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**Deep Learning Driven Simulations of Boundary Layer Clouds over the Southern  
Great Plains**

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

42

## 43 1 Introduction

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

54 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 scales of their operating physics and the complex feedback mechanisms between land  
57 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 compounded when attempting to represent such processes in global and regional  
61 climate models, where the fine-scale interactions are often parameterized in a coarse-  
62 resolution grid due to computational constraints (Bretherton et al., 2007; Moeng et al.,  
63 1996). In addition, different cloud regimes exhibit complex nonlinear cloud-land  
64 interactions, which pose challenges for observational studies and modeling efforts,

65 particularly for physical parameterizations (Tang et al., 2018; Qian et al., 2023;  
66 Sakaguchi et al., 2022; Poll et al., 2022; Tao et al., 2021).

67 As an emerging tool, machine learning (ML) has been widely employed for a  
68 variety of environmental and atmospheric studies (e.g., McGovern et al., 2017; Gagne  
69 et al., 2019; Vassallo et al., 2020; Cadeddu et al., 2009; Molero et al., 2022; Guo et al.,  
70 2024). Specifically, ML techniques are increasingly being employed to simulate and  
71 estimate convection and precipitation, which are crucial for accurate weather  
72 forecasting and climate modeling (Mooers et al., 2021; Wang et al., 2020; O'Gorman et  
73 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 leverage observational data for the refinement of convection parameterizations, offering  
77 more insights into convective triggering (Zhang et al., 2021). In addition, ML has been  
78 used to emulate convection schemes and develop parameterizations using data from  
79 advanced simulations (O'Gorman and Dwyer, 2018; Gentine et al., 2018). Furthermore,  
80 Haynes et al. (2022) develop pixel-based ML-based methods of detecting low clouds,  
81 with a focus on improving detection in multilayer cloud situations and specific attention  
82 given to improving cloud characteristics. Despite the considerable advancements  
83 brought by ML, there are persistent challenges in accurately simulating the vertical  
84 structure of clouds, as well as their complex relationships with land surface.

85 Southern Great Plains (SGP) site, as part of the U.S. Department of Energy  
86 Atmospheric Radiation Measurement (ARM) program, is crucial for cloud evaluation

87 and climatology studies in modeling efforts. Recognized globally as a leading climate  
88 research facility, the ARM SGP site (36.607°N, 97.488°W) has been collecting a wealth  
89 of meteorological and radiative measurements, offering data that spans over two  
90 decades (Sisterson et al. 2016). The rich dataset from the ARM SGP site can help  
91 address persistent challenges in cloud modeling. This study leverages these extensive  
92 observations to build a deep learning model, serving as an observation-based  
93 "emulator" for simulating BLCs. Our model enhances the estimations for cloud fields  
94 of BLCs, particularly cloud occurrence, position, and fraction. Furthermore, the critical  
95 assessment of our model in comparison with existing reanalysis datasets, including  
96 MERRA-2 and ERA-5, highlights the improvement in estimating cloud vertical  
97 structure. Our study analyzed the model's performance across different cloud regimes,  
98 such as stratiform and cumulus. By undertaking this endeavor, we aim to help bridge  
99 the existing gaps between field observations and modeling by a deep learning model of  
100 BLCs, thereby improving diagnostics of model performance and enriching our  
101 understanding of the BLC processes.

102

## 103 **2 Data Description**

### 104 **2.1 Observations for the development of the deep learning model**

105 This study utilized the ARM SGP observations during 1998-2020 to serve as  
106 training, validation, and testing data for the development of the deep learning model.  
107 Note that all the observations are collected at the central facility of SGP, a fixed location,  
108 which is different from other ML studies that use global data from reanalysis or climate

109 model simulations (e.g., O’Gorman and Dwyer, 2018; Shamekh et al. 2023).

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

125 In addition, we also use derived variables based on observations as the input fields  
126 into the deep learning model. LCL is derived from the surface meteorology (Romps,  
127 2017),  $BLH_{\text{parcel}}$  (boundary layer height derived from parcel methods) is calculated  
128 from the morning temperature profiles and surface air temperature (Holzworth, 1964;  
129 Su and Zhang, 2024). Specifically,  $BLH_{\text{parcel}}$  is defined as the height where the morning  
130 potential temperature profile first exceeds the current surface potential temperature by

131 more than 1.5 K. Meanwhile,  $BLH_{SH}$  (boundary layer height derived from sensible heat  
132 flux) is calculated from the morning temperature profiles and surface sensible heat  
133 (Stull, 1988; Su et al. 2023).

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

147 Based on ARM observations, this study develops an advanced deep-learning  
148 framework to simulate the BLCs, using detailed observational data, including SONDE  
149 profiles, surface meteorological measurements, and ARSCL, from the SGP site. This  
150 framework is designed for BLCs, placing a particular emphasis on cloud-land coupling  
151 mechanisms. By integrating morning SONDE observations with diurnally varying  
152 surface fluxes and meteorological data, this deep learning model is capable of

153 diagnosing the initiation and evolution of low clouds, especially those coupled with  
154 land surface processes.

155

## 156 **2.2 Classification of coupled boundary layer clouds from observations**

157 The deep learning model in this study aims to simulate BLCs strongly coupled with  
158 boundary layer and land surface processes. The classification of clouds below is to filter  
159 the BLCs based on the concept of cloud-land coupling and is important for the training  
160 and analysis of the deep learning model. Here, we treat BLCs as synonymous with land-  
161 coupled clouds, in contrast to clouds that are decoupled from the PBL and land surface.

162 Coupled clouds are identified when the cloud base height (CBH), as derived from  
163 the ceilometer, aligns with or is below the lidar-detected PBL top height within 0.2 km,  
164 and the calculated surface-based Lifting Condensation Level (LCL, Romps 2017) falls  
165 within a maximum allowable range of 0.7 km (Su et al. 2022). PBL height data  
166 (<https://doi.org/10.5439/2007149>, Su et al. 2020) are publicly available through the  
167 ARM database. This alignment is indicative of clouds that are directly influenced by  
168 surface-driven processes. Meanwhile, a cloud thickness threshold ( $< 4$  km) is applied  
169 to ensure the occurrence of BLCs (i.e., not deep convective clouds).

170 Within the scope of land-coupled clouds, we further classify the observed daytime  
171 BLCs into cumulus and stratiform categories following the methodology in Su et al.  
172 (2024). Stratiform cloud days are identified by prolonged overcasting conditions during  
173 the daytime, lasting more than three hours, with the maximum cloud fraction exceeding  
174 90% based on ARSCL data. For cumulus cloud days, two criteria are applied: (1) cloud



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

184

### 185 **2.3 Reanalysis data for the application of the deep learning model**

186 To demonstrate how to use the deep learning model, we take advantage of  
187 reanalysis datasets from the European Centre for Medium-Range Weather Forecasts'  
188 fifth-generation global reanalysis (ERA-5, Hersbach et al., 2020) and NASA's Modern-  
189 Era Retrospective analysis for Research and Applications Version 2 (MERRA-2, Gelaro  
190 et al., 2017). Note that unlike observational data aforementioned, reanalysis data are  
191 not used for training the deep learning model, instead they are going to be used to help  
192 illustrate how the deep learning model may disentangle the potential causes leading to  
193 the biased cloud simulations.

194 ERA-5 provides hourly atmospheric states and cloud fraction around SGP by  
195 the Integrated Forecasting System (IFS) and a data assimilation system at a horizontal  
196 resolution of  $0.25^\circ \times 0.25^\circ$  and a vertical resolution of 25 hPa in the lower atmosphere

197 (700 – 1000 hPa). IFS employs a prognostic cloud scheme capable of capturing the  
198 evolution of cloud dynamics over consecutive time steps (Tiedtke 1993), a feature that  
199 enhances its utility in time-dependent climate studies.

200 MERRA-2 provides hourly low cloud fraction and 3-hourly vertical cloud  
201 fraction profiles at a spatial resolution of  $2/3^\circ$  (longitude)  $\times$   $1/2^\circ$  (latitude). MERRA-  
202 2 is based on the Goddard Earth Observing System Data Assimilation System Version  
203 5 and utilizes a diagnostic cloud scheme, focusing on the immediate state of clouds  
204 (Randles et al., 2017), which are widely used in multiple studies (e.g., Yeo et al., 2022;  
205 Kuma, 2020; Miao et al., 2019).

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

213

### 214 **3 Construction of the Deep Learning Model for Boundary Layer Clouds**

#### 215 **3.1 Structure design of the deep learning model**

216 This study develops an integrated deep learning model to simulate BLC over the  
217 SGP site, whose design is illustrated in Figure 1. Traditionally, simulating BLCs  
218 involves solving complex equations related to PBL turbulence and cloud microphysical

219 processes. Our approach, however, leverages deep learning to bypass these intricate  
220 simulations. By using module-specific hidden layers, the deep learning model serves as  
221 an observation-based "emulator" that directly estimates BLCs from early-morning  
222 soundings and surface-related parameters.

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

236 The occurrence module, as the first step, evaluates the likelihood of cloud  
237 formation by producing a number between 0 and 1, which we call "trigger" in the  
238 following, whose value above 0.5 indicates the presence of clouds. The target data for  
239 this module is binary (0 or 1), and the model output is a continuous value between 0  
240 and 1. This occurrence information then feeds into the other two modules in parallel:

241 one for locating cloud boundaries and the other for delineating the vertical shape of the  
242 cloud fraction in cloudy layers. While the cloud-base (or boundary) module and the  
243 fraction-thickness (or fraction) module are independent of each other, they collaborate  
244 to depict the vertical cloud fraction profile.

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

257

### 258 **3.2 Deep Neural Network (DNN) architecture and configuration**

259 The construction of the deep learning model uses the TensorFlow Package,  
260 developed by Google (<https://www.tensorflow.org/>). Each module in the deep learning  
261 model is constructed based on a separate deep neural network (DNN) respectively. The  
262 DNN architecture is designed, beginning with an input layer reflective of the selected

263 feature set, which includes morning sounding profiles, surface meteorology and heat  
264 fluxes data, and the derived variables such as LCL,  $BLH_{\text{parcel}}$  and  $BLH_{\text{SH}}$ . For predicting  
265 the current hour BLC, the inputs of surface conditions include data both at the current  
266 hour and the previous hour. The input variables for training and validating the deep  
267 learning model are detailed in Table 1, including variable names, descriptions, and data  
268 sources, together with the ARMBE cloud fraction profiles as the learning target for  
269 model outputs. Normalization, a preprocessing technique, was applied to both input and  
270 target data to scale them to a zero mean and a standard deviation of one (Klambauer et  
271 al. 2017; Salimans and Kingma, 2016; Raju et al. 2020). This standardization ensures  
272 that the data is scaled to a common range and offers some benefits, such as improving  
273 the stability and efficiency of the training process.

