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2	Deep Learning Driven Simulations of Boundary Layer Clouds over the Southern
3	Great Plains
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5	Tianning Su <sup>1*</sup> , Yunyan Zhang <sup>1</sup>
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7	<sup>1</sup> Lawrence Livermore National Laboratory, Livermore, CA, USA
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15	*Corresponding authors: <u>sul0@llnl.gov</u>
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Abstract. Based on long-term observations at the Southern Great Plains site by the 23 Atmospheric Radiation Measurement (ARM) program for training and validation, a 24 25 deep learning model is developed to simulate the daytime evolution of boundary-layer clouds (BLCs) from the perspective of land-atmosphere coupling. The model takes 26 27 ARM measurements as inputs including early-morning soundings and the diurnalvarying surface meteorological conditions and heat fluxes and predicts hourly estimates 28 as outputs including the determination of cloud occurrence, the positions of cloud 29 boundaries, and the vertical profile of cloud fraction. The deep learning model offers a 30 31 good agreement with the observed cloud fields, especially on the accuracy in reproducing cloud occurrence and base height. If substituting the inputs by reanalysis 32 data from ERA5 and MERRA-2, the outputs of the deep learning model provide a better 33 34 agreement with observation than the cloud fields extracted from ERA5 and MERRA-2 themselves. From such practice, the deep learning model shows great potential to serve 35 as a diagnostic tool on the performance of physics-based models in simulating 36 37 stratiform and cumulus clouds. By quantifying biases in clouds and attributing them to the simulated atmospheric state variables versus the model parameterized cloud 38 processes, this observation-based deep learning model may offer insights on the 39 directions to improve the simulation of BLCs in physics-based models for weather 40 41 forecasting and climate prediction.

43 **1 Introduction** 

Boundary layer clouds (BLCs), comprising primarily of stratiform and shallow 44 45 cumuli, exert a profound influence on the Earth's radiative balance (Betts, 2009; Teixeira and Hogan, 2002; Lu et al., 2013; Golaz et al., 2002). Their formation and 46 evolution are critically shaped by the interactions between surface, planetary boundary 47 layer (PBL) and free troposphere (Miao et al., 2019; Berg and Kassianov, 2008; Zhang 48 and Klein, 2013; Guo et al., 2017, 2019; Zhang et al., 2017). Numerous studies 49 investigated the controlling factors of BLCs, highlighting the pivotal role of the land 50 51 surface in modulating cloud formation and affecting the spatial and temporal distribution of low clouds (Zhang and Klein, 2010; 2013; Rieck et al., 2014; Xiao et al., 52 2018; Lareau et al., 2018; Lee et al., 2019; Tang et al., 2019; Tao et al., 2019; Tian et 53 54 al., 2022).

These clouds, which frequently form in the PBL's entrainment zone, are very 55 challenging to be simulated in weather prediction and climate modeling due to the small 56 57 scales of their operating physics and the complex feedback mechanisms between land surface fluxes, PBL turbulent processes, and cloud microphysics (Miao et al., 2019; Lu 58 et al., 2011; Fast et al., 2019; Morrison et al. 2020; Yang et al., 2018; Nogherotto et al., 59 2016; Caldwell et al., 2021; Wang et al., 2023; Guo et al., 2019). These challenges are 60 61 compounded when attempting to represent such processes in global and regional climate models, where the fine-scale interactions are often parameterized in a coarse-62 63 resolution grid due to computational constraints (Bretherton et al., 2007; Zheng et al. 2021; Moeng et al., 1996; Randall et al., 2003; Prein et al., 2015). In addition, different 64

cloud regimes exhibit complex nonlinear cloud-land interactions, which pose
challenges for observational studies and modeling efforts, particularly for physical
parameterizations (Tang et al., 2018; Qian et al., 2023; Sakaguchi et al., 2022; Poll et
al., 2022; Tao et al., 2021).

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 72 estimate convection and precipitation, which are crucial for accurate weather 73 forecasting and climate modeling (Mooers et al., 2021; Wang et al., 2020; O'Gorman et 74 al., 2018; Gentine et al., 2018; Zhang et al., 2021). For example, Rasp (2020) presents 75 76 algorithms for the implementation of coupled learning in cloud-resolving models and the super parameterization framework. Similarly, ML tools have been applied to 77 leverage observational data for the refinement of convection parameterizations, offering 78 79 more insights into convective triggering (Zhang et al., 2021). In addition, ML has been used to emulate convection schemes and develop parameterizations using data from 80 81 advanced simulations (O'Gorman and Dwyer, 2018; Gentine et al., 2018). Furthermore, Haynes et al. (2022) develop pixel-based ML-based methods of detecting low clouds, 82 with a focus on improving detection in multilayer cloud situations and specific attention 83 given to improving cloud characteristics. Despite the considerable advancements 84 brought by ML, there are persistent challenges in accurately simulating the vertical 85 structure of clouds, as well as their complex relationships with land surface. 86

87	Southern Great Plains (SGP) site, as part of the U.S. Department of Energy
88	Atmospheric Radiation Measurement (ARM) program, is crucial for cloud evaluation
89	and climatology studies in modeling efforts. Recognized globally as a leading climate
90	research facility, the ARM SGP site (36.607°N, 97.488°W) has been collecting a wealth
91	of meteorological and radiative measurements, offering data that spans over two
92	decades (Sisterson et al., 2016). The rich dataset from the ARM SGP site can help
93	address persistent challenges in cloud modeling. This study leverages these extensive
94	observations to build a deep learning model, serving as an observation-based
95	"emulator" for simulating BLCs. Our model enhances the estimations for cloud fields
96	of BLCs, particularly cloud occurrence, position, and fraction. Furthermore, the critical
97	assessment of our model in comparison with existing reanalysis datasets, including
98	MERRA-2 and ERA5, highlights the improvement in estimating cloud vertical
99	structure. Our study analyzed the model's performance across different cloud regimes,
100	such as stratiform and cumulus. By undertaking this endeavor, we aim to help bridge
101	the existing gaps between field observations and modeling by a deep learning model of
102	BLCs, thereby improving diagnostics of model performance and enriching our
103	understanding of the BLC processes.

# 105 2 Data Description

# 106 **2.1 Observations for the development of the deep learning model**

107 This study utilized the ARM SGP observations during 1998-2020 to serve as108 training, validation, and testing data for the development of the deep learning model.

Note that all the observations are collected at the central facility of SGP, a fixed location,
which is different from other ML studies that use global data from reanalysis or climate
model simulations (e.g., O'Gorman and Dwyer, 2018; Shamekh et al., 2023).

