 2014; Yang et al., 60 2018; Nogherotto et al., 2016). These challenges are compounded when attempting to 61





represent such processes in global and regional climate models, where the fine-scale 62 63 interactions are often parameterized in a coarse-resolution grid due to computational constraints (Bretherton et al., 2007; Moeng et al., 1996). In addition, different cloud 64 regimes exhibit varied cloud-land interactions that complicate their representation and 65 66 present challenges for observational studies and modeling efforts (Tang et al., 2018; Qian et al., 2023; Sakaguchi et al., 2022; Poll et al., 2022; Tao et al., 2021). 67 68 As an emerging tool, machine learning (ML) has been widely employed for a 69 variety of environmental and atmospheric studies (e.g., McGovern et al., 2017; Gagne 70 et al., 2019; Vassallo et al., 2020; Cadeddu et al., 2009; Molero et al., 2022; Guo et al., 71 2024). Specifically, ML techniques are increasingly being employed to simulate and estimate convection and precipitation, which are crucial for accurate weather 72 73 forecasting and climate modeling (Mooers et al., 2021; Wang et al., 2020; O'Gorman et al., 2018; Gentine et al., 2018; Zhang et al., 2021). For example, Rasp (2020) presents 74 algorithms for the implementation of coupled learning in cloud-resolving models and 75 the super parameterization framework. Similarly, ML tools have been applied to 76 77 leverage observational data for the refinement of convection parameterizations, offering more insights into convective dynamics (O'Gorman et al., 2018; Gentine et al., 2018; 78 Zhang et al., 2021). Moreover, Haynes et al. (2022) develop pixel-based ML-based 79 methods of detecting low clouds, with a focus on improving detection in multilayer 80 81 cloud situations and specific attention given to improving the cloud characterization. Despite the considerable advancements brought by ML, there are persistent 82 challenges in accurately simulating the vertical structure of clouds, as well as their 83





complex relationships with land surface. To address these complexities, this study 84 developed an advanced deep-learning framework to simulate the BLCs, using 85 comprehensive data from the Atmospheric Radiation Measurement (ARM) program at 86 the Southern Great Plains (SGP) site. This framework is designed to simulate the 87 88 triggers, progression, and structural structure of boundary layer clouds, placing a particular emphasis on cloud-land coupling mechanisms. By assimilating morning 89 90 radiosonde observations with diurnal-varying surface fluxes and meteorological data, 91 this deep learning model is uniquely positioned to unravel the complex initiation and 92 evolution of low clouds, especially those coupled with land surface processes. Furthermore, the critical assessment of our model in comparison with existing 93 reanalysis datasets, including MERRA-2 and ERA-5, highlights the improvement in 94 95 representing cloud vertical structure. Our study analyzed the model's performance 96 across various cloud regimes, such as stratiform and cumulus. By serving as the cloud parameterization in the reanalysis data, this model advanced the capability of low cloud simulations within reanalysis frameworks. By undertaking this endeavor, we strive to 98 99 narrow the existing gaps in boundary layer clouds between field observations and modeling, thereby enriching our understanding of the convective processes. 100

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2 Data and instruments

2.1 Comprehensive observations at the US Southern Great Plains

The ARM program, funded by the U.S. Department of Energy, plays a pivotal role at the SGP site in Oklahoma (36.607°N, 97.488°W). Recognized globally as a leading





107 meteorological and radiative measurements, offering data that spans over two decades. This study utilized these extensive field observations during 1998-2020 to explore the 108 simultions of BLCs from the deep learning techniques. 109 110 Our study employs the Active Remote Sensing of Clouds (ARSCL) product, which integrates lidars, ceilometer, and cloud radar data to define cloud boundaries, utilizing 111 the best estimates from lidar for the lowest cloud bases (Clothiaux et al. 2000, 2001; 112 Kollias et al. 2020). Based on the comprehensive information of cloud vertical structure 113 114 and temporal evolution from the ARSCL dataset, Xie et al. (2010) offers detailed cloud 115 fraction profiles at the hourly resolution in ARM BEST ESTIMATE DATA 116 PRODUCTS (ARMBE). Central to our analysis are the comprehensive thermodynamic profiles obtained 117 from radiosondes (SONDE). Launched routinely at multiple times daily, these SONDE 118 119 measurements offer detailed information into the thermodynamic state of the PBL and the free atmosphere. The operation and technical aspects of the ARM SONDE are 120 121 detailed in Holdridge et al. (2011). Meanwhile, We use a variety of meteorological parameters (i.e., temperature, 122 relative humidity, wind, and pressure) at the surface level from collocated surface 123 meteorology systems (MET) at the ARM SGP site. These surface meteorological 124 parameters play roles in the formation and development of BLCs. Furthermore, the site 125 also provides data on surface sensible and latent heat fluxes. An ARM value-added 126 127 product called the best-estimate fluxes from energy balance Bowen ratio measurements

climate research facility, the ARM SGP site has been collecting a wealth of





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and Bulk Aerodynamic calculations (BAEBBR), was generated to replace the energy balance Bowen ratio flux measurements with a bulk aerodynamic estimation when the Bowen Ratio has a range of -1.6 and -0.45 (Cook, 2018). The replacements generally happen for the measurements at a 30-min temporal resolution under the low sensible heat scenario. We use the BAEBBR data along with the surface meteorology as the key input for the deep learning model.

2.2 Boundary layer clouds

BLCs demonstrate complex evolutions and interact with boundary layer and land surface processes. Tracking the initiation, development, and lifecycle of BLCs is crucial for understanding the convection in our climate system. We treat BLCs as synonymous with land-coupled clouds, in contrast to those clouds are decoupled from PBL and land surface. In this regard, Su et al. (2022) devised a lidar-based method to discern cloud-land coupling, leveraging the vertical coherence and temporal continuity of the PBL. This approach, combined with cloud base height measurements from ceilometers and surface-based Lifting Condensation Level (LCL) calculations as proposed by Romps (2017), forms the foundation for identifying coupled low-level clouds in our study. The methodology for determining PBLH, as outlined by Su et al. (2020), established a long-term record of PBLH at the SGP. The resulting data are publicly available through the ARM database (https://www.arm.gov/data/data-sources/pblht-206). Coupled clouds are identified when the cloud base height (CBH), as derived from ceilometer, aligns with the lidar-detected PBL top and the calculated





LCL within a certain range (Su et al. 2022). This alignment is indicative of clouds that are directly influenced by surface-driven processes. Meanwhile, we apply a cloud thickness threshold of less than 4 km to analyze BLCs.