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

282 As the specific configuration, we utilized the ReLU (Rectified Linear Unit)  
283 activation function to introduce non-linearity into the DNN. L2 regularization with a  
284 strength of 0.01 is applied to mitigate overfitting by penalizing large weights and

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

300

### 301 **3.3 Model Training Process and Examples**

302 The construction of the deep learning model commences with the segregation of the  
303 ARM observations into a training subset (70%) and a validation subset (30%) during  
304 1998-2016. In addition, we save data from 2017-2020 for testing, specifically focusing  
305 on this independent period to assess the model's performance. Upon training completion,  
306 the model is then evaluated, with its performance metrics examined for accuracy and

307 reliability. This methodical and data-driven process balances complexity with precision,  
308 culminating in a robust model capable of simulating BLC features.

309 The modules within the deep learning model operate synergistically, with the  
310 predicted occurrence of clouds extending into the modules for cloud base and the  
311 vertical structure (i.e., cloud thickness and shape of the cloud fraction profile). As the  
312 example of the model output, Figure 2 offers a comparative display of diurnal cloud  
313 fraction profiles over the SGP, contrasting the observed data with the simulated clouds  
314 by the deep learning model. The model accurately simulates the cloud occurrence and  
315 the CBH for these cases, aligning well with observations. However, it falls short in  
316 simulating the cloud top heights, especially significant overestimates for stratiform  
317 clouds. It also underestimates maximum cloud fractions for the stratiform clouds. The  
318 observed maximum cloud fraction for stratiform is close to 1, indicating complete  
319 coverage, however, such an aspect is not fully replicated by the deep learning model.  
320 The third case also falls into the category of stratiform clouds, characterized by an  
321 observed cloud fraction exceeding 0.9. However, the presence of multiple local maxima  
322 within the cloud fraction profile indicates a relatively complex structure. This  
323 complexity poses a challenge to the model, as the DNN is not fully capable of capturing  
324 the internal variations within the convective system. Instead, the model tends to produce  
325 a more uniform cloud fraction across this convective system. Despite these variances,  
326 the model-derived cloud bases and occurrence demonstrate high consistency with  
327 observations, highlighting its value in the cloud simulations.

328

### 329 **3.4 Calculations of Feature Importance and Performance Metric**

330 To elucidate the significance of each input variable within our deep learning models,  
331 we implemented a permutation importance analysis. This robust, model-agnostic  
332 technique assesses each feature's influence on the model's predictive accuracy, which  
333 is crucial for assessing DNN (Date and Kikuchi, 2018; Altmann et al. 2010). In this  
334 study, the permutation importance method differs slightly for each module within the  
335 deep learning model based on whether the module's task is regression (cloud-base and  
336 fraction-thickness) or classification (occurrence).

337 For the modules of cloud-base and fraction-thickness, which are regression tasks,  
338 the Mean Absolute Error (MAE) serves as the performance metric. First, we perform a  
339 test run to establish a baseline performance by calculating the MAE of the module using  
340 the original, unperturbed validation datasets, which comprise early-morning sounding,  
341 surface conditions and the derived variables as the inputs. Then, for every input feature  
342 in the validation set, we disrupt its association with the target cloud fields by shuffling  
343 its values across all instances, creating a permutation of the dataset. This is executed  
344 while maintaining the original order of other features. When performing the  
345 permutation, we shuffle the entire morning profile for each case without altering the  
346 internal height order of values within the profile. This approach ensures that while  
347 profiles are permuted across different cases, the sequential structure of height values  
348 within each profile remains intact. This method allows us to assess the importance of  
349 the profiles as coherent units, rather than disrupting their vertical structures.



350 Furthermore, we re-run the DNN modules with the shuffled feature and all other  
351 features intact as inputs and recalculate the MAE with the new outputs. The difference  
352 between this new MAE and the baseline MAE represents the feature's importance. To  
353 ensure a comprehensive assessment, the permutation and the subsequent MAE  
354 calculation are repeated 20 times with different random shuffles for each input feature.  
355 The final importance score for each feature is then determined as the mean increase in  
356 MAE across these permutations.

357 For the module of cloud occurrence, which is a classification task, the accuracy  
358 score is used as the performance metric. The accuracy score is a measure of the model's  
359 overall correctness and is calculated using the formula:

$$360 \quad Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \quad (1)$$

361 where True Positives (TP) indicates the number of instances correctly predicted as  
362 positive; true Negatives (TN) indicates the number of instances correctly predicted as  
363 negative; False Positives (FP) indicates the number of instances incorrectly predicted  
364 as positive, and False Negatives (FN) indicates the number of instances incorrectly  
365 predicted as negative. After determining the performance metric, other procedures for  
366 determining feature importance remain the same between regression tasks and the  
367 classification task.

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

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

388 In particular, surface relative humidity (RH), surface air temperature (T), and  
389 morning relative humidity profiles are highly influential in BLC simulations. This is  
390 consistent with previous observational and modeling studies (Zhang and Klein, 2013).  
391 Surface RH is a critical factor affecting the occurrence, CBH, and cloud fraction  
392 predictions. As the input conditions for the DNN modules, early-morning atmospheric

393 profiles of different meteorological parameters (i.e., RH, temperature, and wind  
394 components) exert a notable impact on cloud occurrence detection and the  
395 determination of cloud fractions. Surface air temperature is shown to have a substantial  
396 effect on cloud fraction, highlighting the sensitivity of cloud simulations to near-surface  
397 thermal conditions. Meanwhile,  $BLH_{\text{parcel}}$  demonstrates a notable impact, which is  
398 understandable since the PBLH is a critical factor for the formation of BLCs, and  
399  $BLH_{\text{parcel}}$  provides a good representation of PBLH. This approach also recognizes the  
400 interconnectedness of certain features and their collective contribution to the model's  
401 output.

402

## 403 **4 Boundary Layer Cloud Simulations by the Deep Learning Model**

### 404 **4.1 The Occurrence of Boundary Layer Clouds**

405 The occurrence of BLC is a multifaceted process influenced by a variety of  
406 atmospheric parameters and surface processes. As a critical component in the formation  
407 of BLCs, we utilize the deep learning model to identify the BLC trigger using morning  
408 meteorological profiles and observed surface meteorology and fluxes. Figure 4  
409 showcases the model's proficiency in classifying the occurrences (class 1) and non-  
410 occurrences (class 0) of BLC during both a trained period and an independent period.  
411 The classification significantly affects the statistical estimation of cloud fraction, as  
412 cloud fraction is set to 0 if the trigger is less than 0.5. The confusion matrices (Luque  
413 et al. 2019) for the trained period (1998-2016) and for the independent period (2017-  
414 2020) display the model's predictive performance. The matrices reveal the counts and

415 percentages of TP, FP, TN, and FN. For the training period, we use a 70% training and  
416 30% validation split to ensure model validation and use the validation dataset to  
417 generate the statistics. Meanwhile, for the independence period, we use the full dataset  
418 for the validation.

419 Figure 4a represents the trained period, the validation datasets show a high  
420 percentage of TN at 71.2% and TP at 21.1%, indicating that the model is accurate during  
421 the period it was trained. For the independent period (2017-2020), the model still  
422 performs well, with 71.8% TN and 17.4% TP (Figure 4b). However, the rates of FN and  
423 FP are slightly higher at 5.6% and 5.2% respectively, which could indicate that the  
424 model is slightly less accurate when applied to data beyond its training scope. The table  
425 highlights the model's robustness, with overall accuracy rates of 92.3% for the trained  
426 period and a slightly reduced but still substantial 89.2% for the independent period.  
427 Moreover, for the trained period, the model achieved a high precision of 88.1% and a  
428 recall of 81.2%. For the independent period, the precision and recall remained  
429 reasonably high at 76.9% and 75.6%, respectively, demonstrating the model's effective  
430 generalization to new data. These metrics demonstrate the model's predictive  
431 capabilities and reliability for both trained and independent periods.

432 Figure 5 further compares the diurnal frequency of BLC occurrence between  
433 observations (OBS) and the DNN predictions for different seasons. The BLC's strong  
434 diurnal pattern is well-captured by the model, when BLC development peaks between  
435 12-16 local times, aligning closely with observed frequencies. Among different seasons,  
436 the model is notably effective in simulating the pronounced diurnal cycle of summer

437 clouds, which are typically influenced by local convection. Conversely, the winter  
438 season exhibits a weaker diurnal pattern, likely linked to the diminished surface fluxes.  
439 The DNN tends to overestimate BLC presence in the early morning, especially for the  
440 winter season. The overall alignment between observations and the DNN module  
441 represents the model's capability of capturing the diurnal patterns of BLC formation  
442 and development. Determining the occurrence of BLC lays the foundation for the  
443 integrated simulations of BLC features.

444

#### 445 **4.2 Cloud Boundaries and Fraction**

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

450 Figure 6 offer the comparisons between observed values and predictions by the  
451 DNN for CBH, CTH, and cloud fraction. Similarly, as in Section 4.1, these comparisons  
452 are presented for both the training period (a, c, e, based on validation datasets) and an  
453 independent period (b, d, f), revealing the model's ability to generalize beyond its initial  
454 training data. The DNN model demonstrates remarkable performance in simulating  
455 cloud base, boasting a correlation coefficient surpassing 0.9 and an MAE under 0.15  
456 km. Conversely, the model encounters challenges with CTH prediction, evidenced by

457 a lower correlation of about 0.5 and a significantly higher MAE between 0.8 and 0.9  
458 km, aligning with case studies in Figure 2.

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

470 The comparison of cloud fraction between observations and DNN is presented to  
471 consider the model's capability to simulate the vertical distribution of cloud coverage  
472 (Figure 6e-f). The scatterplots comparing observed and modeled cloud fractions at  
473 individual levels in cloudy scenarios show a satisfactory correlation, with an R-value  
474 exceeding 0.77 and an MAE around 0.15. Nevertheless, the DNN model tends to  
475 underestimate the peak cloud fraction, displaying a range up to ~0.8 compared to the  
476 full 0-1 range observed. This underestimation is intrinsically linked to the model's  
477 simulation of cloud boundaries, as both cloud fraction and cloud-base modules operate

478 in tandem. For stratiform clouds, observational data typically exhibit a relatively  
479 uniform vertical extent with cloud fractions close to unity at the central height, whereas  
480 the DNN model tends to generate a broader, more attenuated profile with a reduced  
481 maximum cloud fraction at the center. This points to a need for refining the model's  
482 ability to replicate the pronounced peak cloud fractions characteristic of stratiform  
483 cloud profiles.