The input data to train and validate the deep learning model include early morning 112 sounding data and diurnal varying surface meteorological conditions and surface 113 turbulent heat fluxes. We take radiosondes (SONDE) measurements around 6 a.m. 114 local time to offer thermodynamic and wind profiles in the PBL and the free atmosphere 115 as initial conditions (Holdridge et al., 2011). SONDE launches typically took place four 116 117 times per day at the SGP site, usually at 00, 06, 12, and 18 local times. Local time, defined as daylight saving time, is used consistently throughout the year. Each morning 118 profile comprises 46 levels spanning from 0-8 km, which include levels at intervals of 119 120 50 meters from 0 to 1 km, 0.1 km from 1 to 2 km, 0.25 km from 2 to 4 km, and 0.5 km from 4.5 to 8 km. Meanwhile, the collocated surface meteorology systems (MET, 121 Ritsche, 2011) provide a variety of meteorological measurements (i.e., temperature, 122 123 relative humidity, wind, and pressure) at the surface. Surface sensible and latent heat fluxes are taken from the ARM value-added product called the best-estimate fluxes 124 from the Bulk Aerodynamic calculations of the Energy Balance Bowen ratio 125 measurements (BAEBBR, Cook, 2018). 126

In addition, we also use derived variables based on observations as the input fields into the deep learning model. LCL is derived from the surface meteorology (Romps, 2017), BLH<sub>parcel</sub> (boundary layer height derived from parcel methods) is calculated from the morning temperature profiles and surface air temperature (Holzworth, 1964; Su and Zhang, 2024; Chu et al., 2019). Specifically, BLH<sub>parcel</sub> is defined as the height where the morning potential temperature profile first exceeds the current surface potential temperature by more than 1.5 K. Meanwhile, BLH<sub>SH</sub> (boundary layer height derived from sensible heat flux) is calculated from the morning temperature profiles and surface sensible heat (Stull, 1988; Su et al., 2023).

For the target data of model outputs to train and validate the deep learning model, 136 our study employs hourly cloud fraction data available from the ARM Best Estimate 137 (ARMBE, Xie et al, 2010) dataset. This cloud fraction is developed based on the Active 138 139 Remote Sensing of Clouds (ARSCL, Clothiaux et al., 2000, 2001; Kollias et al., 2020), which utilizes the best estimates from ceilometer for the lowest cloud bases and 140 integrates micro-pulse lidar, ceilometer, and cloud radar data to define cloud tops and 141 142 cloud fraction. In addition, to construct learning targets, the base of BLC is determined at the lowest altitude where the cloud fraction first exceeds 1 %, and the cloud top is 143 identified at the point where the cloud fraction transitions from exceeding 1 % to falling 144 145 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. However, we do not exclude 146 multiple-layer cloudy cases if their vertical fractions are continuous from the lower to 147 upper layer. 148

Based on ARM observations, this study develops an advanced deep-learning framework to simulate the BLCs, using detailed observational data, including SONDE profiles, surface meteorological measurements, and ARSCL, from the SGP site. This framework is designed for BLCs, placing a particular emphasis on cloud-land coupling mechanisms. By integrating morning SONDE observations with diurnally varying surface fluxes and meteorological data, this deep learning model is capable of diagnosing the initiation and evolution of low clouds, especially those coupled with land surface processes.

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### 158 **2.2** Classification of coupled boundary layer clouds from observations

The deep learning model in this study aims to simulate BLCs strongly coupled with 159 boundary layer and land surface processes. The classification of clouds below is to filter 160 161 the BLCs based on the concept of cloud-land coupling and is important for the training and analysis of the deep learning model. Here, we treat BLCs as synonymous with land-162 coupled clouds, in contrast to clouds that are decoupled from the PBL and land surface. 163 164 Coupled clouds are identified when the cloud base height (CBH), as derived from the ceilometer, aligns with or is below the lidar-detected PBL top height within 0.2 km, 165 and the calculated surface-based Lifting Condensation Level (LCL, Romps, 2017) falls 166 167 within a maximum allowable range of 0.7 km (Su et al., 2022). PBL height data (Su et al., 2020; Roldán-Henao et al., 2024) are available through the ARM database. This 168 alignment is indicative of clouds that are directly influenced by surface-driven 169 processes. Meanwhile, a cloud thickness threshold (< 4 km) is applied to ensure the 170 171 occurrence of BLCs (i.e., not deep convective clouds).

Within the scope of land-coupled clouds, we further classify the observed daytime BLCs into cumulus and stratiform categories following the methodology in Su et al. (2024). Stratiform cloud days are identified by prolonged overcasting conditions during

the daytime, lasting more than three hours, with the maximum cloud fraction exceeding 175 90 % based on ARSCL data. For cumulus cloud days, two criteria are applied: (1) cloud 176 177 formations emerge after sunrise, ensuring that they are driven by local convective processes, and (2) there is an absence of stratiform clouds. Based on these criteria, we 178 179 identified 940 days categorized under the cumulus regime, distributed as 21 %, 56 %, 17 %, and 6 % across Spring, Summer, Fall, and Winter, respectively. Similarly, we 180 identified 657 days falling within the stratiform clouds regime, with respective seasonal 181 distributions of 37 %, 12 %, 23 %, and 28 %. Note that this cloud regime classification 182 183 is done on a daily basis. To maintain clarity in our analysis, we excluded days with mixed cloud regimes, focusing only on days that exhibit only stratiform or cumulus 184 clouds during the daytime. 185

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## 187 **2.3 Reanalysis data for the application of the deep learning model**

To demonstrate how to use the deep learning model, we take advantage of 188 189 reanalysis datasets from the European Centre for Medium-Range Weather Forecasts' fifth-generation global reanalysis (ERA5, Hersbach et al., 2020) and NASA's Modern-190 191 Era Retrospective analysis for Research and Applications Version 2 (MERRA-2, Gelaro et al., 2017). Note that unlike observational data aforementioned, reanalysis data are 192 not used for training the deep learning model, instead they are going to be used to help 193 illustrate how the deep learning model may disentangle the potential causes leading to 194 195 the biased cloud simulations.

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ERA5 provides hourly atmospheric states and cloud fraction around SGP by the

Integrated Forecasting System (IFS) and a data assimilation system at a horizontal resolution of  $0.25^{\circ} \ge 0.25^{\circ}$  and a vertical resolution of 25 hPa in the lower atmosphere (700 - 1000 hPa). IFS employs a prognostic cloud scheme capable of capturing the evolution of cloud dynamics over consecutive time steps (Tiedtke, 1993), a feature that enhances its utility in time-dependent climate studies.