Within the scope of land-coupled clouds, we further classify observed BLCs into cumulus and stratiform categories. For cumulus clouds, two criteria are applied: (1) cloud formations emerge after sunrise, ensuring that they are driven by local convective processes, and (2) there is an absence of overcasting clouds. Conversely, stratiform clouds are identified by prolonged overcasting conditions during the daytime, typically lasting more than three hours, with cloud fractions exceeding 90% as per ARSCL data. Based on the criteria, we identified 940 days categorized under the cumulus regime, distributed as 21%, 56%, 17%, and 6% across Spring, Summer, Fall, and Winter, respectively. Similarly, we identified 657 days falling within the stratiform clouds regime, with respective seasonal distributions of 37%, 12%, 23%, and 28%. This classification of cloud types to filter the BLCs based on the concept of cloud-land coupling is important for the training and analysis of the deep learning model. We further attempt to use the comprehensive cloud observations at the SGP to build the deep learning model.

2.3 Reanalysis data

In this study, we also use reanalysis datasets from the European Centre for Medium-Range Weather Forecasts' fifth-generation global reanalysis (ERA-5, Hersbach et al., 2020) and NASA's Modern-Era Retrospective analysis for Research





and Applications Version 2 (MERRA-2, Gelaro et al., 2017).

As the state-of-art reanalysis data, the ERA-5 is produced by the Integrated 173 Forecasting System (IFS) and a data assimilation system at a fine spatial resolution of 174 0.25° x 0.25°. ERA-5 reanalysis data are obtained from the Copernicus Climate Data 175 176 Store. This dataset employs a prognostic cloud scheme capable of capturing the evolution of cloud dynamics over consecutive time steps (Tiedtke 1993), a feature that 177 178 enhances its utility in time-dependent climate studies. We also use ERA-5 data to obtain the cloud and atmospheric information, which provides the hourly measurements at a 179 0.25° - 0.25° longitude-latitude grid. The vertical resolution of ERA-5 data is 25 hPa 180 in the lower atmosphere (700 – 1000 hPa). 181 The MERRA-2 reanalysis data use a new version of the Goddard Earth 182 183 Observing System Data Assimilation System Version 5, which is a advanced system coupling a global atmospheric general circulation model to NCEP's Grid-point 184 Statistical Interpolation analysis (Randles et al., 2017). The MERRA-2 reanalysis has a 185 spatial resolution of 2/3° \times 1/2° (longitude – latitude). MERRA-2 utilizes a 186 diagnostic cloud scheme, focusing on the immediate state of clouds. This dataset 187 specializes in the representation of the hydrological cycle and cloud information, which 188 are widely used in multiple studies (e.g., Yeo et al., 2022; Kuma, 2020; Miao et al., 189 2019). MERRA-2's reanalysis provides detailed hourly low cloud fraction data and tri-190 hourly vertical cloud fraction profiles. 191

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3 Deep Learning Framework for Simulating Boundary Layer Clouds

3.1 Integrated Deep Learning Models for Cloud Simulation

This study developed an integrated deep learning approach to simulate BLC. These models are purpose-built to simulate the initiation, positioning, and vertical extent of BLCs. Figure 1 demonstrates the design of our deep learning framework. The core of this research integrates three distinct deep learning models, each responsible for a critical aspect of cloud simulation: the triggering of cloud formation, the determination of cloud position, and the vertical profile of coverage fraction within cloud boundaries, which jointly yielding the comprehensive features of BLCs through multiple hidden layers. Initially, the triggering model evaluates whether cloud formation is likely, producing a value between 0 and 1, with values above 0.5 indicating the presence of clouds. This triggering information then feeds into the other two models: one for determining the cloud's position and the other for calculating the cloud fraction. While the cloud position and cloud fraction models are independent components, they collaborate to depict the vertical cloud fraction profile.

Morning meteorological profiles set as the initial conditions and then identifying triggers for BLC formation from surface meteorology. Each morning profiles have 46 elements from 0-6km. For surface meteorology and fluxes, the inputs include the data at the current hour and the previous hour. The RH profiles and PBL top are highlighted for their significance in boundary layer development. To represent the vertical structure of BLC, we equally segmented the cloud layer from the base to the top into ten levels.





For each of these levels, our deep learning models calculate individual cloud fraction 214 values. These values are then interpolated to create a continuous vertical profile of cloud 215 fraction within the BLC, offering a detailed depiction of the cloud's vertical extent. This 216 model the TensorFlow Package, developed Google 217 used by 218 (https://www.tensorflow.org/). The deep neural network (DNN) architecture was designed (brown boxes in Figure 219 1), beginning with an input layer reflective of the selected feature set. The detailed 220 221 structures for the three models can be found in Table 1. Normalization is a 222 preprocessing technique that often leads to improvements in model training by scaling the input features and target values to a standard range (Raju et al. 2020). We applied 223 the normalization process to both the input and target data to ensure that they have a 224 zero mean and a standard deviation of one. This standardization scales the data to a 225 common range, allowing for a more stable and efficient training process. Subsequent 226 hidden layers were integrated, each imbued with L2 regularization to mitigate 227 overfitting by penalizing complexity. 228 229 Batch normalization was implemented at each layer to normalize inputs, ensuring consistent data distribution throughout the network, thereby stabilizing the learning 230 process. A dropout rate of 0.2 further prevented overfitting by randomly omitting 231 neuron connections during training, encouraging the network to learn more robust 232 233 features. Training was refined with early stopping, ceasing further epochs when the validation loss ceased to improve, and learning rate reduction, systematically 234





decreasing the learning rate upon encountering plateaus in performance improvement.

236 These callbacks were instrumental in honing the model's performance, ensuring

convergence to the accurate representation of the BLC. Neuron biases are included in

the network's architecture and systematically inserted in the hidden layers (Battaglia et

239 al. 2018).

3.2 Model Training Process and Examples

The construction of our deep learning model suite commenced with the segregation of the comprehensive dataset, sourced from the rich datasets of ARM program, into a training subset (70%) and a validation subset (30%) during 1998-2016. Additionally, we incorporate datasets from 2017-2020 as part of our validation process, specifically focusing on data from the untrained period to assess the model's performance. The training and validations are both using the more than 20-year BLC observations, as well as the ARMBE products. The base of BLC is determined at the lowest altitude where cloud fraction exceeds 1%, and the cloud top is identified at the point where cloud fraction transitions from exceeding 1% to falling below this threshold. In multi-layer systems, the DNN model is trained based on the lowest cloud layer when it is coupled with the land surface. Upon training completion, the model was evaluated, with its performance metrics examined for accuracy and reliability. This methodical and data-driven process balanced complexity with precision, culminating in a robust model capable of simulating BLC features.