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

496 Figures 6 and 7 collectively demonstrate the model's ability to simulate cloud  
497 boundaries and fractions within BLC. It reliably captures CBH yet encounters  
498 challenges with accurately representing cloud top heights and peak cloud fractions on

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

517

## 518 **5 Application of the Deep Learning Model**

### 519 **5.1 Integration with Reanalysis Datasets**

520 As shown in Section 4, the deep learning model can take the conventional



521 meteorological observations (i.e. morning SONDE and surface conditions) as inputs to  
522 simulate the BLC as outputs, reasonably reproduce a good agreement with the observed  
523 vertical structures of BLCs. For its potential application, we may treat it as an “emulator”  
524 of the observed relationships between input and output variables. Here we present an  
525 example by integrating the deep learning model with ERA-5 and MERRA-2 to simulate  
526 BLC with the input of early-morning profiles and surface conditions from the reanalysis.  
527 Here we ask, if inputs are treated as “reality”, what would be the expected responding  
528 cloud fraction simulated by the deep learning model, an observation-based emulator?

529       Following these thoughts, Figure 8 contrasts diurnal cloud fraction patterns from  
530 the observational data and the deep learning model predictions averaged over all  
531 conditions of seasons and years. Figure 8a-b present the observed cloud fractions and  
532 those simulated by the deep learning using ARM data as inputs, respectively. Panels c  
533 and e show the cloud fractions directly extracted from ERA-5 and MERRA-2 reanalysis  
534 datasets, while panels d and f illustrate the simulated cloud fraction by the deep learning  
535 model using inputs from ERA (ERA<sub>DNN</sub>) and MERRA (MERRA<sub>DNN</sub>) reanalysis data.  
536 Observing fluctuations in surface temperature and humidity data in ERA-5 for this  
537 region, we smoothed ERA-5 surface air temperature and humidity data with a  $\pm 1$ -hour  
538 window to mitigate potential variability from assimilation before using them as input  
539 for the DNN modules. To eliminate sampling biases in comparison, we averaged only  
540 those samples for which both observations and reanalysis are concurrently available.

541       Note that here we adopt the deep learning model as a complementary tool rather  
542 than a replacement for any existing cloud representations in reanalysis data. The DNN

543 outputs serve a diagnostic purpose, identifying biases in BLCs and aiding in  
544 understanding deficiencies within reanalysis data.

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

557 Furthermore, Figure 9 provides a detailed examination of stratiform clouds,  
558 utilizing the same comparative approach as in Figure 8. The observed stratiform clouds  
559 display a layered structure with expansive coverage and maximum cloud fractions  
560 typically exceeding 0.6. The DNN model using ARM data as inputs reproduces these  
561 observed characteristics fairly well, albeit with minor overestimations in cloud vertical  
562 extent. Conversely, the original ERA-5 and MERRA-2 stratiform cloud data exhibit  
563 limitations, particularly in underestimating cloud fraction. The integration of the DNN  
564 model with reanalysis data as inputs enhances the estimations of stratiform cloud

565 fractions, as depicted in the heatmaps of Figure 9, showcasing improved agreement  
566 with observational data and underscoring the enhancement potential for cloud fraction  
567 simulations in reanalysis datasets.

568 In addition, Figure 10 extends the comparative study to cumulus clouds. Cumulus  
569 clouds pose significant challenges for modeling and parameterization partly due to their  
570 typically small spatial extent compared to the model grid, often spanning from a few  
571 hundred meters to several kilometers (Zhang et al. 2017; Tao et al., 2021; Bogenschutz  
572 et al. 2023; Gustafson et al. 2020). In line with expectations, the original ERA-5 and  
573 MERRA-2 cloud fields exhibit significant biases in representing cumulus clouds when  
574 compared to observational data. In contrast, the DNN model with ARM data as inputs  
575 achieves commendable success in capturing the diurnal variability of cumulus clouds,  
576 including cloud base, vertical extension, and cloud fraction, by leveraging local  
577 convective signals derived from surface meteorology data. When the DNN model is  
578 integrated with ERA-5 as inputs, it significantly improves the estimation of vertical  
579 cloud fields of cumulus. However, the original MERRA-2 data, which tend to overlook  
580 the majority of cumulus clouds, continue to significantly underrepresent them even  
581 after the application of DNN, suggesting that additional biases in the input variables  
582 such as meteorological factors may contribute to this discrepancy.

583 The integration of deep learning with ERA-5 and MERRA-2 reanalysis datasets  
584 demonstrates the notable refinement in the simulation of BLC, and achieves more  
585 accurate estimations of cloud fractions for both stratiform and cumulus clouds.

586

## 587 5.2 Applying Deep Learning for Bias Attribution in Cloud Simulation

588 We further examine the remaining disparities in cloud fraction simulations within  
589 reanalysis datasets, despite the integration of deep learning models (as shown in Figures  
590 8-10), indicating persisting meteorological biases. Deep learning is utilized to quantify  
591 and attribute these biases for BLC simulations.

592 Figure 11 offers a comparative analysis of vertical cloud fraction profiles for both  
593 stratiform and cumulus clouds. It presents cloud fractions directly taken from reanalysis  
594 data (RD), including ERA-5 and MERRA-2, and their corresponding deep learning-  
595 informed simulations. While the application of deep learning to use reanalysis data as  
596 inputs ( $RD_{DNN}$ ) yields improvements, remaining cloud biases are evident, particularly  
597 in MERRA-2. Acknowledging the significant influence of surface RH on BLC  
598 simulations (as indicated by Figure 3e, we refine the inputs into the DNN model by  
599 replacing the reanalysis surface RH with the ARM observed surface RH (the model  
600 output is labeled as  $RD_{DNN-RH}$ ). This modification leads to a much better simulation for  
601 MERRA-2, closing the gap with observational data, especially for stratiform clouds.  
602 For ERA-5,  $RD_{DNN-RH}$  and  $RD_{DNN}$  show negligible differences for cumulus clouds, but  
603 for stratiform clouds,  $RD_{DNN-RH}$  also exhibits a reduced bias. These refined profiles of  
604 cloud fraction attest to the benefits of using the observed surface moisture data as input,  
605 confirming its important role in achieving a more accurate representation of BLC.

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

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

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

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

623 We get the bias attributed to different meteorological factors and parameterization  
 624 schemes in the ERA-5 and MERRA-2 datasets, respectively (Figure 12). Each bar  
 625 indicates the normalized bias contributed by factors such as morning meteorological  
 626 profiles, surface pressure, surface fluxes, various surface meteorology variables, and  
 627 parameterization schemes. Notably, parameterization stands out as a significant  
 628 contributor to bias, accounting for 14.45% and 19.05% of the discrepancy in stratiform  
 629 clouds between observations versus ERA-5 and MERRA-2 respectively. For cumulus  
 630 clouds, the parameterization biases are more pronounced, contributing 22.23% and

631 30.94% for ERA-5 and MERRA-2, respectively.

632 In addition to parameterization, RH, RH profiles, and sensible heat are identified as  
633 major factors contributing to the differences between observations and reanalysis data.  
634 For instance, aligning MERRA-2's RH with observed surface RH could potentially  
635 reduce bias by 23.13% for stratiform and 10.26% for cumulus clouds. Meanwhile,  
636 surface RH and morning RH profiles in ERA-5 lead to 11.25% and 3.96% of biases for  
637 the stratiform clouds. The bias between ERA-5 and observed cumulus clouds is largely  
638 driven by parameterization, which suggests that employing the DNN model with ERA-  
639 5 can lead to a more accurate simulation of cumulus clouds.

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

646

## 647 **6. Summary**

648 This study has developed a deep learning model to estimate the evolution of BLCs  
649 over the SGP. The model utilizes over two decades of meteorological data to simulate  
650 BLC formation and characteristics, including the occurrence of BLCs, cloud boundaries,  
651 and vertical structures of cloud fraction. As this model is built based on the perspective  
652 of cloud-land coupling, the DNN approach demonstrates the capability to diagnose

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

662 The application of this model on the reanalysis datasets like ERA-5 and MERRA-  
663 2 has resulted in enhanced cloud field estimations for stratiform clouds and cumulus,  
664 and an accurate vertical structure of clouds in terms of climatology, providing a  
665 promising diagnostic tool for improving weather forecasting and climate modeling. The  
666 deep learning model notably addresses the limitation in cumulus simulations in the  
667 reanalysis data, Meanwhile, this approach is much more cost-effective compared to  
668 traditional parameterizations and schemes at various scales, as it can simulate two  
669 decades of BLCs with vertical information over the SGP within 1-minute using a single  
670 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,  
674 morning RH profiles, and surface sensible heat are the three major factors that lead to

675 the mismatches in BLC representation in ERA-5 and MERRA-2. These findings  
676 underscore the importance of incorporating more accurate humidity information in  
677 reanalysis datasets, which is crucial for refining BLC simulations. This analysis also  
678 sheds light on the necessity to update reanalysis datasets with improved  
679 parameterization of boundary layer convection.

680 Moving forward, future work is warranted to test and extend this diagnostic tool to  
681 different synoptic patterns over a large region, which can be integrated into multiple-  
682 scale 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 of clouds and radiosonde profiles globally. This scarcity of data can hinder the model's  
685 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 model trained in one region to other regions with limited data. Integrating data from  
688 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

694

695 ***Code and data availability.*** The code package of DNN models and for the simulation  
696 outputs of BLCs from observed meteorological data and ERA-5 and MERRA-2 is  
697 available under the GNU General Public License v3.0 at



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707 [levels?tab=form](https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-pressure-levels?tab=form) (Hersbach et al. 2023).  
708

709

710 ***Author contributions.*** TS designed this study and carried out the analysis and model  
711 training. TS and YZ interpreted the data and wrote the manuscript. YZ supervised the  
712 project.