MERRA-2 provides hourly low cloud fraction and 3-hourly vertical cloud fraction profiles at a spatial resolution of  $2/3^{\circ}$  (longitude)  $\times 1/2^{\circ}$  (latitude). MERRA-2 is based on the Goddard Earth Observing System Data Assimilation System Version 5 and utilizes a diagnostic cloud scheme, focusing on the immediate state of clouds (Randles et al., 2017), which are widely used in multiple studies (e.g., Yeo et al., 2022; Kuma, 2020; Miao et al., 2019).

Here we acknowledge the local heterogeneity of cloud fields in the area covered by an ERA5 or MERRA-2 grid cell. This inherent discrepancy between the reanalysis data and the ARM SGP observations may arise from the difference between point-based measurements and area-based assimilated grid-averages. However, observations at the SGP site, representative of plain regions, have been widely used for evaluating models across scales from climatological and statical perspectives (e.g., Song et al., 2014; Zhao et al., 2017; Zheng et al., 2023; Zhang et al., 2017).

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## **3** Construction of the Deep Learning Model for Boundary Layer Clouds

## 217 **3.1 Structure design of the deep learning model**

This study develops an integrated deep learning model to simulate BLC over the SGP site, whose design is illustrated in Fig. 1. Traditionally, simulating BLCs involves solving complex equations related to PBL turbulence and cloud microphysical processes. Our approach, however, leverages deep learning to bypass these intricate simulations. By using module-specific hidden layers, the deep learning model serves as an observation-based "emulator" that directly estimates BLCs from early-morning soundings and surface-related parameters.

The model is purpose-built to consist of three distinct deep learning modules, each 225 responsible for a critical aspect of the cloud simulation: 1) the determination of the 226 227 BLC occurrence, 2) the height position of the cloud base, and 3) the cloud thickness and the normalized 10-layered shape of cloud fraction within cloud boundaries, which 228 jointly yield the hourly-averaged vertical structures of BLCs. This modular approach 229 230 ensures that the estimations are specific for each aspect of the BLCs. Combining cloud 231 thickness and cloud fraction in one module is logical because the thickness for 10layered clouds varies based on cloud thickness, and thickness is potentially related to 232 the fraction, as thicker clouds are sometimes associated with larger cloud fractions. 233 234 Naturally, cloud top is considered as the cloud base plus the thickness. This separation of tasks enhances the overall reliability and clarity of the model in capturing the various 235 236 characteristics of BLCs. Note that each of the three deep learning modules is built upon a deep neural network (DNN) with multiple hidden layers. 237

The occurrence module, as the first step, evaluates the likelihood of cloud 238 formation by producing a number between 0 and 1, which we call "trigger" in the 239 240 following, whose value above 0.5 indicates the presence of clouds. The target data for this module is binary (0 or 1), and the model output is a continuous value between 0 241 and 1. This occurrence information then feeds into the other two modules in parallel: 242 one for locating cloud boundaries and the other for delineating the vertical shape of the 243 cloud fraction in cloudy layers. While the cloud-base (or boundary) module and the 244 fraction-thickness (or fraction) module are independent of each other, they collaborate 245 246 to depict the vertical cloud fraction profile.

To represent the vertical structure of BLC in the fraction-thickness module, we 247 segmented the cloud layer from the base to the top into ten levels, with each level's 248 249 thickness varying according to the overall cloud thickness. These values are then interpolated to create a continuous vertical profile of cloud fraction within the BLC 250 boundaries, offering a detailed depiction of the cloud's vertical extent. The vertical 251 252 position of the layer changes based on the predicted cloud base and top to accurately represent the vertical structure of BLCs. This dynamic approach allows the fraction 253 module to adjust and focus on the relevant portions of cloud fraction within cloudy 254 layers. Compared to a static height-level approach, which requires the prediction of 255 256 cloud fraction across a fixed vertical extent (e.g., multiple levels between 0-6 km), our method focuses on the shape of the fraction profile. This ensures the model is not 257 258 constrained by fixed vertical levels, allowing for more efficient and robust estimations.

#### 260 **3.2 Deep Neural Network (DNN) architecture and configuration**

The construction of the deep learning model uses the TensorFlow Package, 261 262 developed by Google (https://www.tensorflow.org/). Each module in the deep learning model is constructed based on a separate deep neural network (DNN) respectively. The 263 264 DNN architecture is designed, beginning with an input layer reflective of the selected feature set, which includes morning sounding profiles, surface meteorology and heat 265 fluxes data, and the derived variables such as LCL, BLHparcel and BLHSH. For predicting 266 the current hour BLC, the inputs of surface conditions include data both at the current 267 268 hour and the previous hour. The input variables for training and validating the deep learning model are detailed in Table 1, including variable names, descriptions, and data 269 sources, together with the ARMBE cloud fraction profiles as the learning target for 270 271 model outputs. Normalization, a preprocessing technique, was applied to both input and target data to scale them to a zero mean and a standard deviation of one (Klambauer et 272 al. 2017; Salimans and Kingma, 2016; Raju et al. 2020). This standardization ensures 273 274 that the data is scaled to a common range and offers some benefits, such as improving the stability and efficiency of the training process. 275

The architecture of the DNN models was structured and tailored for each module: occurrence, cloud-base, and fraction (or fraction-thickness) estimation. Each module's structure is defined by the number of neurons in its hidden layers. For the occurrence module, the structure consists of four hidden layers with 108, 64, 36, and 24 neurons, respectively. The CBH prediction module is similarly structured with four hidden layers, but consisting of 96, 56, 32, and 24 neurons, respectively. The module for predicting cloud fraction and thickness has a slightly simpler structure, with three hidden layerscontaining 56, 32, and 24 neurons, respectively.

284 As the specific configuration, we utilized the ReLU (Rectified Linear Unit) activation function to introduce non-linearity into the DNN. L2 regularization with a 285 286 strength of 0.01 is applied to mitigate overfitting by penalizing large weights and encouraging simpler models. Batch normalization is implemented at each layer to 287 normalize the inputs, ensuring consistent data distribution and stabilizing the learning 288 process. A dropout rate of 0.2 is used to randomly omit neuron connections during 289 290 training, preventing overfitting and encouraging the network to learn more robust features. The training process was refined with early stopping, ceasing further epochs 291 when the validation loss ceased to improve, and learning rate reduction, systematically 292 293 decreasing the learning rate upon encountering plateaus in performance improvement. These callbacks were instrumental in honing the model's performance, ensuring 294 convergence to the accurate estimation of the BLC. Neuron biases are included in the 295 296 network's architecture and systematically inserted in the hidden layers (Battaglia et al. 2018). The model is compiled using the Adam optimizer with an initial learning rate of 297 0.01. The loss functions used are mean squared error for regression tasks and Binary 298 Cross-Entropy for binary classification tasks. The batch size during training is set to 32. 299 Early stopping with a patience of 37 epochs is implemented to prevent overfitting and 300 to restore the best weights when the validation loss ceases to improve. 301

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### **303 3.3 Model Training Process and Examples**

The construction of the deep learning model commences with the segregation of the ARM observations into a training subset (70 %) and a validation subset (30 %) during 1998-2016. In addition, we save data from 2017-2020 for testing, specifically focusing on this independent period to assess the model's performance. Upon training completion, the model is then evaluated, with its performance metrics examined for accuracy and reliability. This methodical and data-driven process balances complexity with precision, culminating in a robust model capable of simulating BLC features.