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These models operate synergistically, with the predicted cloud trigger extending into the models for cloud position and vertical structure (i.e., cloud fraction and cloud thickness). As the example of the model output, Figure 2 offers a comparative display of diurnal cloud fraction profiles over the SGP, contrasting observed data with deep learning simulations. The model accurately simulates the cloud occurrence and cloud base for these cases, aligning well with observations. However, it falls short in simulating cloud top position, especially for stratiform clouds, overestimating cloud tops. It also underestimates maximum cloud fractions for the stratiform clouds. The maximum cloud fraction for stratiform is close to 1, indicating complete coverage, an aspect not fully replicated by the model. The third case also falls into the category of stratiform clouds, characterized by a cloud fraction exceeding 0.9. However, the presence of multiple local maxima within the cloud fraction profile indicates a relatively complex structure. This complexity poses a challenge to the model, as the DNN is not fully capable of capturing the internal variations within the convective system. Instead, the model tends to produce a more uniform cloud fraction across this convective system. Despite these variances, the model-derived cloud bases and occurrence demonstrates high consistency with observations, highlighting its value in the cloud simulations.

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3.3 Calculations of Feature Importance and Performance Metric

To elucidate the significance of each variable within our deep learning models, we implemented a permutation importance analysis. This robust, model-agnostic technique assesses each feature's influence on the model's predictive accuracy, which is crucial





for assessing DNN (Date and Kikuchi, 2018; Altmann et al. 2010). In this study, the permutation importance method differs slightly based on whether the model's task is regression (cloud position and fraction) or classification (trigger).

For the models predicting cloud position and cloud fraction, which are regression tasks, the Mean Absolute Error (MAE) serves as the performance metric. First, we perform a test run to establish a baseline performance by calculating the MAE of the model using the original, unperturbed validation datasets, which comprises morning sounding and surface meteorology data as the input. Then, for every feature in the validation set, we disrupt its association with the target by shuffling its values across all instances, creating a permutation of the dataset. This is executed while maintaining the original order of all other features. Furthermore, we recalculate the MAE with the shuffled data. The difference between this new MAE and the baseline MAE represents the feature's importance. To ensure a comprehensive assessment, the permutation and subsequent MAE calculation are repeated 20 times with different random shuffles. The final importance score for each feature is then determined as the mean increase in MAE across these permutations.

However, for the model classifying cloud triggers, which is a classification task, the accuracy score is used as the performance metric. The accuracy score is a measure of the model's overall correctness and is calculated using the formula:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \tag{1}$$

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where True Positives (TP) indicates the number of instances correctly predicted as positive; true Negatives (TN) indicates the number of instances correctly predicted as negative; False Positives (FP) indicates the number of instances incorrectly predicted as positive, and False Negatives (FN) indicates the number of instances incorrectly predicted as negative. After determining the performance metric, other procedures for determining feature importance remain the same between regression tasks and the classification task. In the model, we filter individual input parameters from the consideration of importance score. By using this methodology, Figure 3 illustrates these importance scores from different features, underscoring the most influential factors for predicting the presence, position, and vertical fraction of BLCs. These factors are ranked from most important factors to least important factors. BLC trigger is a special factor since it is the output of the classification model. Notably, the importance scores are not computed as a simple sum but are determined by collectively shuffling groups of features and observing the impact on model performance. Table 1 complements Figure 3 by providing the model's structure and the precise importance values assigned to each feature across the three cloud prediction tasks. Among these factors, LCL is derived from the surface meteorology (Romps, 2017), BLH_{parcel} is derived from the morning temperature profiles and surface air temperature based on the Parcel method (Holzworth, 1964; Su et al. 2020). Specifically, BLH_{parcel} is defined as the height where the morning potential temperature profile first exceeds the current surface potential temperature by more than

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heat (Stull, 1988; Su et al. 2023). 320 In particular, surface relative humidity (RH), surface air temperature (T), and 321 morning relative humidity profiles are highly influential in BLC simulations. This is 322 323 consistent with previous observational and modeling studies (Zhang and Klein, 2013). Surface RH is a critical factor affecting the trigger, CBH, and cloud fraction predictions. 324 325 As the boundary condition for the DNN model, morning atmospheric profiles of different meteorological parameters (i.e., RH, temperature, and wind components) exert 326 327 a notable impact on cloud trigger detection and the determination of cloud fractions. Surface air temperature is shown to have a substantial effect on cloud fraction, 328 highlighting the sensitivity of cloud simulations to near-surface thermal conditions. 329 330 This approach recognizes the interconnectedness of certain features and their collective contribution to the model's output. 331 332 4 Modeling Boundary Layer Clouds with Deep Learning 333 4.1 Boundary Layer Clouds Trigger 334 The occurrence of BLC is a multifaceted process influenced by a variety of 335 atmospheric parameters and surface processes. The BLC trigger, a critical component 336

1.5 K. BLH_{SH} is derived from the morning temperature profiles and surface sensible

in the formation of BLCs, is a dynamic phenomenon that our deep learning model seeks

to identify and simulate from the surface meteorology.





By using the morning SONDE and measurements of surface meteorology and 339 fluxes, Figure 4 showcases the model's proficiency in classifying the occurrences (class 340 1) and non-occurrences (class 0) of BLC during both a trained period and an untrained, 341 future period. The confusion matrices (Luque et al. 2019) for the trained period (1998-342 343 2016) and for the untrained period (2017-2020) display the model's predictive performance. The matrices reveal the counts and percentages of TP, FP, TN, and FN. 344 345 Figure 4a represents the trained period, we use 30% dataset for the validation and see a high percentage of TN at 71.2% and TP at 21.1%, indicating that the model is accurate 346 347 during the period it was trained on. For the untrained period (2017-2020), the model still performs well, with 71.8% TN and 17.4% TP (Figure 4b). However, the rates of 348 FN and FP are slightly higher at 5.6% and 5.2% respectively, which could indicate that 349 350 the model is slightly less accurate when applied to data beyond its training scope. TP, FP, TN, and FN, further offer insights into the model's precision, recall, and 351 overall accuracy in detecting the presence of BLC. Precision, which gauges the 352 accuracy of positive predictions, recall, which assesses the detection of actual positives, 353 354 and the F1 score, which balances the two, are consistently above 75% across both periods. This high performance across key metrics demonstrates the model's robustness 355 and reliability in identifying the onset of BLCs. 356 Table 2 complements the Figure 4 and provides a detailed quantitative number of 357 358 the model's classification performance. It presents the number of instances and their corresponding percentages of different matrices (i.e., TN, FP, FN, and TP). The high 359

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percentages of correct predictions (TP and TN) underscore the model's effectiveness, while the lower FP and FN rates reflect its reliability. The table highlights the model's robustness, with overall accuracy rates of 92.3% for the trained period and a slightly reduced but still substantial 89.2% for the untrained period. These metrics demonstrate the model's predictive capabilities and reliability for both trained and untrained periods. Figure 5 further compares the diurnal frequency of BLC occurrence between observations (OBS) and DNN predictions for different seasons. The BLC's strong diurnal pattern is well-captured by the model, when BLC development peaks between 12-16 local times, aligning closely with observed frequencies. Among different seasons, the model is notably effective in simulating the pronounced diurnal cycle of summer clouds, which are typically influenced by local convection. Conversely, the winter season exhibits a weaker diurnal pattern, likely linking to the diminished surface fluxes. The DNN tends to overestimate BLC presence in the early morning, especially for the winter season. The overall alignment between observations and the DNN model represents the model's capability of capturing the diurnal patterns of BLC formation and development. Determining the triggers of BLC lays the foundation for the integrated simulations of BLC features.