713

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727

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1050 **TABLE LIST:**

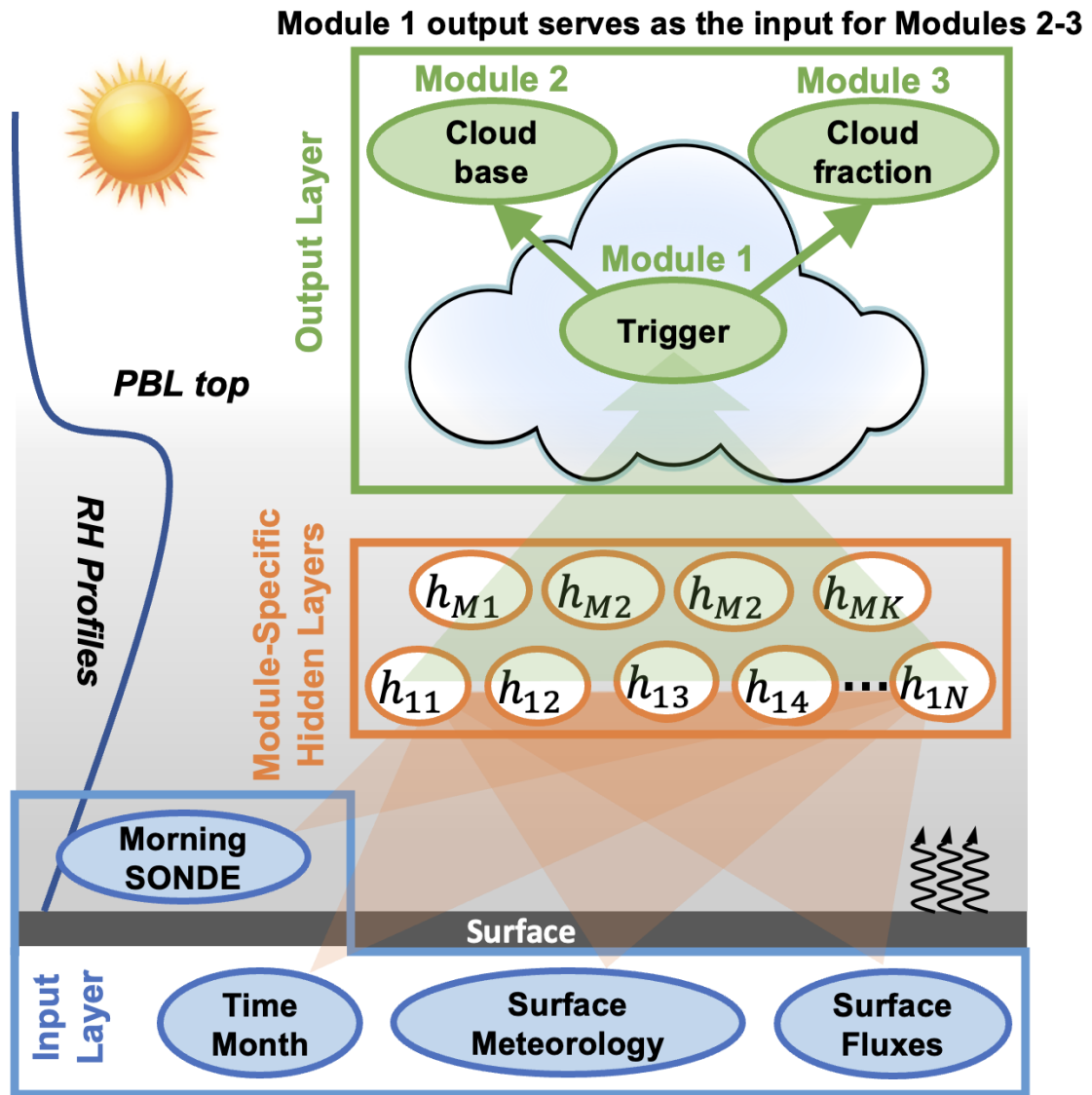
1051 **Table 1:** Detailed descriptions of input and output variables used in the deep learning  
 1052 models for predicting boundary layer clouds (BLCs). The table includes the variable  
 1053 names, descriptions, and data sources. For the input parameters, surface meteorology  
 1054 and fluxes are taken from the current and previous hours, while morning profiles  
 1055 comprises 46 values spanning from 0-8 km at 06 LT. Note that the output data is derived  
 1056 from ARSCL (Active Remote Sensing of Clouds). The three outputs correspond to the  
 1057 trigger module, cloud-base module, and fraction-thickness module, respectively.

<b>Variable</b>	<b>Description</b>	<b>Data Source</b>
<b><i>Input</i></b>		
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
T	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
RH Profile	Morning RH profiles	Radiosonde
U Profile	Morning U wind profiles	Radiosonde
V Profile	Morning V wind profiles	Radiosonde
$\theta$ Profile	Morning potential temperature profiles	Radiosonde
BLH <sub>SH</sub>	PBLH derived from sensible heat	Derived from $\theta$ Profile and SH
BLH <sub>Parcel</sub>	PBLH derived from parcel method	Derived from $\theta$ Profile and T
<b><i>Output</i></b>		
Trigger	Cloud occurrence	ARSCL
Position	Cloud-base height	ARSCL
Fraction Profiles	Cloud fraction and thickness	ARSCL

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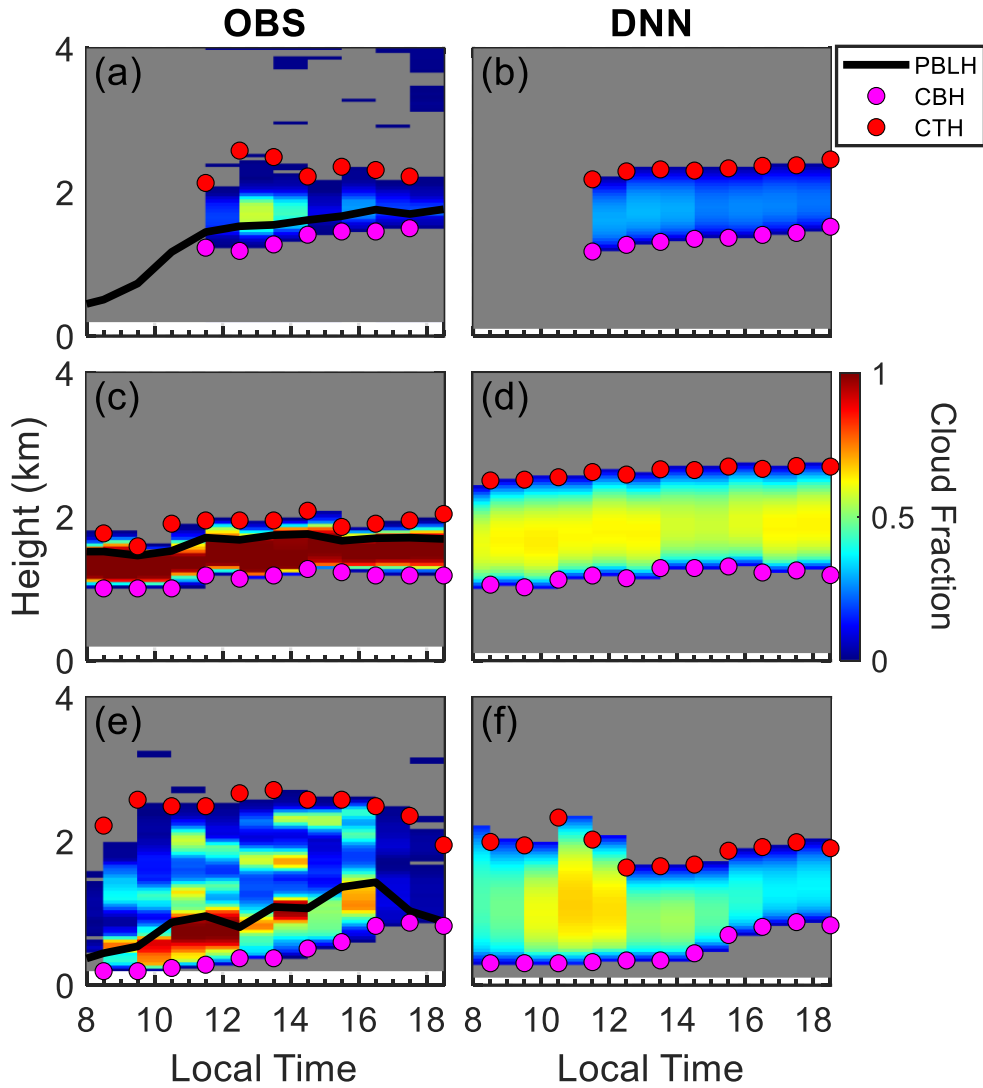
1071

