On the estimation of boundary layer heights: A machine learning approach

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Abstract. The planetary boundary-layer height (z_i) is a key parameter used in atmospheric models for estimating the exchange
10 of heat, momentum and moisture between the surface and the free troposphere. Near-surface atmospheric and subsurface
    properties (such as soil temperature, relative humidity etc.) are known to have an impact on z_i. Nevertheless, precise
    relationships between these surface properties and z_i are less well known and not easily discernible from the multi-year dataset.
    Machine learning approaches, such as Random Forest (RF), which use a multi-regression framework, help to decipher some
    of the physical processes linking surface-based characteristics to z_i. In this study, a four-year dataset from 2016 to 2019 at the
15 Southern Great Plains site is used to develop and test a machine learning framework for estimating z_i. Parameters derived
    from Doppler lidars are used in combination with over 20 different surface meteorological measurements as inputs to a RF
    model. The model is trained using radiosonde-derived z_i values spanning the period from 2016 through 2018, and then
    evaluated using data from 2019. Results from 2019 showed significantly better agreement with the radiosonde compared to
    estimates derived from a thresholding technique using Doppler lidars only. Noteworthy improvements in daytime z_i estimates
20 were observed using the RF model, with a 50% improvement in mean absolute error and an R^2 of greater than 85% compared
    to the Tucker method z_i. We also explore the effect of z_i uncertainty on convective velocity scaling and present preliminary
    comparisons between the RF model and z_i estimates derived from atmospheric models.

1 Introduction

25   Measuring the growth of the Planetary Boundary Layer (PBL) height is crucial for understanding the turbulent transfer
    of air mass, which in turn strongly influences the winds, temperature, and moisture within the atmospheric boundary layer.
    During daytime, the air within the PBL is well mixed due to convection and results in weakening of turbulence at the top of
    the PBL (entrainment zone). One of the characteristics of the top of the PBL during clear sky conditions is that the turbulence
    is near zero, while in cases with boundary-layer clouds, significant up and downdrafts can be observed at the top of the

30   boundary layer (typically the cloud base height). Routine, continuous, long-term monitoring of the PBL height, z_i, is crucial for evaluating climate, weather, and air quality models skill in representing near-surface turbulent mixing, entrainment across the PBL top, the development of shallow cumulus, understanding effects of morning or evening transitions (Grant 1997), and nocturnal convection initiation (Reif et al., 2017). Profiles of potential temperature, water vapor mixing ratio, and particulate concentration often exhibit strong gradients at or near the top of the PBL. Typically, estimates of z_i are obtained from an

35   analysis of temperature and humidity profiles obtained from radiosondes. Indeed, radiosondes continue to be the de facto standard due to their long operational history, fine vertical resolution, accuracy, and reliability. However, major limitations are the poor temporal resolution and large sampling error because radiosondes are typically only launched twice daily at operational centers around the world. The launch time periods are generally not optimal for looking at various boundary layer properties. As a result, the diurnal variation in z_i is usually poorly represented in radiosonde data.

40   Modern remote sensing instruments can provide continuous estimates of the boundary layer dynamics. Space-based remote sensing instruments, such as Moderate Resolution Imaging Spectroradiometer, Tropical Rainfall Measuring Mission data, and Multiangle Imaging SpectroRadiometer have also shown the ability to estimate PBL height (Wood and Bretherton 2004, Karlsson et al. 2010).

          Ground-based lidar systems, such as the Raman lidars (Turner et al., 2014), ceilometer, micro pulse lidar (Campbell

45   et al. 2002), atmospheric emitted radiance interferometer (Knuteson et al., 2004; Sawyer and Li, 2013), Doppler lidar (Tucker et al., 2009, Berg et al., 2017, Bonin et al., 2018, Vakkari et al., 2015, Banakh et al., 2021) and high spectral resolution lidar, have been commonly used to provide PBL height estimates (Quan et al., 2013, McNicholas and Turner 2014). For elastic lidar systems such as the micro pulse lidar, z_i is estimated by locating the height where the range-corrected signal-to-noise ratio (SNR) or attenuated backscatter profile experiences a strong decrease with height (Emeis et al., 2008). A similar approach is

50   used to estimate z_i from profiles of water vapor mixing ratio from Raman lidar (Summa et al., 2013) or differential absorption lidar systems (Hennemuth and Lammert 2006); however, the peak in the water vapor variance has also been used as an estimate of z_i (Turner et al. 2014).