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4.2 Simulating Cloud Positions and Cloud Fractions

A key aspect of cloud modeling involves the accurate simulation of cloud positions and fractions, which are indicative of a cloud's vertical extent and fractional coverage.





Our deep learning model demonstrates capabilities in predicting these key attributes of 381 382 BLC. Figure 6 offer the comparisons between observed values and predictions by the 383 DNN for CBH, CTH, and cloud fraction. These comparisons are presented for both the 384 385 training period (a, c, e) and an independent period (b, d, f), revealing the model's ability to generalize beyond its initial training data. DNN model demonstrates remarkable 386 performance in simulating cloud base, boasting a correlation coefficient surpassing 0.9 387 and an MAE under 0.15 km. Conversely, the model encounters challenges with CTH 388 389 prediction, evidenced by a lower correlation of about 0.5 and a significantly higher 390 MAE between 0.8 and 0.9 km, aligning with case studies in Figure 2. The discrepancy in accurately simulating CBH and CTH may stem from two main 391 factors. Firstly, CBH determinations are generally more precise due to the effectiveness 392 of laser-based methods (Pal et al., 1992), while CTH estimations often suffer from 393 reduced accuracy, partly attributed to signal attenuation issues (Clothiaux et al., 2000). 394 Secondly, our DNN simulations are developed from the perspective of cloud-land 395 coupling, primarily utilizing surface meteorology. This can introduce inherent 396 limitations, as the tops of many clouds may be decoupled from surface influences 397 despite a coupled base, leading to potential gaps in the model's parameterization to 398 accurately define the cloud top. 399 400 The comparison of cloud fraction between observations and DNN are presented to consider the model's capability to simulate the vertical distribution of cloud coverage 401

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(Figure 6e-f). The scatterplots comparing observed and modeled cloud fractions at individual levels in cloudy scenarios show a satisfactory correlation, with an R-value exceeding 0.77 and an MAE around 0.15. Nevertheless, the DNN model tends to underestimate the peak cloud fraction, displaying a range up to ~0.8 compared to the full 0-1 range observed. This underestimation is intrinsically linked to the model's simulation of cloud position, as both cloud fraction and position models operate in tandem. For stratiform clouds, observational data typically exhibit a relatively uniform vertical extent with cloud fractions close to unity at the central height, whereas the DNN model tends to generate a broader, more attenuated profile with a reduced maximum cloud fraction at the center. This points to a need for refining the model's ability to replicate the pronounced peak cloud fractions characteristic of stratiform cloud profiles. The diurnal patterns of cloud base and top heights, captured through daily profiles, showcase the model's adeptness at simulating the temporal changes in cloud positions for all BLCs, the cumulus regime, and the stratiform regime (as shown in Figure 7). These profiles, derived from both observational data and DNN outputs, include shaded regions representing the variability (one standard deviation) around the average heights. Cumulus clouds exhibit a marked diurnal cycle, whereas stratiform clouds typically maintain a relatively consistent position and smaller variations throughout the day. A close alignment is observed between the mean and standard deviation of the cloud base between observed and simulated data for different regimes. In contrast, while the mean cloud top heights follow a similar diurnal trend in both cases, the variability presented





by the observed data exhibits more pronounced variabilities compared to the relatively small variabilities in DNN simulations.

Figures 6 and 7 collectively demonstrate the model's ability to simulate cloud positions and fractions within BLC. It reliably captures cloud base heights yet encounters challenges with accurately representing cloud top heights and peak cloud fractions on an individual basis. These constraints are somewhat expected, given that even very fine-scale model struggle to entirely capture the vertical extent of clouds, as evidenced in Large-Eddy Simulations or Convection-Permitting Models (Zhang et al. 2017; Gustafson et al. 2020; Bogenschutz et al. 2023).

4.3 Integrating Deep Learning Models into Reanalysis Datasets

The DNN model can use the conventional meteorological data (i.e. morning SONDE and surface meteorology data) to diagnose the BLC. Meanwhile, it also can be used in reanalysis data (i.e., ERA-5 and MERRA-2) to serve as the convection parameterization to simulate BLC with the input of morning profiles and meteorology data from the reanalysis. Thus, we can assess the integration of Deep Learning Models with reanalysis datasets to refine the simulation of BLCs.

Following this thoughts, Figure 8 contrasts diurnal cloud fraction patterns from observational data and deep learning model predictions across all conditions of seasons and years. Figure 8a-b present the observed cloud fractions and those simulated by our deep learning neural network (DNN), respectively. Panels c and e display cloud fractions directly available from ERA and MERRA reanalysis datasets, while panels d

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and f illustrate the enhanced simulation results after the application of DNN to ERA 445 446 (ERA_{DNN}) and MERRA (MERRA_{DNN}) data. To eliminate sampling biases, we averaged only those samples for which both observational and reanalysis datasets are concurrently available. Observing fluctuations in surface temperature and humidity 448 449 data in ERA-5 for this region, we smoothed ERA-5 surface air temperature and humidity data with a ± 1-hour window to mitigate potential variability from 450 451 assimilation before using them as input for the DNN. 452 The DNN simulations with observed meteorological data align closely in cloud 453 fraction profiles within the 0-2 km range, reflecting the model's ability to capture landcoupled clouds. As this model are designed for diagnosing land-coupled clouds, the 454 model does not simulate decoupled clouds, which often have bases occurring above the 455 456 2-km (Su et al. 2022). Original reanalysis data show significant underestimations of cloud fractions for low clouds, particularly evident in MERRA-2. The implementation 457 of DNN enhances cloud fraction representation compared to original reanalysis data, 458 demonstrating the DNN model's strength in simulating BLC. Given that the DNN 459 model specializes in simulating BLC, when utilizing reanalysis data, the portion of 460 cloud profiles that are decoupled are preserved as they are in the original datasets—that 461 is, for the cloud layers above the BLC-tops or for clouds that rooted above the PBL. 462 Furthermore, Figure 9 provides a detailed examination of stratiform clouds, 463 utilizing the same comparative approach as in Figure 8. The observed stratiform clouds 464 display a layered structure with expansive coverage and maximum cloud fractions 465 typically exceeding 0.6. The DNN model reproduce these observed characteristics 466