1072 **Figures**



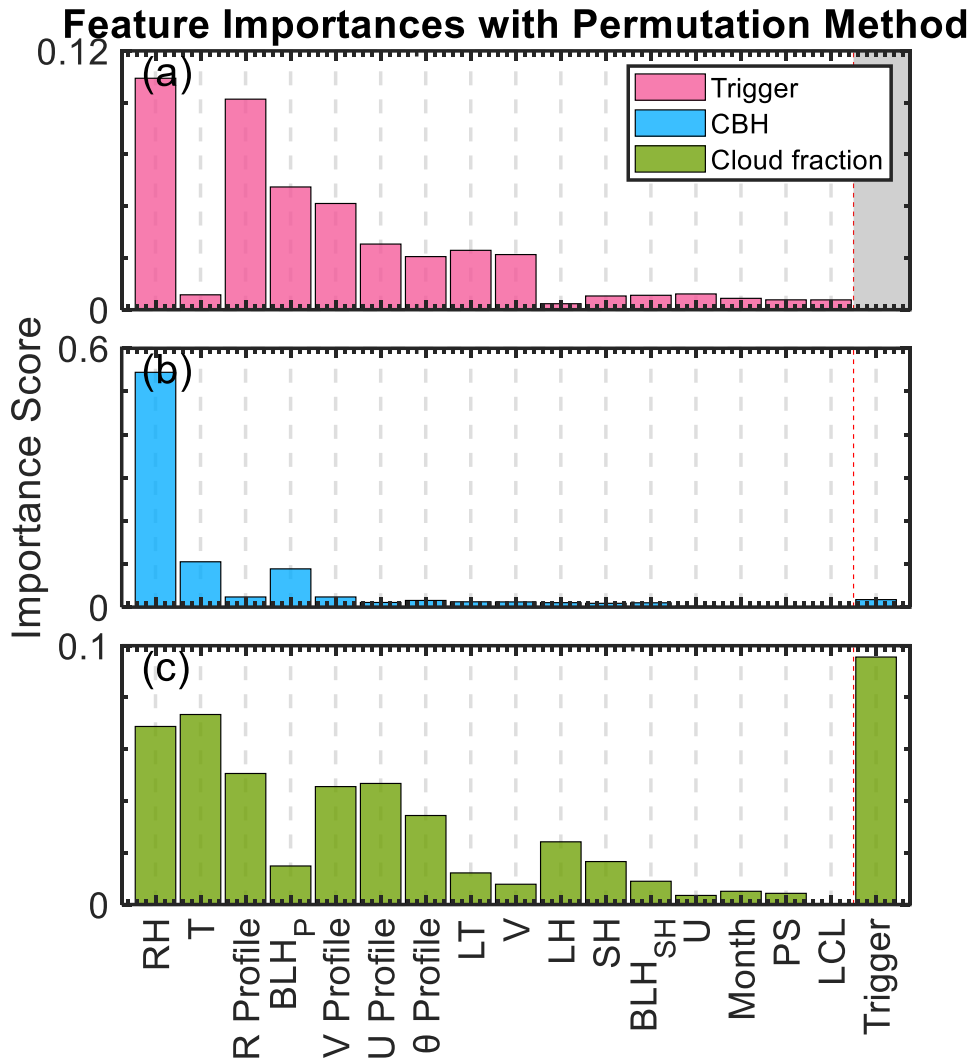
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1074 **Figure 1:** Conceptual diagram of the deep learning framework for simulating boundary  
 1075 layer cloud (BLC) characteristics over the US Southern Great Plains. Inputs for the deep  
 1076 neural networks (DNN) include morning meteorological profiles from radiosonde  
 1077 (SONDE), time indicators (i.e., local time and month), and surface conditions such as  
 1078 fluxes (curved black arrows) and meteorological data. The relevance of relative  
 1079 humidity (RH) profiles and the planetary boundary layer (PBL) top is emphasized due  
 1080 to their critical role in BLCs development. These variables are processed through  
 1081 multiple layers of hidden neurons ( $h_{11}$  to  $h_{MK}$ ). Both input and output parameters are  
 1082 hourly, except for the morning SONDE. Separate DNN modules are constructed for  
 1083 each task: Module 1 handles the initiation (trigger) of BLC; Module 2 estimates the  
 1084 cloud base; and Module 3 estimates cloud fraction and thickness. Together, these  
 1085 models synergize to predict the presence, altitude, and stratification of BLC.



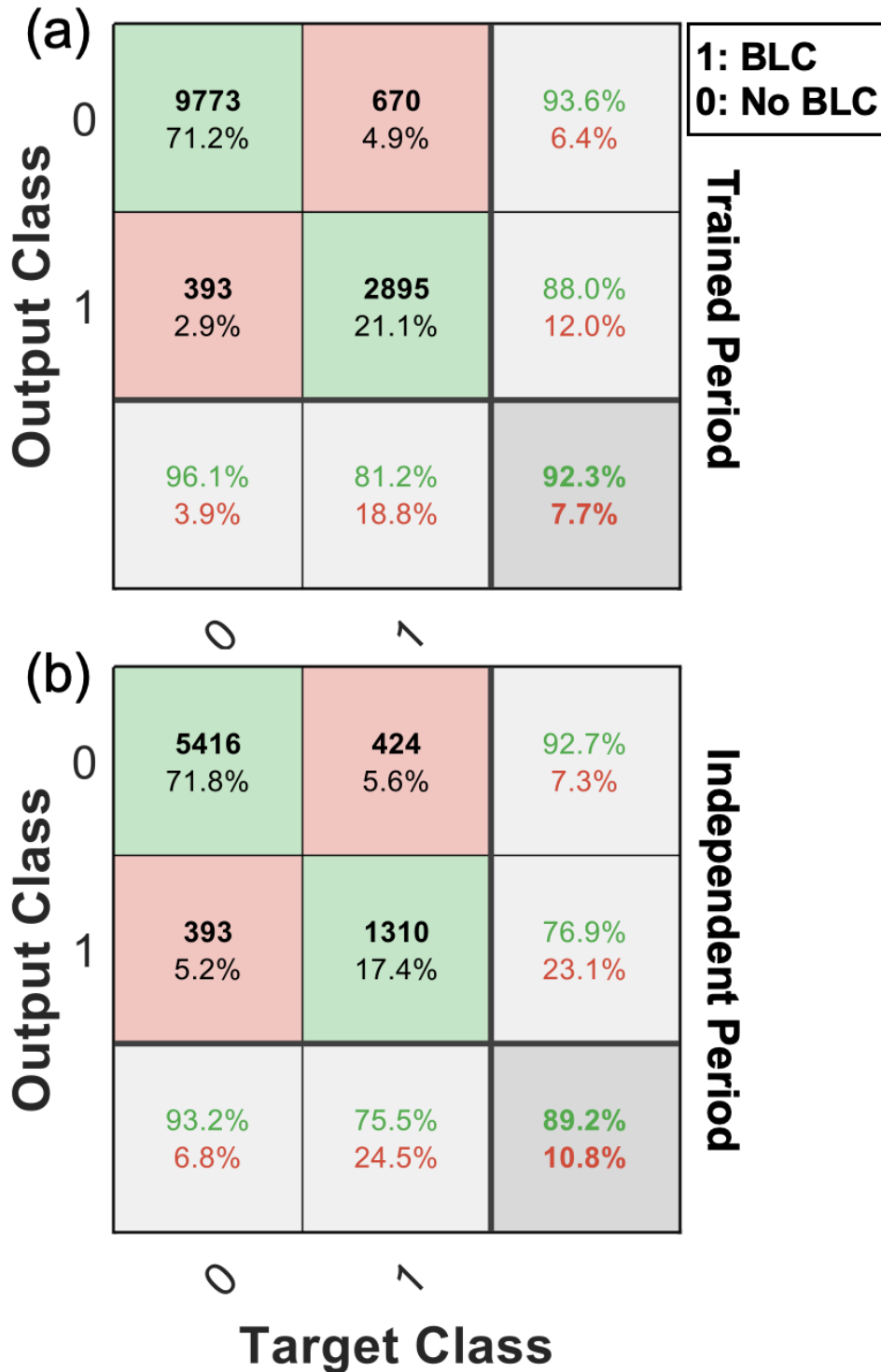
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1087 **Figure 2:** Examples of diurnal cloud fraction profiles for cumulus (a, b), stratiform (c,  
 1088 d), and complex cloud structures (e, f) over the US Southern Great Plains. Observed  
 1089 data (OBS) are shown alongside deep learning neural network (DNN) simulations.  
 1090 Black lines represent the observed PBL height (PBLH), with cloud base (CBH) and  
 1091 cloud top heights (CTH) marked by pink and red dots, respectively. The color gradient  
 1092 indicates the cloud fraction.



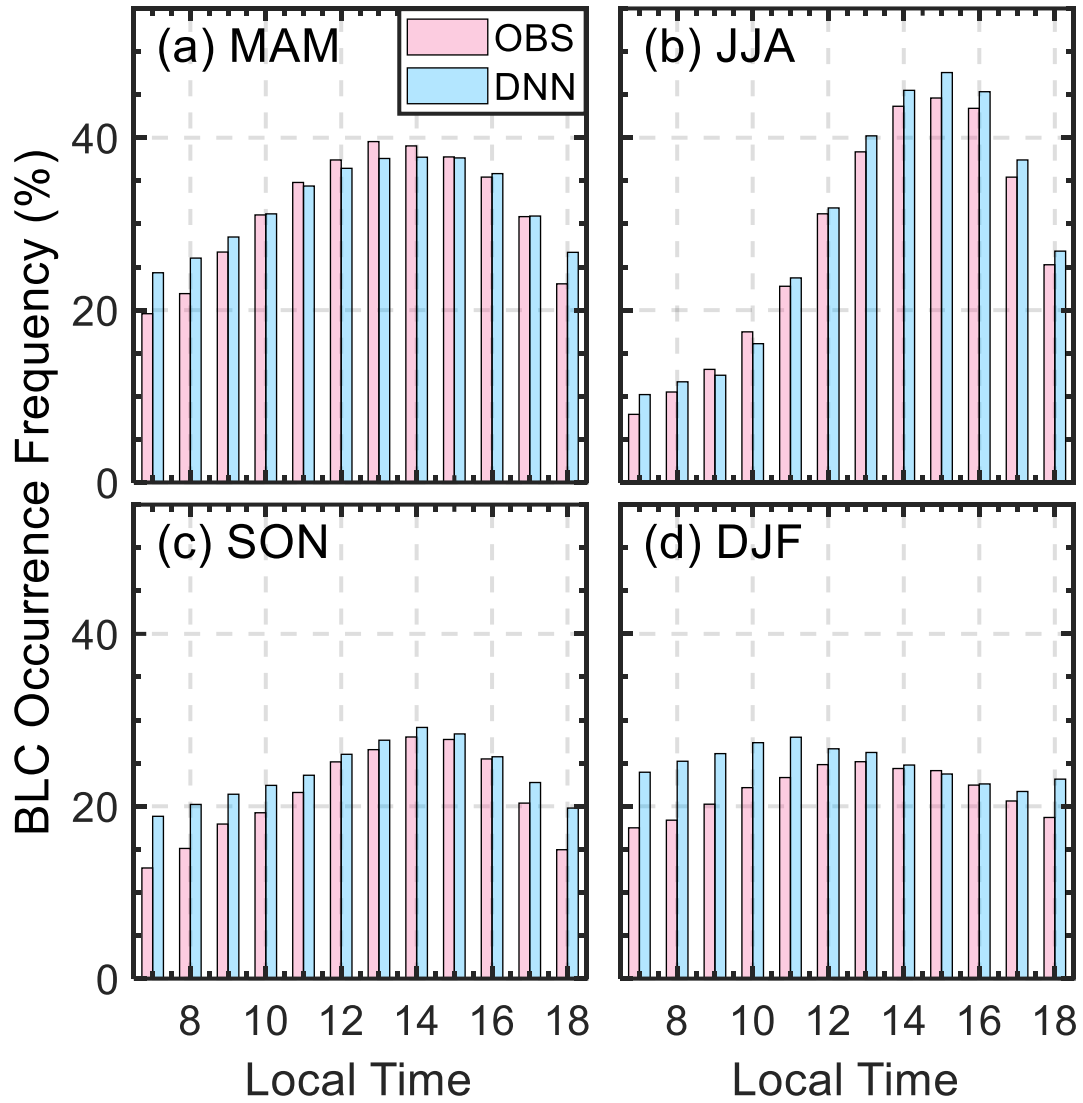
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1094 **Figure 3.** Feature importance scores for predicting cloud occurrence (a), cloud base  
 1095 height (CBH) (b), and cloud fraction (c) in the deep learning simulations of BLCs. Each  
 1096 panel presents the relative contribution of input features, includes month, local time  
 1097 (LT), surface pressure (PS), relative humidity (RH), zonal (U) and meridional (V) wind  
 1098 components, temperature (T), lifting condensation level (LCL), boundary layer height  
 1099 derived from sensible heat (BLH<sub>SH</sub>) and parcel methods (BLH<sub>parcel</sub>), sensible heat (SH),  
 1100 latent heat (LH), and morning profiles of relative humidity (R Profile), U wind (U  
 1101 Profile), V wind (V Profile), and potential temperature ( $\theta$  Profile). These factors are  
 1102 ranked based on their overall importance. The importance scores are calculated with  
 1103 permutation method and quantify the relative contribution of each feature to the model's  
 1104 predictive accuracy.