          Doppler lidars provide range-resolved measurements of radial velocity, attenuated backscatter, and SNR. When staring vertically, a ground-based Doppler lidar measures height-resolved profiles of vertical velocity in the lower atmosphere

55   with a temporal resolution of 1 second or less. Profiles of the vertical velocity variance can then be computed by averaging over an appropriate time interval (typically 15 to 30 minutes). The primary advantage of Doppler lidars is that they measure the turbulence directly and thus provide a more defensible measure of z_i. Other systems rely on gradients of aerosol loading or moisture that are used to infer z_i.

          One method for estimating the convective boundary layer (CBL) depth using Doppler lidars is to find the height

60   where the vertical velocity variance profile falls below some prescribed threshold, which in some cases can vary with time (Lenschow et al., 2000, Tucker et al., 2009, Lenschow et al., 2012, Berg et al., 2017). This method, which we refer to as the Tucker method, is simple to implement and provides a direct measure of z_i. However, the estimates are sensitive to the choice of variance threshold, which is somewhat arbitrary. Also, this method fails under stable nocturnal conditions due to weak

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turbulence and the fact that the lowest gate of the lidar is often above the depth of the nocturnal z_i. Horizontal velocity variance
65 and dissipation rate profiles from a Doppler lidar can be used to estimate z_i in nocturnal conditions (Vakkari et al., 2015, Banakh et al., 2021). Alternatively, one can estimate the PBL height based on wind shear and Turbulence Kinetic Energy (TKE), but there has been limited research on this topic (Brost and Wyngaard, 1978, Teixeira and Cheinet, 2004, Le Mone et al., 2018).

Due to different measurement approaches between multiple remote sensing instruments, considerable uncertainties
70 exist when comparing z_i to standard radiosonde retrievals. PBL heights from different instruments provide expected trends during certain atmospheric conditions (mostly daytime convective time periods) but differ slightly due to measurement uncertainties and thresholds chosen associated with each instrument. Therefore, a framework independent of threshold techniques used in previous studies is warranted. Although this paper does not directly address a unified approach to estimate z_i, it is a step in that direction.

75 In view of these limitations, we investigate the potential of using a machine learning (ML) approach for continuous monitoring of z_i, with a focus on CBL. ML enables us to bring together various observations to arrive at a consensus answer. ML models, such as RF and Neural Networks, have been used for classifying various atmospheric phenomena (McGovern et al. 2017, Gagne II et al., 2019, Vassalo et al., 2020) or retrieving atmospheric variables (e.g., Solheim 1998, Cadeddu et al. 2009). The RF model is versatile, simple to implement, and robust. Training the RF model entails providing it with
80 observations (i.e. features) that aid in predicting z_i. Examples of such observations include surface sensible and latent heat flux, soil temperature, soil moisture, surface potential temperature, surface humidity etc. These features have all been shown to exhibit some degree of correlation with z_i (Santanello et al., 2005; Zhang et al., 2013).

Here we use a RF model to predict z_i using input features derived from vertically-staring Doppler lidar data and various surface and sub-surface observations. We use a multi-year dataset from the U.S. Department of Energy (DOE)'s
85 Southern Great Plains (SGP) site (Sisterson et al., 2016) for training and evaluating the RF model. Reference z_i measurements from radiosondes are used in the RF training process (Sivaraman et al., 2013). Specifically, the RF model is trained using observations from 2016 through 2018, and its performance is evaluated using data from 2019.

In this paper, Section 2 describes the observations that are used in this study, Section 3 describes the details of the RF model, including the training method, data conditioning and performance. Results of the RF model's performance are presented
90 in Section 4, and in Section 5 we examine how RF model-derived z_i estimates affect the scaling of the vertical velocity variance profiles. PBL heights estimates from Energy Exascale Earth System Model (E3SM) Atmosphere Model version 1 (EAMv1), large-eddy simulations (LESs), and observations are compared in Section 6. Finally, a summary and future work are provided in Section 7.