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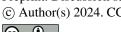
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fairly well, albeit with minor overestimations in cloud vertical extent. Conversely, the original ERA-5 and MERRA-2 data exhibit limitations, particularly in underestimating cloud fraction. The integration of the DNN model with reanalysis data enhances the representation of stratiform cloud fractions, as depicted in the heatmaps of Figure 9, showcasing improved agreement with observational data and underscoring the enhancement potential for cloud fraction simulations in reanalysis datasets. Additionally, Figure 10 extends the comparative study to cumulus clouds. Cumulus clouds pose significant challenges for modeling and parameterization partly due to their typically small spatial extent compared to the model grid, often spanning from a few hundred meters to several kilometers (Zhang et al. 2017; Tao et al., 2021; Bogenschutz et al. 2023; Gustafson et al. 2020). In line with expectations, ERA-5 and MERRA-2 exhibit significant biases in representing cumulus clouds when compared to observational data, possibly related to the large grid of the reanalysis that might not fully capture the fine-scale characteristics of cumulus formations. In contrast, the DNN model achieves commendable success in capturing the diurnal variability of cumulus clouds, including cloud base, vertical extension, and cloud fraction, by leveraging local convective signals derived from surface meteorology data. When the DNN methodology is applied to ERA-5, it significantly improves the representation of cumulus clouds. However, the original MERRA-2 data, which tend to overlook the majority of cumulus clouds, continue to significantly underrepresent them even after the application of DNN, suggesting that additional biases in meteorological factors may contribute to this discrepancy.





The integration of deep learning with ERA and MERRA reanalysis datasets demonstrates the notable refinement in the simulation of BLC. By integrating our deep learning models with reanalysis data, we achieve a more accurate representation of cloud fractions for both stratiform and cumulus clouds.

We further examine the remaining disparities in cloud fraction simulations within

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4.4 Applying Deep Learning for Bias Attribution in Cloud Simulation

reanalysis datasets, despite the integration of deep learning models (as shown in Figures 8-10), indicating persisting meteorological biases. Deep learning is utilized to quantify and attribute these biases for BLC simulations. Figure 11 offers a comparative analysis of vertical cloud fraction profiles for both stratiform and cumulus clouds. It presents cloud fractions observed with those from reanalysis data (RD), including ERA-5, MERRA-2, and their corresponding deep learning-informed simulations. While the application of deep learning to reanalysis data (RD_{DNN}) yields improvements, remaining biases are evident, particularly in MERRA-2. Acknowledging the significant influence of surface RH on BLC simulations (as indicated by Figure 3e, input observed surface relative humidity (RH) instead of reanalysis RH into the DNN models (the output is RD_{DNN-RH}). This modification leads to a more accurate simulation for MERRA-2, closing the gap with observational data, especially for stratiform clouds. For ERA-5, RD_{DNN-RH} and RD_{DNN} show negligible differences for cumulus clouds, but for stratiform clouds, RD_{DNN-RH} exhibits a reduced bias. These refined profiles attest to the benefits of using observed surface moisture





data, confirming its important role in achieving a more accurate representation BLC. 511 We can further dissect the bias in cloud fraction simulations attributed to various 512 meteorological factors and parameterization schemes within ERA and MERRA 513 reanalysis datasets: 514 515 Bias due to parameterization = $|RD - OBS| - |RD_{DNN} - OBS|$ (2) Bias due to surface $RH = |RD_{DNN} - OBS| - |RD_{DNN-RH} - OBS|$ (3) 516 517 where RD and OBS are the cloud fraction derived from reanalysis data and observations, 518 respectively. The definition of RD_{DNN} and RD_{DNN-RH} are the same with the above. For 519 getting a representative value, these biases are layer-averaged from 0-4 km over different local times, and then normalized by the observed mean cloud fraction, offering 520 a climatological perspective on the discrepancies between observed and simulated data 521 522 across seasons and years. 523 We get the bias attributed to different meteorological factors and parameterization schemes in the ERA-5 and MERRA-2 datasets, respectively (Figure 12). Each bars 524 indicate the normalized bias contributed by factors such as morning meteorological 525 526 profiles, surface pressure, surface fluxes, various surface meteorology variables, and parameterization schemes. Notably, parameterization stands out as a significant 527 contributor to bias, accounting for 14.45%/19.05% of the discrepancy in stratiform 528 clouds between observations and ERA-5/MERRA-2. For cumulus clouds, the 529 parameterization biases are more pronounced, contributing 22.23% and 30.94% for 530 ERA-5 and MERRA-2, respectively. 531 In addition to parameterization, RH, RH profiles, and sensible heat are identified as 532





major factors contributing to the differences between observations and reanalysis data. For instance, aligning MERRA-2's RH with observed surface RH could potentially reduce bias by 23.13% for stratiform and 10.26% for cumulus clouds. Meanwhile, surface RH and morning RH profiles in ERA-5 lead to 11.25% and 3.96% of biases for the stratiform clouds. The bias between ERA-5 and observed cumulus clouds is largely driven by parameterization, which suggests that employing the DNN model with ERA-5 can lead to a more accurate simulation of cumulus clouds.

The detailed bias attribution analysis facilitated by the deep learning model elucidates the individual impact of meteorological factors on the discrepancies in cloud fraction between observations and reanalysis data. It underscores the necessity for more accurate humidity data within reanalysis datasets to refine BLC simulations. Furthermore, this deep learning approach illuminates pathways for improved parameterization of boundary layer convection.

5 Summary

This study has developed a deep learning model to estimate the evolution of BLCs over the SGP. The model utilizes over two decades of meteorological data to simulate BLC formation and characteristics, including timing of convection initiation (BLC onset), their positions, and vertical structures. As this model is built based on the perspective of cloud-land coupling, the DNN approach demonstrates the capability to diagnose land-coupled convective systems from surface meteorology. The DNN model is built on the cloud-land interactions and serves as the testimony for the coupling





between BLCs and land surface. The proficiency and reliability of the DNN model is 555 evident in its robustness during both the training period and subsequent independent 556 periods. 557 The implementation of this model within reanalysis datasets like ERA-5 and 558 559 MERRA-2 has resulted in enhanced representation for stratiform clouds and cumulus and an accurate vertical structure of clouds in term of climatology, providing a 560 561 promising tool for improving weather forecasting and climate modeling. The deep 562 learning model notably address the limitation in cumulus simulations in the reanalysis 563 data, Meanwhile, this approach is much cost-effective compared to traditional parameterizations and schemes at various scales, as it can simulate two decades of BLC 564 with vertical information over the SGP in ~30-second using a single GPU node. 565 In addition to the BLC simulations, the deep learning model developed in this study 566 also is used to attribute discrepancies between observational data and reanalysis 567 datasets to different meteorological factors. Besides parameterization, surface RH, 568 morning RH profiles, and surface sensible heat are the three major factors lead to the 569 570 mismatches in BLC representation in ERA-5 and MERRA-2. These findings underscore the importance of incorporating more accurate humidity information in 571 reanalysis datasets, which is crucial for refining BLC simulations. This analysis also 572 sheds light on the necessity to update reanalysis datasets with improved 573 574 parameterization of boundary layer convection. 575 By leveraging deep learning, the model addressed the simulation of cloud vertical structure, among one of the key challenges in the field. They highlight the value of deep 576