311 The modules within the deep learning model operate synergistically, with the predicted occurrence of clouds extending into the modules for cloud base and the 312 vertical structure (i.e., cloud thickness and shape of the cloud fraction profile). As the 313 314 example of the model output, Fig. 2 offers a comparative display of diurnal cloud fraction profiles over the SGP, contrasting the observed data with the simulated clouds 315 by the deep learning model. The model accurately simulates the cloud occurrence and 316 317 the CBH for these cases, aligning well with observations. However, it falls short in simulating the cloud top heights, especially significant overestimates for stratiform 318 clouds. It also underestimates maximum cloud fractions for the stratiform clouds. The 319 observed maximum cloud fraction for stratiform is close to 1, indicating complete 320 coverage, however, such an aspect is not fully replicated by the deep learning model. 321 The third case also falls into the category of stratiform clouds, characterized by an 322 observed cloud fraction exceeding 0.9. However, the presence of multiple local maxima 323 within the cloud fraction profile indicates a relatively complex structure. This 324

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 demonstrate high consistency with
observations, highlighting its value in the cloud simulations.

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## **331 3.4 Calculations of Feature Importance and Performance Metric**

To elucidate the significance of each input 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 for each module within the deep learning model based on whether the module's task is regression (cloud-base and fraction-thickness) or classification (occurrence).

For the modules of cloud-base and fraction-thickness, 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 module using the original, unperturbed validation datasets, which comprise early-morning sounding, surface conditions and the derived variables as the inputs. Then, for every input feature in the validation set, we disrupt its association with the target cloud fields by shuffling its values across all instances, creating a permutation of the dataset. This is executed

while maintaining the original order of other features. When performing the 346 permutation, we shuffle the entire morning profile for each case without altering the 347 348 internal height order of values within the profile. This approach ensures that while profiles are permuted across different cases, the sequential structure of height values 349 within each profile remains intact. This method allows us to assess the importance of 350 the profiles as coherent units, rather than disrupting their vertical structures. 351 Furthermore, we re-run the DNN modules with the shuffled feature and all other 352 features intact as inputs and recalculate the MAE with the new outputs. The difference 353 354 between this new MAE and the baseline MAE represents the feature's importance. To ensure a comprehensive assessment, the permutation and the subsequent MAE 355 calculation are repeated 20 times with different random shuffles for each input feature. 356 357 The final importance score for each feature is then determined as the mean increase in MAE across these permutations. 358

For the module of cloud occurrence, 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:

362 
$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$
(1)

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 368 determining feature importance remain the same between regression tasks and the369 classification task.

After determining the importance scores from the test run, in refining the model, features contributing a negligible or negative effect on performance (i.e., importance scores less than zero) are excluded to ensure only beneficial data is used.

By using this methodology, Fig. 3 illustrates these importance scores from different 373 features, underscoring the most influential factors for predicting the BLC occurrence, 374 the cloud-base, and the thickness and the shape of the vertical fraction of BLCs. These 375 376 factors are ranked from most important factors to least important factors. Notably, the importance scores are not computed as a simple sum but are determined by collectively 377 shuffling groups of features and observing the impact on model performance. The BLC 378 379 trigger of occurrence is a special factor since it is the output of the classification model. The trigger value, which indicates the likelihood of cloud occurrence, is used as an input 380 to the estimations of cloud boundaries and fractions. Sometimes, the trigger value 381 382 hovers around 0.5, indicating uncertainty about the presence of clouds. This situation 383 often corresponds to scenarios like broken clouds or residual clouds, typically associated with relatively small cloud fractions. Incorporating the trigger value as an 384 input for cloud fraction estimation helps the model account for these ambiguous 385 situations, thereby enhancing its ability to estimate cloud fraction. Specifically, only 386 trigger values greater than 0.5 indicate cloud presence and are used for cloud fraction 387 388 predictions. While including the trigger value is beneficial for the cloud fraction model, it does not affect the CBH estimation. 389

In particular, surface relative humidity (RH), surface air temperature (T), and 390 morning relative humidity profiles are highly influential in BLC simulations. This is 391 392 consistent with previous observational and modeling studies (Zhang and Klein, 2013). Surface RH is a critical factor affecting the occurrence, CBH, and cloud fraction 393 predictions. As the input conditions for the DNN modules, early-morning atmospheric 394 profiles of different meteorological parameters (i.e., RH, temperature, and wind 395 components) exert a notable impact on cloud occurrence detection and the 396 determination of cloud fractions. Surface air temperature is shown to have a substantial 397 398 effect on cloud fraction, highlighting the sensitivity of cloud simulations to near-surface thermal conditions. Meanwhile, BLH<sub>parcel</sub> demonstrates a notable impact, which is 399 understandable since the PBLH is a critical factor for the formation of BLCs, and 400 401 BLH<sub>parcel</sub> provides a good representation of PBLH. This approach also recognizes the interconnectedness of certain features and their collective contribution to the model's 402 output. 403

404

## 405 **4** Boundary Layer Cloud Simulations by the Deep Learning Model

# 406 4.1 The Occurrence of Boundary Layer Clouds

The occurrence of BLC is a multifaceted process influenced by a variety of atmospheric parameters and surface processes. As a critical component in the formation of BLCs, we utilize the deep learning model to identify the BLC trigger using morning meteorological profiles and observed surface meteorology and fluxes. Figure 4 showcases the model's proficiency in classifying the occurrences (class 1) and non-

occurrences (class 0) of BLC during both a trained period and an independent period. 412 The classification significantly affects the statistical estimation of cloud fraction, as 413 414 cloud fraction is set to 0 if the trigger is less than 0.5. The confusion matrices (Luque et al. 2019) for the trained period (1998-2016) and for the independent period (2017-415 2020) display the model's predictive performance. The matrices reveal the counts and 416 percentages of TP, FP, TN, and FN. For the training period, we use a 70 % training and 417 30 % validation split to ensure model validation and use the validation dataset to 418 generate the statistics. Meanwhile, for the independence period, we use the full dataset 419 420 for the validation.