1105

1106 **Figure 4:** Confusion matrices on the classification performance of the deep learning  
 1107 model in predicting the occurrence of boundary layer clouds (BLCs) during the trained  
 1108 period (1998-2016) in panel (a), and the independent period (2017-2020) in panel (b).  
 1109 The matrices in the trained period are calculated using the 30% dataset for the validation.  
 1110 The matrices in the black color display the counts and percentages of true positive (TP),  
 1111 false positive (FP), true negative (TN), and false negative (FN) predictions. The overall  
 1112 accuracy, precision, and recall scores for each class are also included, demonstrating  
 1113 the model's ability in identifying BLC occurrence.



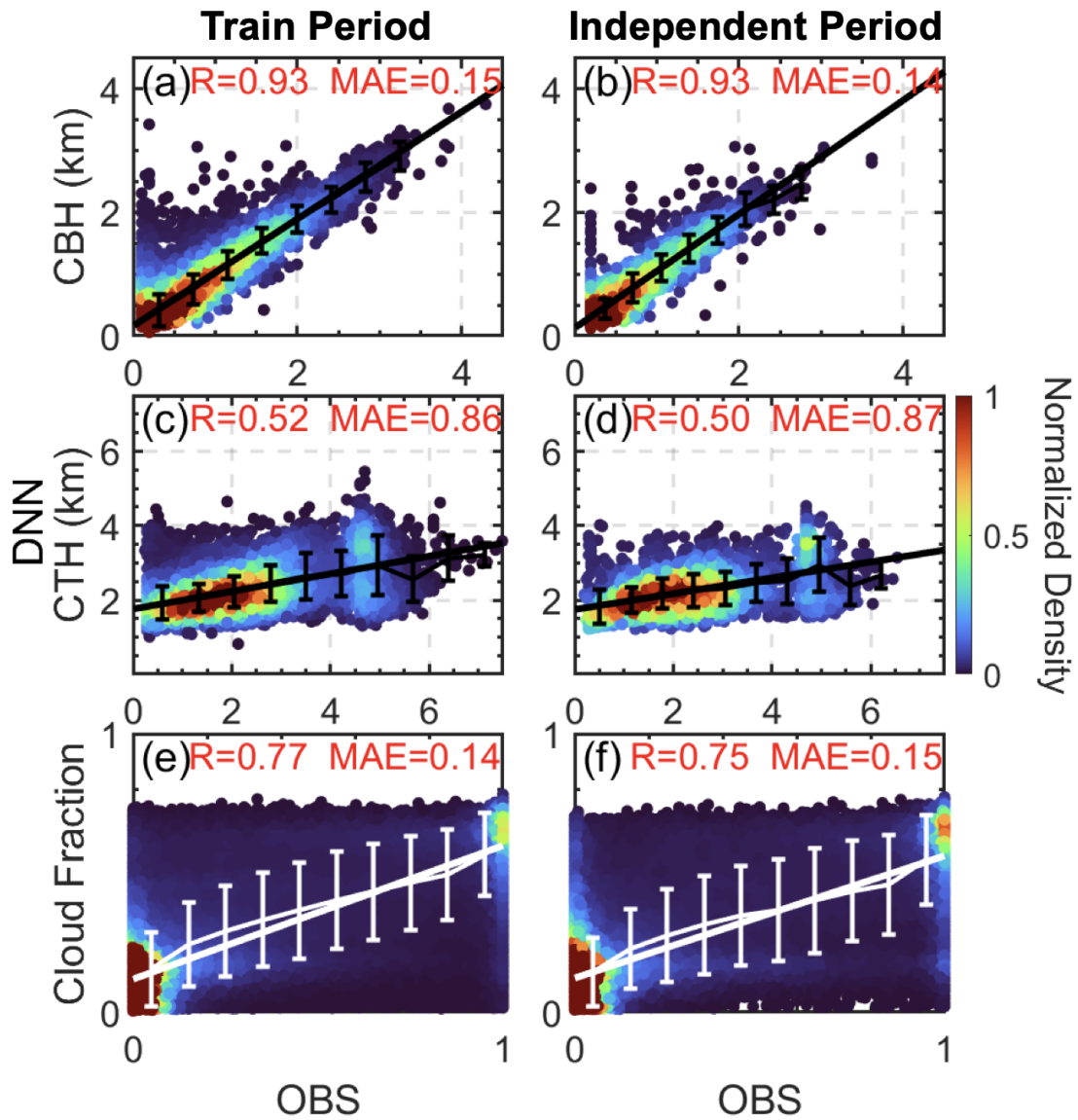
1114

1115 **Figure 5.** Bar graph comparison on the occurrence frequency of boundary layer clouds  
 1116 (BLC) between the observed (OBS, red) and the predicted by the deep learning neural  
 1117 network (DNN, blue) across different local times of the day, segmented by seasons: (a)  
 1118 MAM (Spring), (b) JJA (Summer), (c) SON (Fall), and (d) DJF (Winter).

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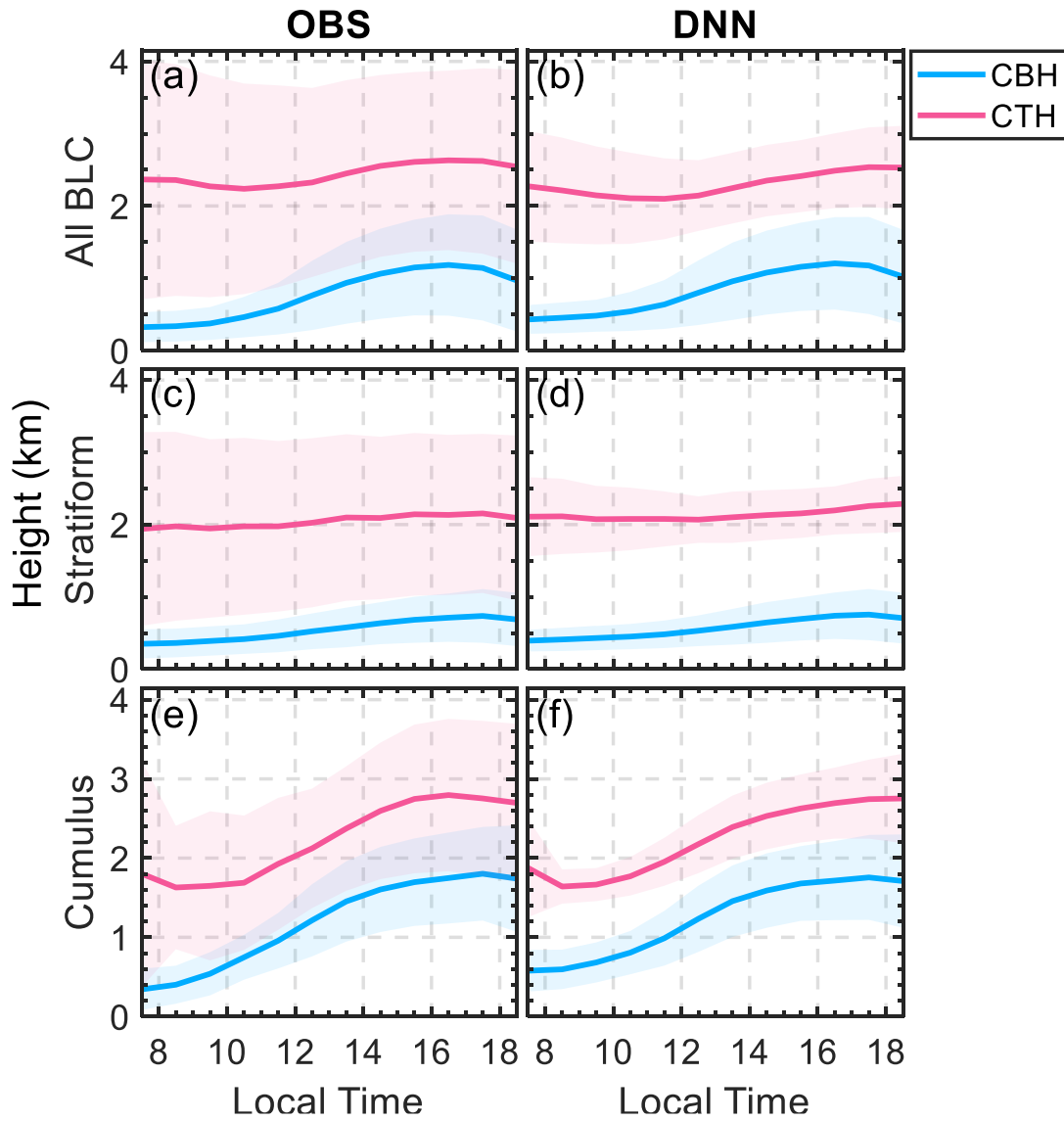


1122

1123 **Figure 6.** Scatter density comparison between the observed (OBS) and the predicted  
 1124 values by the deep learning neural network (DNN) for cloud base height (CBH), cloud  
 1125 top height (CTH), and cloud fraction during the trained period (a, c, e) and an  
 1126 independent period (b, d, f). Note that the BLC is segmented into ten layers, yielding  
 1127 ten separate cloud fraction values per BLC instance for analysis. The correlation  
 1128 coefficient (R) and mean absolute error (MAE) are indicated for each comparison. The  
 1129 color scale represents the normalized density of data points. The solid lines and error  
 1130 bars denoting the linear regression and standard deviations in each bar.