learning in advancing our understanding of BLC dynamics and improving the 577 representation of low clouds in atmospheric models. This work not only narrows the 578 observational-modeling divide but also paves the way for future developments in cloud 579 parameterization. Moving forward, future work is warranted to test and extend this 580 581 parameterization to different synoptic regions. The goal is to develop a versatile model capable of simulating BLC on a global scale, which can be integrated into multiple scale 582 583 models or reanalysis data. 584 Code and data availability. The code package of DNN models and for the The 585 simulation outputs of BLCs from observed meteorological data and ERA-5 and 586 MERRA-2 can be found in https://doi.org/10.5281/zenodo.10719342 (Su, 2024). ARM 587 fluxes, cloud 588 radiosonde data, surface and masks available https://adc.arm.gov/discovery/#/results/instrument_class_code::armbe 589 (ARM user 590 facility, 1994). ARSCL (Active Remote Sesning of Cloud) can be found in 591 https://adc.arm.gov/discovery/#/results/instrument class code::arscl (ARM 592 facility, 1996). MERRA-2 reanalysis data can be downloaded obtained from 593 https://disc.gsfc.nasa.gov/datasets/M2T1NXRAD 5.12.4/summary?keywords%E2%8 0%89=%E2%80%89MERRA-2%20tavg1 2d rad Nx (GMAO, 2015). ERA-5 594 reanalysis from 595 data are obtained https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-pressure-596 levels?tab=form (Hersbach et al. 2023). 597 598 Author contributions. TS designed this study and carried out the analysis and model 599 600 training. TS and YZ interpreted the data and wrote the manuscript. YZ supervised the 601 project.





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TABLE LIST:

Table 1: Feature Importance and Structure in the Deep Learning Models. This table details the structure and importance of features for each DNN model applied to predict cloud trigger, cloud base height (CBH), and cloud fraction. The structure of each model is defined by the number of neurons in sequential layers, and the importance scores reflect the predictive contribution of each feature, which includes month, local time (LT), surface pressure (PS), relative humidity (RH), zonal (U) and meridional (V) wind components, temperature (T), lifting condensation level (LCL), boundary layer height derived from sensible heat (BLH_{SH}) and parcel methods (BLH_{Parcel}), sensible heat (SH), latent heat (LH), and morning profiles of relative humidity (RH Profile), U wind (U Profile), V wind (V Profile), and potential temperature (θ Profile). The trigger feature is applicable only to the CBH and cloud fraction models.

Feature		Trigger	СВН	Cloud fraction
Structure		[108, 64, 36, 24]	[96, 56, 32, 24]	[56, 32, 24]
· ·	Month	0.00527286	0.001389318	0.005121363
	LT	0.02753033	0.012310212	0.012221336
	PS	0.004575528	0.00105115	0.004330988
	RH	0.107300553	0.54430006	0.06879726
	U	0.007313414	0.002259621	0.003518908
	V	0.025564082	0.012099721	0.00784819
	T	0.006910447	0.105152747	0.073418902
Importance	LCL	0.00455838	-0.001687665	-0.000544992
ort	BLH _{SH}	0.006687529	0.010036585	0.008999221
uĎ	BLHParcel	0.056904017	0.088704497	0.014904008
1	SH	0.006364585	0.008868474	0.016607784
	LH	0.002783613	0.010357209	0.024233806
	RH Profile	0.097609351	0.02356447	0.050633957
	U Profile	0.030436833	0.010810712	0.04678593
	V Profile	0.049247653	0.023581766	0.045574382
	θ Profile	0.024626684	0.015502336	0.034399533
	Trigger	N.A.	0.017457138	0.095616528





Table 2: Classification Performance of the Deep Learning Model for Boundary Layer Clouds (BLC) Trigger. This table present the performance metrics of the deep learning model during both the trained and untrained periods. It lists the number of samples and corresponding percentages for true negatives (TN), false positives (FP), false negatives (FN), and true positives (TP). The overall accuracy for each period is also provided, indicating the model's overall effectiveness in predicting the presence of boundary layer clouds.

Performance	Trained Period (1998-2016)		Untrained Period (2017-2020)	
Metrics	Sample #	Percentage (%)	Sample #	Percentage (%)
TN	9773	71.1747142	5416	71.8016704
FP	393	2.8621368	393	5.2101286
FN	670	4.8794698	424	5.6211057
TP	2895	21.0836793	1310	17.3670953
Overall Accuracy	N.A.	92.2583934	N.A.	89.1687657



914 Figures

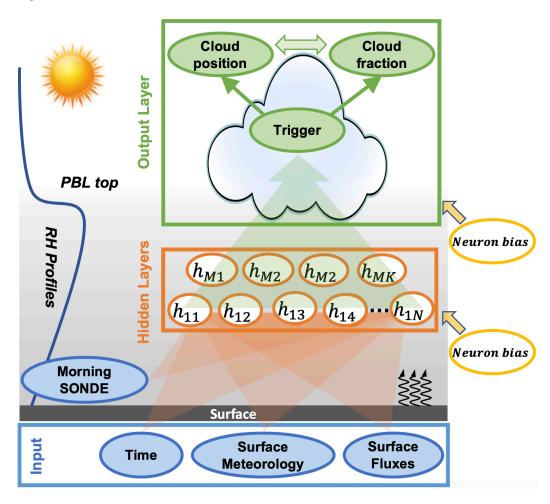


Figure 1: Conceptual diagram of the deep learning framework for simulating boundary layer cloud (BLC) characteristics over the US Southern Great Plains. Inputs for the deep neural networks (DNN) include morning radiosonde (SONDE) profiles, time indicators, and surface conditions such as fluxes (curved black arrows) and meteorological data. The relevance of relative humidity (RH) profiles and the planetary boundary layer (PBL) top is emphasized due to their critical role in boundary layer development. These variables are processed through multiple layers of hidden neurons (h_{11} to h_{MK}), each with neuron bias adjustments to optimize the network's predictive capability. Separate DNN models are constructed for the initiation (trigger) of boundary layer clouds (BLC), their vertical positioning, and cloud fraction across ten atmospheric layers. Together, these models synergize to predict the presence, altitude, and stratification of BLC.