2 Data Sources

The U.S. DOE Atmospheric Radiation Measurement (ARM) User Facility operates the SGP site in north-central Oklahoma (Mather and Voyles, 2013; Sisterson et al., 2016). The site contains an extensive suite of instrumentation for monitoring the atmosphere and surface properties. Most of these instruments operate continuously and the data are freely available from the ARM website (https://adc.arm.gov/discovery; McCord and Voyles 2016). The SGP site contains several heavily instrumented subsites or "facilities" that are geographically dispersed over Oklahoma and Kansas (Mather and Voyles, 2013). For this study, we use observations from the central facility (C1), which also contains the largest number and most diverse suite of instruments in ARM. Figure 1 shows the layout of the SGP C1 site and the locations of instruments used in this study. Additionally, Table 1 lists the instruments, ARM data stream names, and specific measurements that were used. In ML, independent variables, or inputs, are often referred to as features. A model can have multiple features/inputs and for this project, the measurements from the observations will be referred to as features in the RF model.
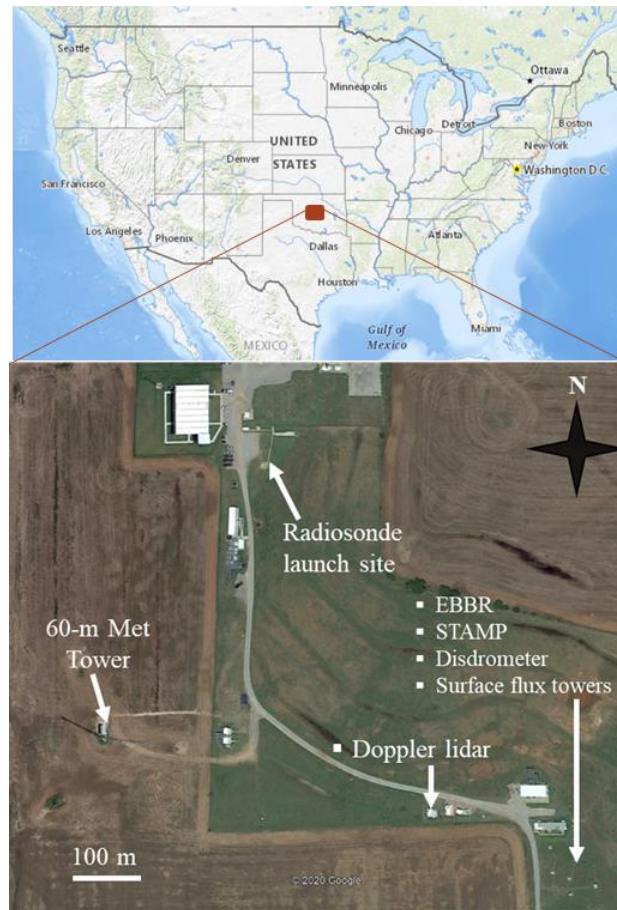
Figure 1. ARM SGP site C1 layout and instruments used in this study in Oklahoma, USA. Maps are extracted from © Google Earth and © Google Maps.

Table 1: Instruments, ARM data stream names, and measurements used in this study.

Instrument	ARM data stream	Measurements or features	Measurement height/range	References
Radiosonde	sgppblhtsonde1mcfarlC1.c1	PBL height estimates (m)	100 m to 5000 m AGL	Sivaraman et al., 2013
Surface eddy correlation station	sgp30co2flx25mC1.b1	Sensible heat flux (Wm^{-2})	25 m AGL	Cook et al., 2018 and Tang et al., 2019
		Latent heat flux (Wm^{-2})		
		Vertical velocity variance (m^2s^{-2})		
		Friction velocity (ms^{-1})		
		Turbulence Kinetic Energy (m^2s^{-2})		
		Monin-Obukhov length (m)		
		Wind speed (ms^{-1})		
		Wind direction (degrees from north)		
Surface meteorological station	sgpmetE13.b1	Air temperature (deg K)	4 m AGL	Ritsche and Prell, 2011
		Relative humidity (%)		
Soil temperature and moisture probes	sgpstampE13.b1 or sgpswatsE13.b1	Soil moisture (m^3m^{-3}) Soil temperature (deg C)	-5 cm below surface	Cook, 2018
Surface energy balance system / solar infrared radiation station	sgpqcrad1longE13.c1 and sgpqcrad1longE13.c2	Best estimate of longwave, shortwave and normal radiation (Wm^{-2})	2 m AGL	Cook and Sullivan, 2019
Doppler lidar	sgpdlfptC1.b1	Range-corrected attenuated backscatter variance ($m^{-1}sr^{-1}$), SNR variance (dB), and average eddy dissipation rate (m^2s^{-3}).	90 m to 800 m AGL	Champagne et al., 1977, Newsom and Krishnamurthy, 2020
	sgpdlprofwstats4newsC1.c1	Cloud base height (m) CBL depth from Tucker method (m) Year, month and hour of day	0 m to 9000 m AGL	Newsom et al., 2019b, Tucker et al., 2009
	sgpdlprofwinds4newsC1.c1	Wind shear exponent ($\alpha = \log_{10}\left(\frac{U_1}{U_2}\right)/\log_{10}\left(\frac{Z_1}{Z_2}\right)$), where U_i and Z_i are wind speed and height at altitude i.	$z_1 = 90$ m to $z_2 = 300$ m AGL (or lower, depending on data availability)	Wharton and Lundquist, 2012.