1131

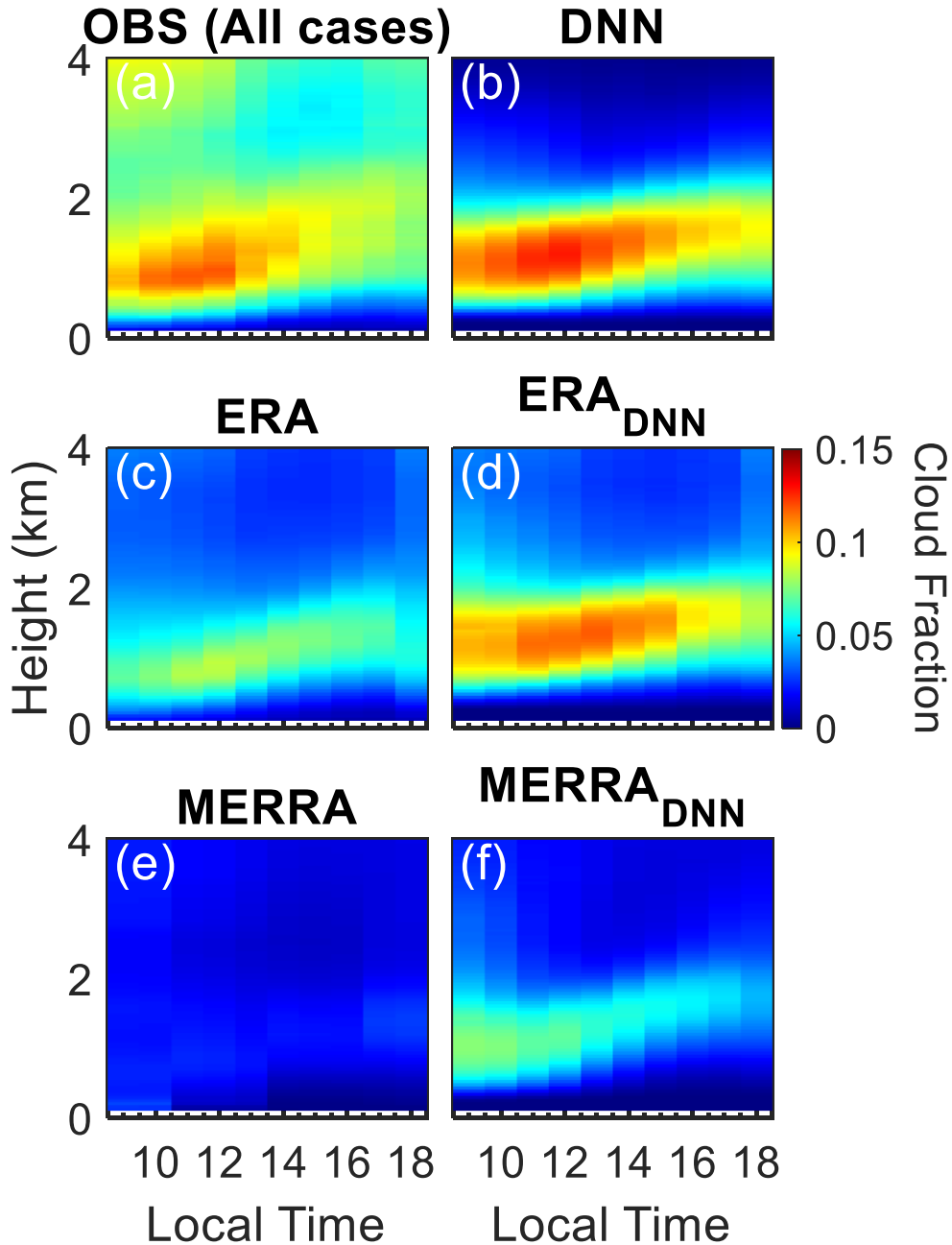




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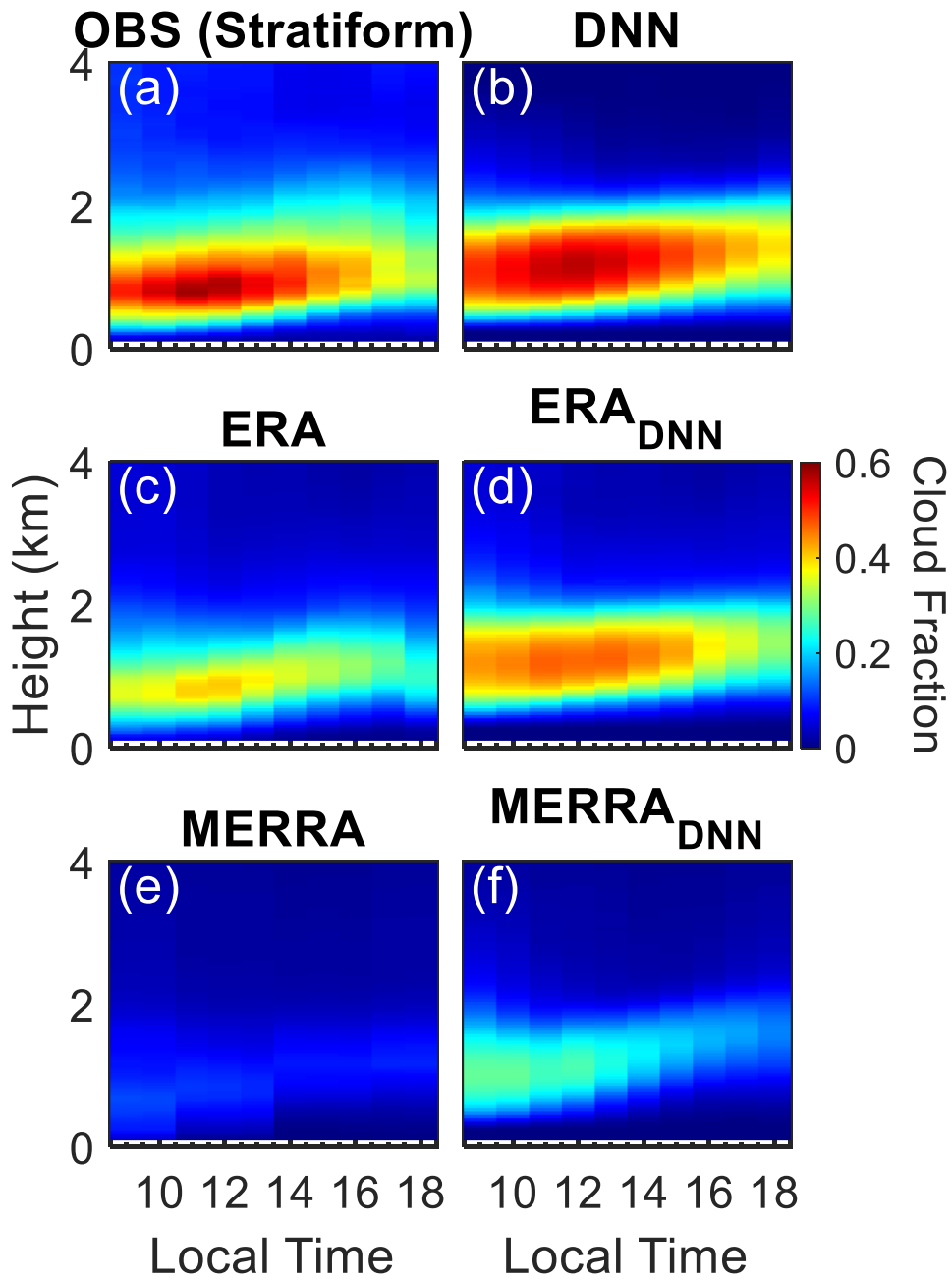
1133 **Figure 7.** Diurnal profiles of cloud base height (CBH) and cloud top height (CTH) as  
 1134 determined by the observations (OBS) and deep learning simulations for all BLC (a-b),  
 1135 stratiform clouds (c-d), and cumulus (e-f). The shaded areas represent the variability  
 1136 (one standard deviation) around the mean heights.

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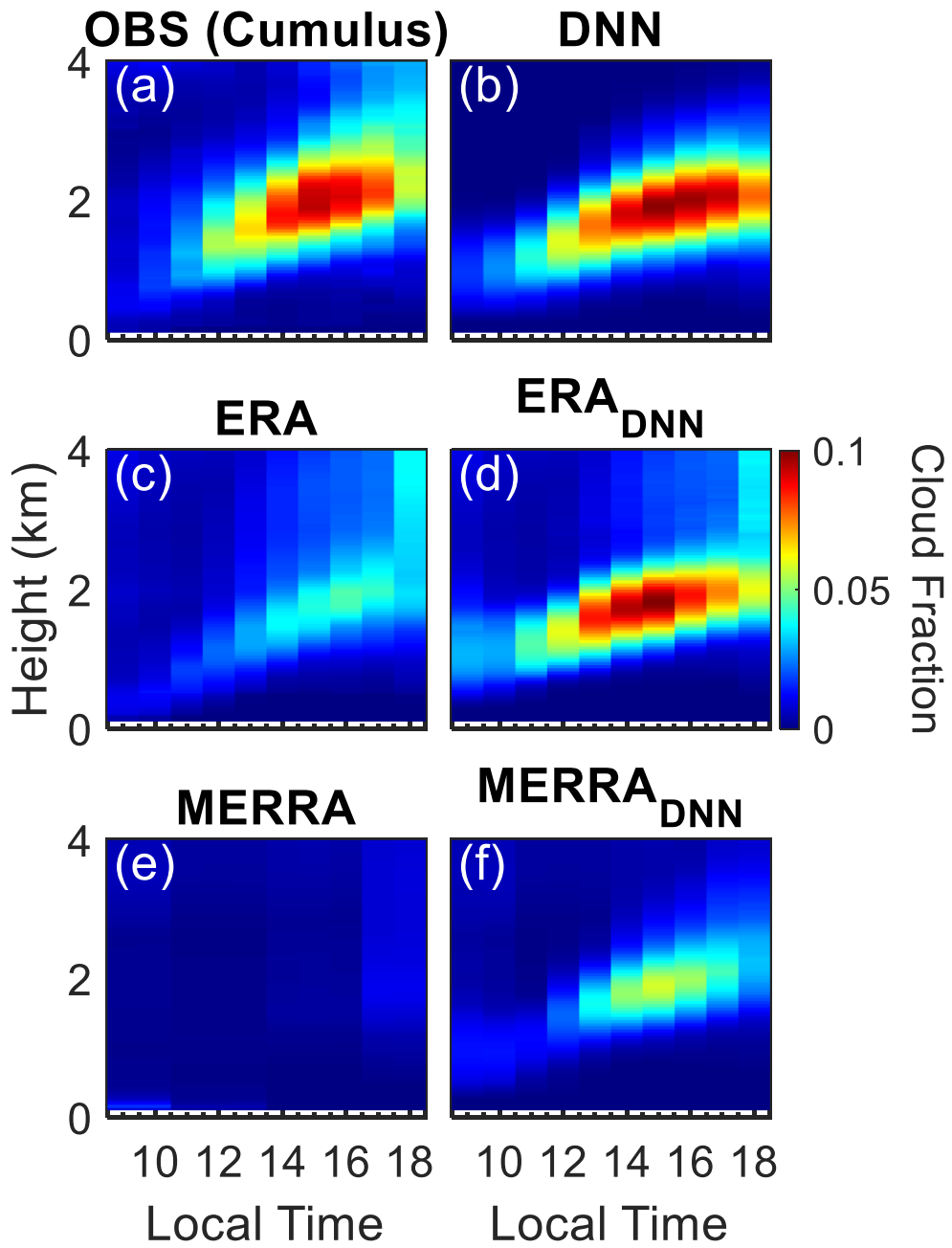
1138