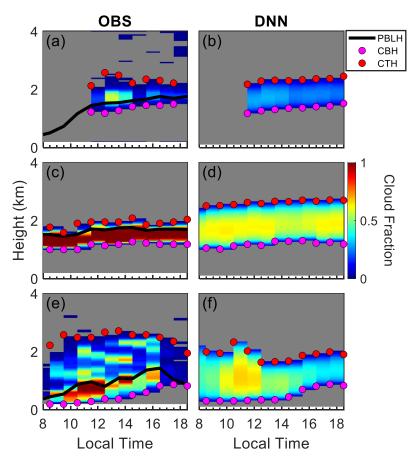


Figure 2: Examples of diurnal cloud fraction profiles for cumulus (a, b), stratiform (c, d), and complex cloud structures (e, f) over the US Southern Great Plains. Observed data (OBS) are shown alongside deep learning neural network (DNN) simulations. Black lines represent the observed PBL height (PBLH), with cloud base (CBH) and cloud top heights (CTH) marked by pink and red dots, respectively. The color gradient indicates the cloud fraction.

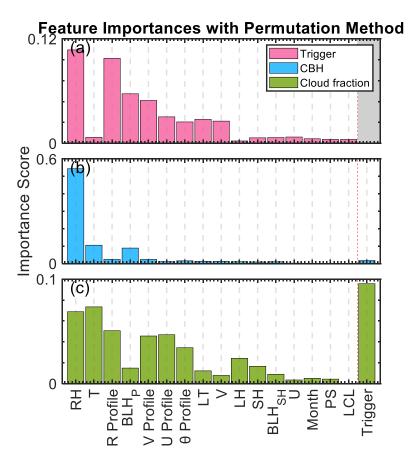


Figure 3. Feature importance scores for predicting cloud trigger (a), cloud base height (CBH) (b), and cloud fraction (c) in deep learning simulations of BLCs. Each panel presents the relative contribution of input features, includes month, local time (LT), surface pressure (PS), relative humidity (RH), zonal (U) and meridional (V) wind components, temperature (T), lifting condensation level (LCL), boundary layer height derived from sensible heat (BLH_{SH}) and parcel methods (BLH_{Parcel}), sensible heat (SH), latent heat (LH), and morning profiles of relative humidity (R Profile), U wind (U Profile), V wind (V Profile), and potential temperature (θ Profile). These factors are ranked based on their overall importance. The importance scores are calculated with permutation method and quantify the relative contribution of each feature to the model's predictive accuracy.

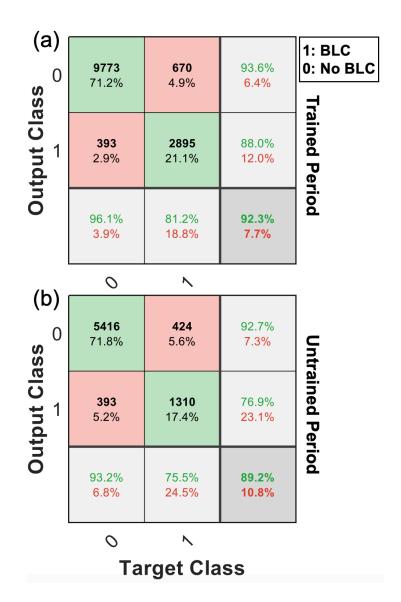


Figure 4: Confusion matrices representing the classification performance of the deep learning model for the presence of boundary layer clouds (BLCs) during the trained period (1998-2016) in panel (a), and the untrained period (2017-2020) in panel (b). For the trained period, we use 30% dataset for the validation. The matrices in the black color display the counts and percentages of true positive (TP), false positive (FP), true negative (TN), and false negative (FN) predictions. The overall precision, recall, and F1 scores for each class are also included, demonstrating the model's ability in identifying BLC occurrence.





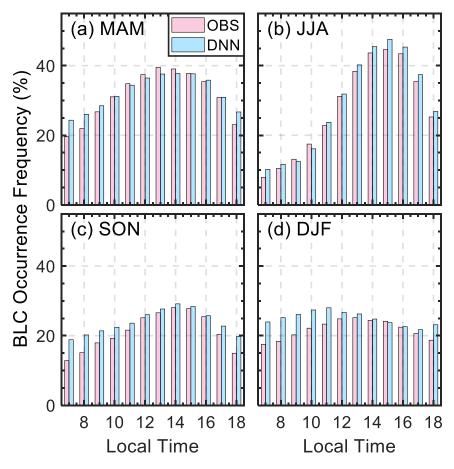


Figure 5. Bar graph comparing the frequency of boundary layer cloud (BLC) occurrence as observed (OBS, red) and as predicted by the deep learning neural network (DNN, blue) across different local times of the day, segmented by seasons: (a) MAM (Spring), (b) JJA (Summer), (c) SON (Fall), and (d) DJF (Winter). The bars present the diurnal pattern of BLC development.





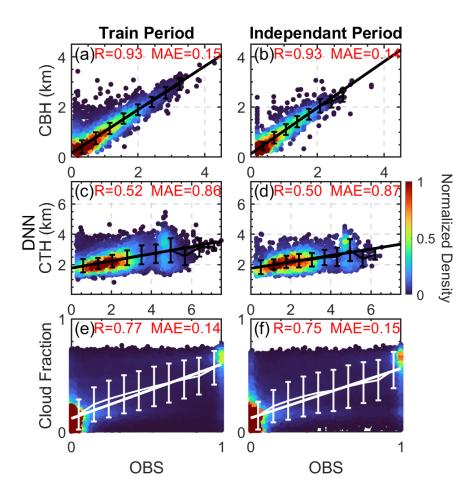


Figure 6. Scatter density plots comparing observed (OBS) and deep learning neural network (DNN) predicted values for cloud base height (CBH), cloud top height (CTH), and cloud fraction during the train period (a, c, e) and an independent period (b, d, f). Note that the BLC is segmented into ten layers, yielding ten separate cloud fraction values per BLC instance for analysis. The correlation coefficient (R) and mean absolute error (MAE) are indicated for each comparison. The color scale represents the normalized density of data points. The solid lines and error bars denoting the linear regression and standard deviations in each bar.





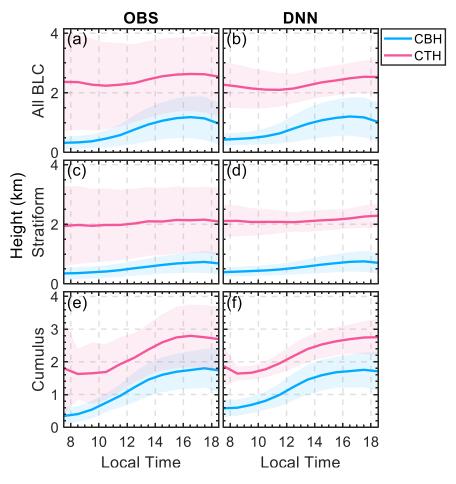


Figure 7. Diurnal profiles of cloud base height (CBH) and cloud top height (CTH) as determined by the observations (OBS) and deep learning simulations for all BLC (a-b), stratiform clouds (c-d), and cumulus (e-f). The shaded areas represent the variability (one standard deviation) around the mean heights.