421 Figure 4a represents the trained period, the validation datasets show a high percentage of TN at 71.2 % and TP at 21.1 %, indicating that the model is accurate 422 during the period it was trained. For the independent period (2017-2020), the model 423 424 still performs well, with 71.8 % TN and 17.4 % TP (Fig. 4b). However, the rates of FN and FP are slightly higher at 5.6 % and 5.2 % respectively, which could indicate that 425 the model is slightly less accurate when applied to data beyond its training scope. The 426 427 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 independent 428 period. Moreover, for the trained period, the model achieved a high precision of 88.1 % 429 430 and a recall of 81.2 %. For the independent period, the precision and recall remained reasonably high at 76.9 % and 75.6 %, respectively, demonstrating the model's effective 431 generalization to new data. These metrics demonstrate the model's predictive 432 capabilities and reliability for both trained and independent periods. 433

Figure 5 further compares the diurnal frequency of BLC occurrence between 434 observations (OBS) and the DNN predictions for different seasons. The BLC's strong 435 436 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, 437 the model is notably effective in simulating the pronounced diurnal cycle of summer 438 clouds, which are typically influenced by local convection. Conversely, the winter 439 season exhibits a weaker diurnal pattern, likely linked to the diminished surface fluxes. 440 The DNN tends to overestimate BLC presence in the early morning, especially for the 441 442 winter season. The overall alignment between observations and the DNN module represents the model's capability of capturing the diurnal patterns of BLC formation 443 and development. Determining the occurrence of BLC lays the foundation for the 444 445 integrated simulations of BLC features.

446

## 447 **4.2 Cloud Boundaries and Fraction**

A key aspect of cloud modeling involves the accurate simulation of cloud boundaries and fraction, which are indicative of a cloud's vertical extent and fractional coverage at different height levels. Our deep learning model demonstrates capabilities in predicting these key attributes of BLC.

Figure 6 offer the comparisons between observed values and predictions by the DNN for CBH, CTH, and cloud fraction. Similarly, as in Sect. 4.1, these comparisons are presented for both the training period (a, c, e, based on validation datasets) and an independent period (b, d, f), revealing the model's ability to generalize beyond its initial
training data. The DNN model demonstrates remarkable performance in simulating
cloud base, boasting a correlation coefficient surpassing 0.9 and an MAE under 0.15
km. Conversely, the model encounters challenges with CTH prediction, evidenced by
a lower correlation of about 0.5 and a significantly higher MAE between 0.8 and 0.9
km, aligning with case studies in Fig. 2.

461 The discrepancy in accurately simulating CBH and CTH may stem from two main factors. Firstly, observed CBH determinations are generally more precise due to the 462 effectiveness of laser-based methods (Pal et al., 1992), while observed CTH estimations 463 often suffer from reduced accuracy, partly attributed to signal attenuation issues 464 (Clothiaux et al., 2000). For the observed shallow cumulus, cloud top is often 465 contaminated by insect signals, further complicating accurate CTH measurements 466 467 (Chandra et al, 2010). Secondly, our DNN simulations are developed from the perspective of cloud-land coupling, primarily utilizing surface meteorology. This can 468 introduce inherent limitations, as the tops of many clouds may be decoupled from 469 470 surface influences despite a coupled base, potentially leading to gaps in the DNN's ability to accurately define and estimate the cloud top. 471

The comparison of cloud fraction between observations and DNN is presented to consider the model's capability to simulate the vertical distribution of cloud coverage (Fig. 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 476 underestimate the peak cloud fraction, displaying a range up to ~0.8 compared to the 477 478 full 0-1 range observed. This underestimation is intrinsically linked to the model's simulation of cloud boundaries, as both cloud fraction and cloud-base modules operate 479 in tandem. For stratiform clouds, observational data typically exhibit a relatively 480 uniform vertical extent with cloud fractions close to unity at the central height, whereas 481 the DNN model tends to generate a broader, more attenuated profile with a reduced 482 maximum cloud fraction at the center. This points to a need for refining the model's 483 484 ability to replicate the pronounced peak cloud fractions characteristic of stratiform cloud profiles. 485

The diurnal patterns of cloud base and top heights, captured through daily profiles, 486 showcase the model's adeptness at simulating the temporal changes in cloud positions 487 488 for all BLCs, the cumulus regime, and the stratiform regime (as shown in Fig. 7). These profiles, derived from both observational data and DNN outputs, include shaded regions 489 representing the variability (one standard deviation) around the average heights. 490 491 Cumulus clouds exhibit a marked diurnal cycle, whereas stratiform clouds typically maintain a relatively constant cloud boundaries and smaller variations throughout the 492 day. A close alignment is observed between the mean and standard deviation of the 493 494 cloud base between the observed and the simulated data for different cloud regimes. In contrast, while the mean cloud top heights follow a similar diurnal trend in both cases, 495 the observed data exhibits more pronounced variabilities compared to the relatively 496 small variabilities in the DNN simulations. 497

Figures 6 and 7 collectively demonstrate the model's ability to simulate cloud 498 boundaries and fractions within BLC. It reliably captures CBH yet encounters 499 500 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-501 scale models struggle to entirely capture the vertical extent of clouds, as evidenced in 502 Large-Eddy Simulations or Convection-Permitting Models (Zhang et al. 2017; 503 Gustafson et al. 2020; Bogenschutz et al. 2023). In addition to the discussion of deep 504 learning models, we also acknowledge the role of mixed-layer (single-column) models 505 506 in representing boundary layer processes (Lilly 1968, Pelly and Belcher, 2001; Clayson and Chen, 2002; Zhang et al, 2005, 2009; De Roode et al., 2014). Mixed-layer models 507 have several advantages: they are inherently grounded in physical principles and are 508 509 readily integrated into many large-scale models. These models are effective at capturing the diurnal evolution of the PBL given an initial state and time series of surface fluxes. 510 However, the DNN approach offers distinct benefits that complement this theoretical 511 512 approach. DNNs might be able to capture complex, nonlinear relationships between various controlling factors and the cloud fraction. These may be difficult to capture by 513 the single (for the overcast stratocumulus-topped mixed layer) or multiple mixed-layer 514 models (for the broken trade cumulus clouds), which are still subject to assumptions, 515 e.g., on entrainment processes. By training on large observational datasets, DNNs can 516 learn from real-world examples, potentially identifying patterns and relationships not 517 518 explicitly encoded in physical models.