1139 **Figure 8.** Color shaded areas demonstrate the diurnal variation in cloud fraction for all  
 1140 cases as observed and simulated. Panel (a) shows the observed cloud fraction (OBS),  
 1141 while panel (b) illustrates the cloud fraction simulated by the deep learning neural  
 1142 networks (DNN) using ARM observational data as inputs. (c, e): cloud fractions directly  
 1143 extracted from ERA and MERRA reanalysis datasets, respectively. (d, f): the cloud  
 1144 fractions simulated by the DNN model using ERA (ERA<sub>DNN</sub>) and MERRA  
 1145 (MERRA<sub>DNN</sub>) data as inputs.



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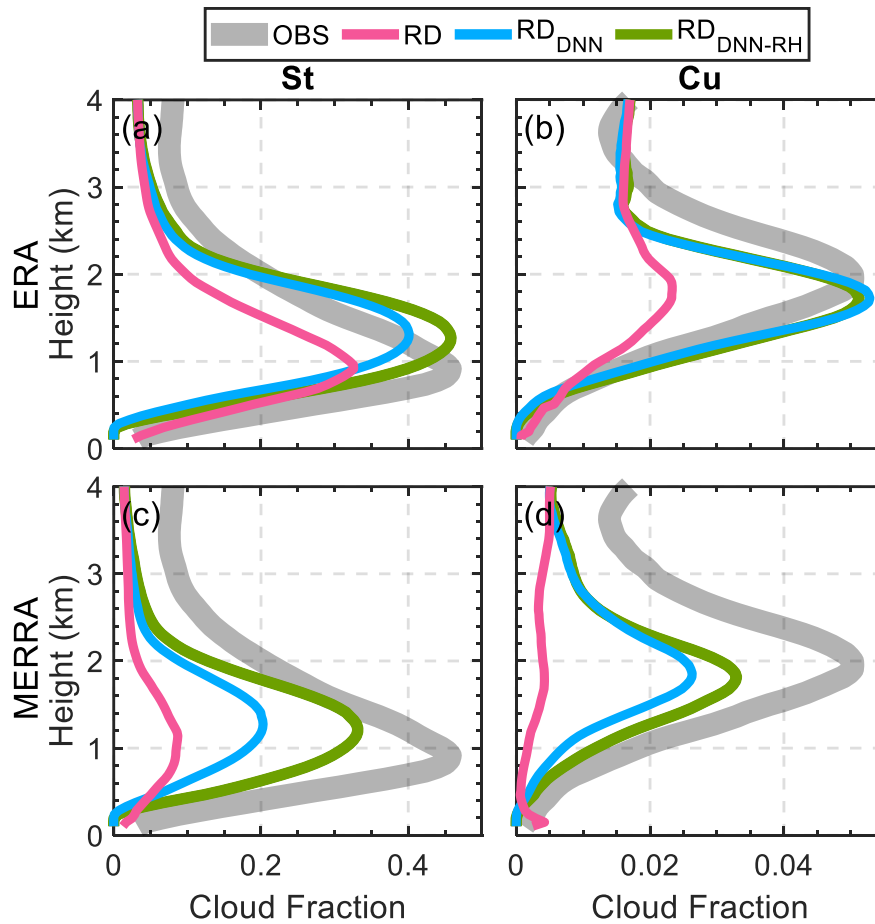
1147 **Figure 9.** Same to Figure 8, but for stratiform clouds.



1148

1149 **Figure 10.** Same to Figure 8, but for cumulus.

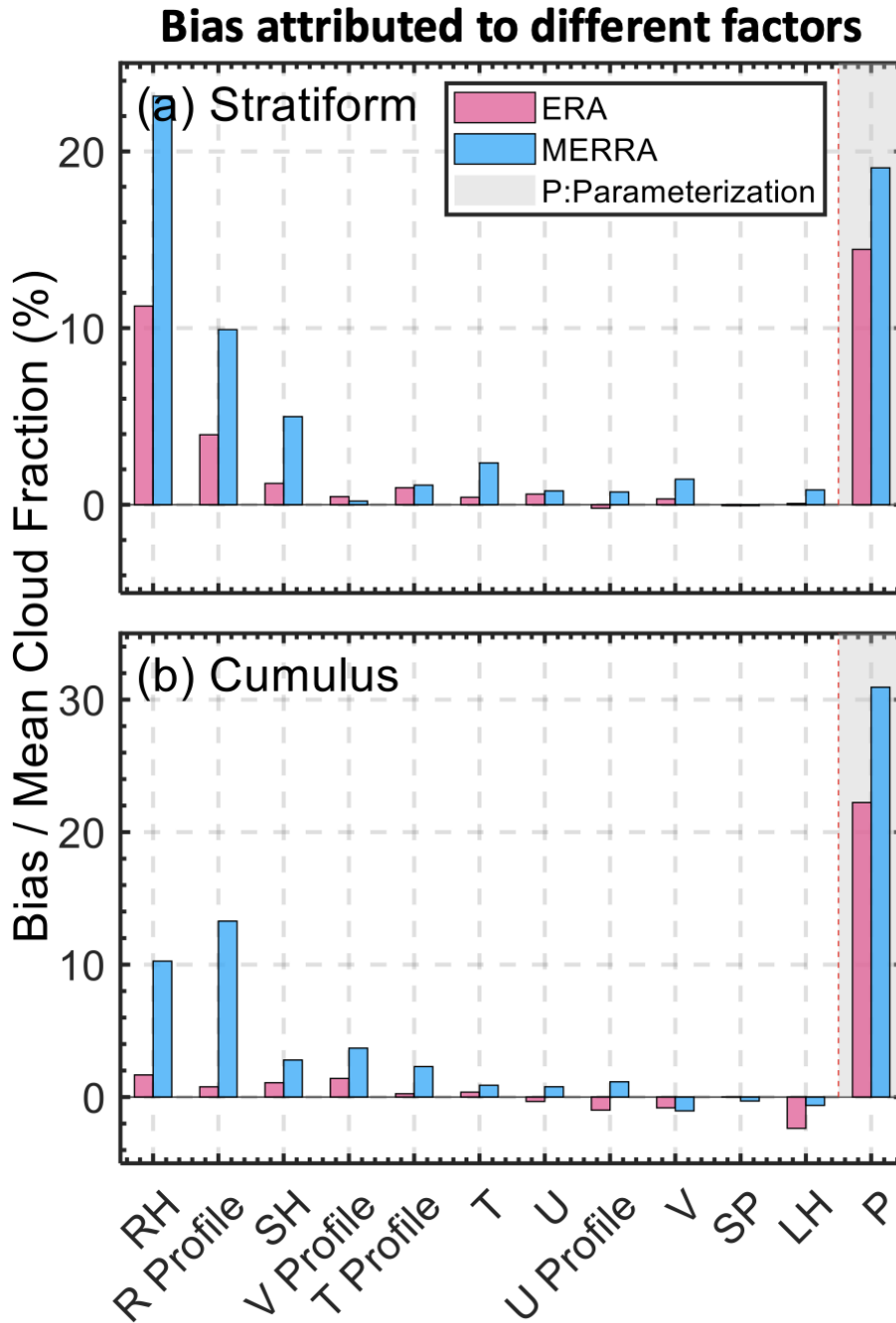
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1153 **Figure 11:** Vertical profiles of cloud fraction for stratiform (St) and cumulus (Cu)  
 1154 scenarios over the US Southern Great Plains. Panels (a) and (b) display ERA reanalysis  
 1155 data comparisons, while panels (c) and (d) show MERRA reanalysis data comparisons.  
 1156 The observed cloud fractions (OBS) are represented by the shaded grey area, illustrating  
 1157 the averaged cloud coverage recorded by field observations. The original reanalysis  
 1158 data (RD) is indicated in pink, indicating the baseline cloud fraction profiles as  
 1159 simulated by the reanalysis. The  $RD_{DNN}$  profiles in blue depict the new simulation  
 1160 results after applying the DNN models to the reanalysis data for boundary layer cloud  
 1161 (BLC) simulation. The  $RD_{DNN-RH}$  profiles in green show the simulation results when  
 1162 the surface relative humidity (RH) from the reanalysis data is replaced with observed  
 1163 values, indicating the impact of accurate surface moisture representation on cloud  
 1164 fraction simulations.



1165

1166 **Figure 12:** Attribution of bias between observed and reanalysis on cloud fractions to  
 1167 various meteorological factors and parameterization schemes for stratiform (a) and  
 1168 cumulus (b) cloud scenarios. The bars represent the normalized bias (bias divide mean  
 1169 cloud fraction) contributed by each factor: relative humidity profile (RH), meridional  
 1170 wind profile (V Profile), temperature profile (T Profile), zonal wind profile (U Profile),  
 1171 surface pressure (SP), latent heat flux (LH), and parameterization (P). All profiles took  
 1172 on morning (06:00 LT). Light blue bars indicate biases identified in the ERA reanalysis  
 1173 dataset, while pink bars represent biases in the MERRA reanalysis dataset. The dashed  
 1174 red line marked 'P' denotes biases attributed specifically to the parameterization within  
 1175 the reanalysis models. This analysis uses the DNN to discern the impact of each factor  
 1176 (ranked from highest to lowest) on the discrepancy in cloud fraction estimates between  
 1177 observations and reanalysis models.