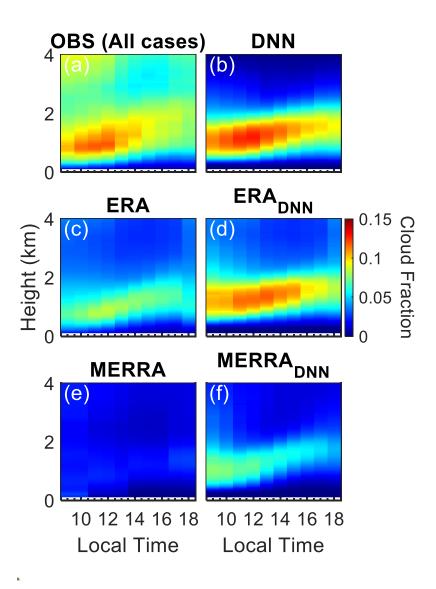
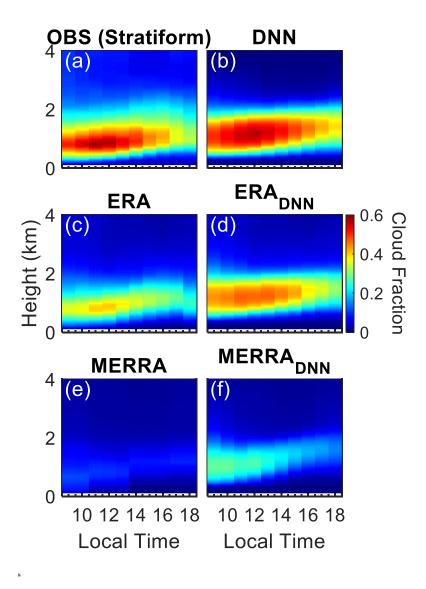


Figure 8. Cloud shaded areas demonstrate the diurnal variation in cloud fraction for all cases as observed and simulated. Panel (a) shows the observed cloud fraction (OBS), while panel (b) illustrates the cloud fraction simulated by the deep learning neural networks (DNN). (c, e): cloud fractions from ERA and MERRA reanalysis datasets, respectively. (d, f): the cloud fractions after the application of the DNN model to ERA (ERA_{DNN}) and MERRA (MERRA_{DNN}) data.





988 Figure 9. Same to Figure 8, but for stratiform clouds.



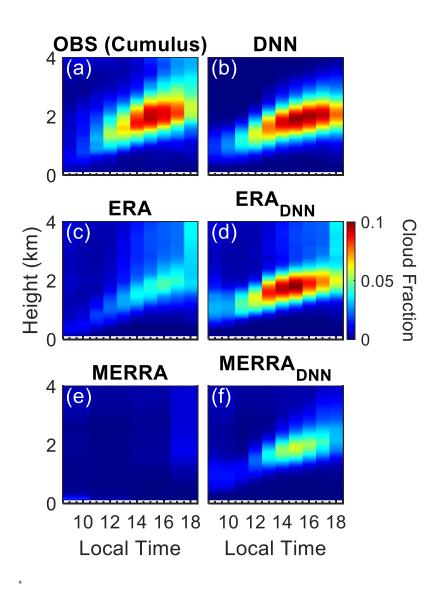


Figure 10. Same to Figure 8, but for cumulus.





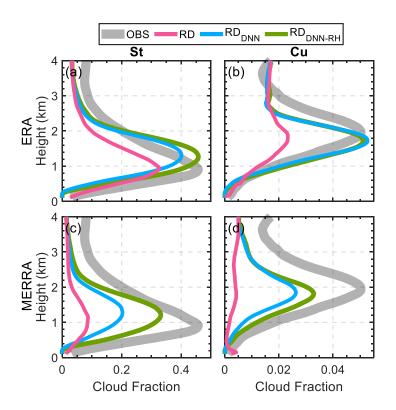


Figure 11: Vertical profiles of cloud fraction for stratiform (St) and cumulus (Cu) scenarios over the US Southern Great Plains. Panels (a) and (b) display ERA reanalysis data comparisons, while panels (c) and (d) show MERRA reanalysis data comparisons. The observed cloud fractions (OBS) are represented by the shaded grey area, illustrating the averaged cloud coverage recorded by field observations. The original reanalysis data (RD) is indicated in pink, indicating the baseline cloud fraction profiles as simulated by the reanalysis. The RD_{DNN} profiles in blue depict the new simulation results after applying the DNN models to the reanalysis data for boundary layer cloud (BLC) simulation. The RD_{DNN-RH} profiles in green show the simulation results when the surface relative humidity (RH) from the reanalysis data is replaced with observed values, indicating the impact of accurate surface moisture representation on cloud fraction simulations.

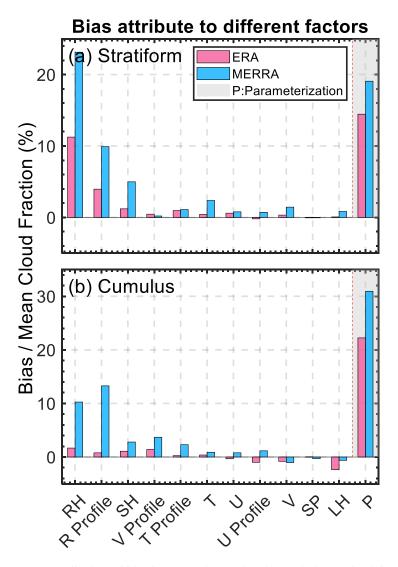


Figure 12: Attribution of bias between observed and reanalysis on cloud fractions to various meteorological factors and parameterization schemes for stratiform (a) and cumulus (b) cloud scenarios. The bars represent the normalized bias (bias divide mean cloud fraction) contributed by each factor: relative humidity profile (RH), meridional wind profile (V Profile), temperature profile (T Profile), zonal wind profile (U Profile), surface pressure (SP), latent heat flux (LH), and parameterization (P). All profiles took on morning (06:00 LT). Light blue bars indicate biases identified in the ERA reanalysis dataset, while pink bars represent biases in the MERRA reanalysis dataset. The dashed red line marked 'P' denotes biases attributed specifically to the parameterization within the reanalysis models. This analysis uses the DNN to discern the impact of each factor (ranked from highest to lowest) on the discrepancy in cloud fraction estimates between observations and reanalysis models.