## 520 **5** Application of the Deep Learning Model

## 521 5.1 Integration with Reanalysis Datasets

522 As shown in Sect. 4, the deep learning model can take the conventional meteorological observations (i.e. morning SONDE and surface conditions) as inputs to 523 524 simulate the BLC as outputs, reasonably reproduce a good agreement with the observed vertical structures of BLCs. For its potential application, we may treat it as an "emulator" 525 of the observed relationships between input and output variables. Here we present an 526 example by integrating the deep learning model with ERA5 and MERRA-2 to simulate 527 528 BLC with the input of early-morning profiles and surface conditions from the reanalysis. Here we ask, if inputs are treated as "reality", what would be the expected responding 529 cloud fraction simulated by the deep learning model, an observation-based emulator? 530 531 Following these thoughts, Fig. 8 contrasts diurnal cloud fraction patterns from the observational data and the deep learning model predictions averaged over all conditions 532 of seasons and years. Figure 8a-b present the observed cloud fractions and those 533 simulated by the deep learning using ARM data as inputs, respectively. Panels c and e 534 show the cloud fractions directly extracted from ERA5 and MERRA-2 reanalysis 535 datasets, while panels d and f illustrate the simulated cloud fraction by the deep learning 536 model using inputs from ERA (ERA<sub>DNN</sub>) and MERRA (MERRA<sub>DNN</sub>) reanalysis data. 537 Observing fluctuations in surface temperature and humidity data in ERA5 for this 538 region, we smoothed ERA5 surface air temperature and humidity data with a  $\pm 1$ -hour 539 window to mitigate potential variability from assimilation before using them as input 540 for the DNN modules. To eliminate sampling biases in comparison, we averaged only 541

those samples for which both observations and reanalysis are concurrently available.

Note that here we adopt the deep learning model as a complementary tool rather than a replacement for any existing cloud representations in reanalysis data. The DNN outputs serve a diagnostic purpose, identifying biases in BLCs and aiding in understanding deficiencies within reanalysis data.

The DNN simulations with ARM observations as inputs align closely with the ARM 547 observed cloud fraction profiles within the 0-2 km range, reflecting the model's ability 548 to capture land-coupled clouds. As this model is designed for diagnosing land-coupled 549 550 clouds, the model does not simulate decoupled clouds, which often have bases occurring above 2-km (Su et al., 2022). Original cloud data directly from reanalysis 551 show significant underestimations of BLC fractions, particularly evident in MERRA-2. 552 553 The application of the deep learning model using reanalysis data as inputs enhances cloud fraction estimations compared to the original cloud data directly from reanalysis, 554 demonstrating the DNN model's strength in simulating BLC. Given that the DNN 555 556 model specializes in simulating BLC, when utilizing reanalysis data, the portion of cloud profiles that are decoupled are preserved as they are in the original datasets-that 557 is, for the cloud layers above the BLC-tops or as those clouds rooted above the PBL. 558

559 Furthermore, Fig. 9 provides a detailed examination of stratiform clouds, utilizing 560 the same comparative approach as in Fig. 8. The observed stratiform clouds display a 561 layered structure with expansive coverage and maximum cloud fractions typically 562 exceeding 0.6. The DNN model using ARM data as inputs reproduces these observed 563 characteristics fairly well, albeit with minor overestimations in cloud vertical extent. 564 Conversely, the original ERA5 and MERRA-2 stratiform cloud data exhibit limitations, 565 particularly in underestimating cloud fraction. The integration of the DNN model with 566 reanalysis data as inputs enhances the estimations of stratiform cloud fractions, as 567 depicted in the heatmaps of Fig. 9, showcasing improved agreement with observational 568 data and underscoring the enhancement potential for cloud fraction simulations in 569 reanalysis datasets.

In addition, Fig. 10 extends the comparative study to cumulus clouds. Cumulus 570 clouds pose significant challenges for modeling and parameterization partly due to their 571 572 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 573 et al. 2023; Gustafson et al. 2020). In line with expectations, the original ERA5 and 574 575 MERRA-2 cloud fields exhibit significant biases in representing cumulus clouds when compared to observational data. In contrast, the DNN model with ARM data as inputs 576 achieves commendable success in capturing the diurnal variability of cumulus clouds, 577 578 including cloud base, vertical extension, and cloud fraction, by leveraging local convective signals derived from surface meteorology data. When the DNN model is 579 integrated with ERA5 as inputs, it significantly improves the estimation of vertical 580 cloud fields of cumulus. However, the original MERRA-2 data, which tend to overlook 581 the majority of cumulus clouds, continue to significantly underrepresent them even 582 after the application of DNN, suggesting that additional biases in the input variables 583 such as meteorological factors may contribute to this discrepancy. 584

585 The integration of deep learning with ERA5 and MERRA-2 reanalysis datasets

demonstrates the notable refinement in the simulation of BLC, and achieves moreaccurate estimations of cloud fractions for both stratiform and cumulus clouds.

588

## 589 5.2 Applying Deep Learning for Bias Attribution in Cloud Simulation

We further examine the remaining disparities in cloud fraction simulations within reanalysis datasets, despite the integration of deep learning models (as shown in Figs. 8-10), indicating persisting meteorological biases. Deep learning is utilized to quantify and attribute these biases for BLC simulations.

594 Figure 11 offers a comparative analysis of vertical cloud fraction profiles for both stratiform and cumulus clouds. It presents cloud fractions directly taken from reanalysis 595 data (RD), including ERA5 and MERRA-2, and their corresponding deep learning-596 597 informed simulations. While the application of deep learning to use reanalysis data as inputs (RD<sub>DNN</sub>) yields improvements, remaining cloud biases are evident, particularly 598 in MERRA-2. Acknowledging the significant influence of surface RH on BLC 599 600 simulations (as indicated by Fig. 3e, we refine the inputs into the DNN model by replacing the reanalysis surface RH with the ARM observed surface RH (the model 601 output is labeled as RD<sub>DNN-RH</sub>). This modification leads to a much better simulation for 602 MERRA-2, closing the gap with observational data, especially for stratiform clouds. 603 604 For ERA5, RD<sub>DNN-RH</sub> and RD<sub>DNN</sub> show negligible differences for cumulus clouds, but for stratiform clouds, RD<sub>DNN-RH</sub> also exhibits a reduced bias. These refined profiles of 605 606 cloud fraction attest to the benefits of using the observed surface moisture data as input, confirming its important role in achieving a more accurate representation of BLC. 607

608 With such methodology, we may further dissect the bias in cloud fraction 609 simulations attributed to various meteorological factors and the parameterization 610 schemes within ERA and MERRA reanalysis datasets:

 $Bias due to parameterization = |RD - OBS| - |RD_{DNN} - OBS|$ (2)

612 Bias due to surface 
$$RH = |RD_{DNN} - OBS| - |RD_{DNN-RH} - OBS|$$
 (3)

where RD and OBS are the cloud fraction taken directly from reanalysis data and 613 observations, respectively. The definitions of RD<sub>DNN</sub> and RD<sub>DNN-RH</sub> are the same as the 614 above. For getting a representative value, these biases are layer-averaged from 0-4 km 615 616 over different local times, and then normalized by the observed mean cloud fraction, offering a climatological perspective on the discrepancies between observed and 617 simulated data across seasons and years. For equation (2), we assume that the 618 619 climatology of observations used as input to the DNN model (OBS<sub>DNN</sub>) matches the observed cloud fraction climatology (i.e., OBS<sub>DNN</sub>~OBS), which has been 620 demonstrated in Figs. 9-11. Therefore, we exclude the term representing the difference 621 622 between the DNN-predicted observations and the actual observations. This assumption justifies our approach by ensuring the input observations align with the observed cloud 623 fraction in equations. 624

We get the bias attributed to different meteorological factors and parameterization schemes in the ERA5 and MERRA-2 datasets, respectively (Fig. 12). Each bar indicates the normalized bias contributed by factors such as morning meteorological profiles, surface pressure, surface fluxes, various surface meteorology variables, and parameterization schemes. Notably, parameterization stands out as a significant contributor to bias, accounting for 14.45 % and 19.05 % of the discrepancy in stratiform
clouds between observations versus ERA5 and MERRA-2 respectively. For cumulus
clouds, the parameterization biases are more pronounced, contributing 22.23 % and
30.94 % for ERA5 and MERRA-2, respectively.

In addition to parameterization, RH, RH profiles, and sensible heat are identified as 634 major factors contributing to the differences between observations and reanalysis data. 635 For instance, aligning MERRA-2's RH with observed surface RH could potentially 636 reduce bias by 23.13 % for stratiform and 10.26 % for cumulus clouds. Meanwhile, 637 638 surface RH and morning RH profiles in ERA5 lead to 11.25 % and 3.96 % of biases for the stratiform clouds. The bias between ERA5 and observed cumulus clouds is largely 639 driven by parameterization, which suggests that employing the DNN model with ERA5 640 641 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.

648

649 6. Summary

650 This study has developed a deep learning model to estimate the evolution of BLCs651 over the SGP. The model utilizes over two decades of meteorological data to simulate

BLC formation and characteristics, including the occurrence of BLCs, cloud boundaries, 652 and vertical structures of cloud fraction. As this model is built based on the perspective 653 654 of cloud-land coupling, the DNN approach demonstrates the capability to diagnose land-coupled convective systems from early-morning sounding and surface conditions. 655 The DNN model is built on the cloud-land interactions and serves as the testimony for 656 the coupling between BLCs and the land surface. The proficiency and reliability of the 657 DNN model are evident in its robustness during both the training period and the 658 subsequent independent periods. The deep learning model addresses the simulation of 659 660 cloud vertical structure, among one of the key challenges in physics-based large-scale models. It should be noted that the current DNN model cannot produce detailed cloud 661 microphysics and turbulence information. We propose using the DNN model alongside 662 663 traditional physical models to obtain comprehensive information on BLCs.

The application of this model on the reanalysis datasets like ERA5 and MERRA-2 664 has resulted in enhanced cloud field estimations for stratiform clouds and cumulus, and 665 666 an accurate vertical structure of clouds in terms of climatology, providing a promising diagnostic tool for improving weather forecasting and climate modeling. The deep 667 learning model notably addresses the limitation in cumulus simulations in the reanalysis 668 data, Meanwhile, this approach is much more cost-effective compared to traditional 669 parameterizations and schemes at various scales, as it can simulate two decades of 670 BLCs with vertical information over the SGP within 1-minute using a single GPU node. 671 In addition to the BLC simulations, the deep learning model developed in this study 672 also is used to attribute discrepancies between observational data and reanalysis 673

datasets to different meteorological factors. Besides parameterization, surface RH, morning RH profiles, and surface sensible heat are the three major factors that lead to the mismatches in BLC representation in ERA5 and MERRA-2. These findings underscore the importance of incorporating more accurate humidity information in reanalysis datasets, which is crucial for refining BLC simulations. This analysis also sheds light on the necessity to update reanalysis datasets with improved parameterization of boundary layer convection.

Moving forward, future work is warranted to test and extend this diagnostic tool to 681 682 different synoptic patterns over a large region, which can be integrated into multiplescale models or reanalysis data. However, several challenges need to be addressed to 683 achieve this. One significant limitation is the lack of high-quality, detailed observations 684 685 of clouds and radiosonde profiles globally. This scarcity of data can hinder the model's ability to generalize effectively across different regions. To overcome this, there are 686 several potential strategies. First, using transfer learning techniques can help adapt the 687 688 model trained in one region to other regions with limited data. Integrating data from global observational networks (i.e., ARM) can also create a more diverse and 689 representative training dataset, capturing a wider range of atmospheric conditions and 690 cloud characteristics. Meanwhile, leveraging satellite data can provide broader 691 coverage and enhance the robustness of the model. We plan to explore these approaches 692 in future work to enhance the model's performance and applicability on a global scale. 693

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Code and data availability. The code package of DNN models and for the simulation 696 outputs of BLCs from observed meteorological data and ERA5 and MERRA-2 is 697 the GNU General Public v3.0 698 available under License at https://doi.org/10.5281/zenodo.10719342 (Su, 2024). ARM radiosonde data, surface 699 fluxes. cloud masks available 700 and are at https://adc.arm.gov/discovery/#/results/instrument class code::armbe (ARM 701 user facility, 1994). ARSCL (Active Remote Sensing of Clouds) can be found in 702 703 https://adc.arm.gov/discovery/#/results/instrument class code::arscl (ARM user facility, 1996). MERRA-2 reanalysis data can be downloaded obtained from 704 https://disc.gsfc.nasa.gov/datasets/M2T1NXRAD 5.12.4/summary?keywords%E2%8 705 0%89=%E2%80%89MERRA-2%20tavg1 2d rad Nx (GMAO, 706 2015). ERA5 reanalysis data obtained from 707 are https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-pressure-708 levels?tab=form (Hersbach et al. 2023). 709

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*Author contributions.* TS designed this study and carried out the analysis and model
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project.

714

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717

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# **TABLE LIST:**

**Table 1:** Detailed descriptions of input and output variables used in the deep learning models for predicting boundary layer clouds (BLCs). The table includes the variable names, descriptions, and data sources. For the input parameters, surface meteorology and fluxes are taken from the current and previous hours, while morning profiles comprises 46 values spanning from 0-8 km at 06 LT. Note that the output data is derived from ARSCL (Active Remote Sensing of Clouds). The three outputs correspond to the trigger module, cloud-base module, and fraction-thickness module, respectively.

Variable	Description	Data Source
Input		
Month	Range from 1-12	Time Record
LT	Local Time	Time Record
PS	Pressure at surface level (2m)	Surface Meteorology Station
RH	Relative Humidity at 2m	Surface Meteorology Station
U	Zonal wind at 2m	Surface Meteorology Station
V	Meridional wind at 2m	Surface Meteorology Station
Т	Temperature at 2m	Surface Meteorology Station
LCL	Lifted Condensation Level	Derived from T, RH, PS
SH	Sensible Heat	Energy Balance Bowen Ratio
LH	Latent Heat	Energy Balance Bowen Ratio
<b>RH</b> Profile	Morning RH profiles	Radiosonde
U Profile	Morning U wind profiles	Radiosonde
V Profile	Morning V wind profiles	Radiosonde
θ Profile	Morning potential temperature profiles	Radiosonde
BLH <sub>SH</sub>	PBLH derived from sensible heat	Derived from $\theta$ Profile and SH
<b>BLH</b> <sub>Parcel</sub>	PBLH derived from parcel method	Derived from $\theta$ Profile and T
Output		
Trigger	Cloud occurrence	ARSCL
Position	Cloud-base height	ARSCL
Fraction Profiles	Cloud fraction and thickness	ARSCL



Module 1 output serves as the input for Modules 2-3

1095

Figure 1: Conceptual diagram of the deep learning framework for simulating boundary 1096 layer cloud (BLC) characteristics over the US Southern Great Plains. Inputs for the deep 1097 neural networks (DNN) include morning meteorological profiles from radiosonde 1098 (SONDE), time indicators (i.e., local time and month), and surface conditions such as 1099 fluxes (curved black arrows) and meteorological data. The relevance of relative 1100 humidity (RH) profiles and the planetary boundary layer (PBL) top is emphasized due 1101 to their critical role in BLCs development. These variables are processed through 1102 multiple layers of hidden neurons ( $h_{11}$  to  $h_{MK}$ ). Both input and output parameters are 1103 hourly, except for the morning SONDE. Separate DNN modules are constructed for 1104 each task: Module 1 handles the initiation (trigger) of BLC; Module 2 estimates the 1105 cloud base; and Module 3 estimates cloud fraction and thickness. Together, these 1106 1107 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 occurrence (a), cloud base 1116 1117 height (CBH) (b), and cloud fraction (c) in the deep learning simulations of BLCs. Each panel presents the relative contribution of input features, includes month, local time 1118 (LT), surface pressure (PS), relative humidity (RH), zonal (U) and meridional (V) wind 1119 components, temperature (T), lifting condensation level (LCL), boundary layer height 1120 1121 derived from sensible heat (BLH<sub>SH</sub>) and parcel methods (BLH<sub>Parcel</sub>), sensible heat (SH), latent heat (LH), and morning profiles of relative humidity (R Profile), U wind (U 1122 Profile), V wind (V Profile), and potential temperature ( $\theta$  Profile). These factors are 1123 ranked based on their overall importance. The importance scores are calculated with 1124 permutation method and quantify the relative contribution of each feature to the model's 1125 predictive accuracy. 1126





Figure 4: Confusion matrices on the classification performance of the deep learning 1128 model in predicting the occurrence of boundary layer clouds (BLCs) during the trained 1129 period (1998-2016) in panel (a), and the independent period (2017-2020) in panel (b). 1130 The matrices in the trained period are calculated using the 30 % dataset for the 1131 validation. The matrices in the black color display the counts and percentages of true 1132 1133 positive (TP), false positive (FP), true negative (TN), and false negative (FN) predictions. The overall accuracy, precision, and recall scores for each class are also 1134 included, demonstrating the model's ability in identifying BLC occurrence. 1135



Figure 5. Bar graph comparison on the occurrence frequency of boundary layer clouds
(BLC) between the observed (OBS, red) and the 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).



1145 Figure 6. Scatter density comparison between the observed (OBS) and the predicted 1146 values by the deep learning neural network (DNN) for cloud base height (CBH), cloud top height (CTH), and cloud fraction during the trained period (a, c, e) and an 1147 independent period (b, d, f). Note that the BLC is segmented into ten layers, yielding 1148 ten separate cloud fraction values per BLC instance for analysis. The correlation 1149 coefficient (R) and mean absolute error (MAE) are indicated for each comparison. The 1150 1151 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. 1152



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.** Color 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) using ARM observational data as inputs. (c, e): cloud fractions direcly extracted from ERA and MERRA reanalysis datasets, respectively. (d, f): the cloud fractions simulated by the DNN model using ERA (ERA<sub>DNN</sub>) and MERRA (MERRA<sub>DNN</sub>) data as inputs.



1167 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) 1173 1174 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. 1175 The observed cloud fractions (OBS) are represented by the shaded grey area, illustrating 1176 the averaged cloud coverage recorded by field observations. The original reanalysis 1177 data (RD) is indicated in pink, indicating the baseline cloud fraction profiles as 1178 simulated by the reanalysis. The RD<sub>DNN</sub> profiles in blue depict the new simulation 1179 results after applying the DNN models to the reanalysis data for boundary layer cloud 1180 (BLC) simulation. The RD<sub>DNN-RH</sub> profiles in green show the simulation results when 1181 the surface relative humidity (RH) from the reanalysis data is replaced with observed 1182 values, indicating the impact of accurate surface moisture representation on cloud 1183 fraction simulations. 1184



Figure 12: Attribution of bias between observed and reanalysis on cloud fractions to 1186 various meteorological factors and parameterization schemes for stratiform (a) and 1187 cumulus (b) cloud scenarios. The bars represent the normalized bias (bias divide mean 1188 cloud fraction) contributed by each factor: relative humidity profile (RH), meridional 1189 wind profile (V Profile), temperature profile (T Profile), zonal wind profile (U Profile), 1190 surface pressure (SP), latent heat flux (LH), and parameterization (P). All profiles took 1191 on morning (06:00 LT). Light blue bars indicate biases identified in the ERA reanalysis 1192 dataset, while pink bars represent biases in the MERRA reanalysis dataset. The dashed 1193 red line marked 'P' denotes biases attributed specifically to the parameterization within 1194 1195 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 1196 observations and reanalysis models. 1197