The ARM User Facility has operated a Halo Photonics Stream Line XR (Pearson et al., 2009) at C1 since April 2011. The instrument provides height- and time-resolved measurements of radial velocity, attenuated backscatter, and SNR. The range resolution is set to 30 m and the temporal resolution is about 1-s. The instrument is configured to stare vertically most of the time. Once every 15 minutes, it executes a plan-position-indicator scan, from which profiles of the wind speed and direction are computed. The vertical staring data are used to compute profiles of noise-corrected vertical velocity variance using a 30-minute averaging period. More details about the instrument are provided by Newsom and Krishnamurthy (2020). Details about the vertical velocity statistics value-added product (VAP) are provided by Newsom et al. (2019a), and detail about the Doppler lidar wind VAP are given by Newsom et al. (2019b).

Doppler lidar-derived features used in this study are listed in Table 1. The list includes raw height-resolved measurements of attenuated backscatter and range-corrected SNR, which are known to be directly correlated with z_i (Cohn and Angevine 2000, Brooks 2003). Also listed are several derived quantities such as cloud base height, wind shear, turbulence eddy dissipation rate, and z_i estimated using the Tucker method (Tucker et al., 2009). Typically, the nocturnal vertical velocity variance estimates are too small, and the threshold used in the Tucker method is not applicable. During certain rare nocturnal convection initiation events, larger vertical velocity variance estimates are observed and the same threshold (0.04 m^{2}s^{-2}) is used to estimate nighttime values of z_i from the lidar. For consistency in terminology being used here, we refer to all z_i estimates from the lidar as the Tucker method (both nighttime and daytime). Because the range of the Doppler lidars at SGP C1 is often less than 1 km (see Appendix A), estimates of eddy dissipation rate (using 1 Hz vertical velocity stares, Champagne et al., 1977) above 800 m were affected by system noise. Thus, features such as the eddy dissipation rate, attenuated backscatter, and SNR from the Doppler lidar were limited to 800 m AGL. Reducing the height from 800 m to 500 m AGL did not impact the results. Moreover, RF models used in this study are only capable of ingesting 1-dimensional timeseries data; therefore, 2-dimensional Doppler lidar features were averaged over the vertical column (90 m [lowest range gate] to 800 m AGL). Adding these features increased the overall variance explained by the RF model (82% of the total variance compared to 74% of the total variance without using lidar derived parameters).

The ARM PBL VAP (sgppblhtsonde1mcfarlC1.c1) contains estimates of z_i derived from radiosondes launched at SGP C1. We note that radiosondes are typically launched four times daily from SGP C1, nominally at 0530, 1130, 1730 and 2330 UTC each day (local time = UTC - 0600 hours). The PBL VAP uses three different algorithms for estimating z_i. These include the Heffter 1980, two bulk Richardson thresholds methods, and Liu and Liang (2010). The Heffter (1980) method is a well-established and widely used algorithm (e.g., Marsik et al. 1995, Delle Monache et al., 2004) that determines z_i from potential temperature gradients using criteria related to the strength of an inversion and the potential temperature difference across the inversion. The bulk Richardson number (Ri_b) is a dimensionless number relating vertical stability to vertical shear. It represents the ratio of thermally produced turbulence to that generated by vertical shear. Methods using Ri_b to estimate z_i assume that there is no turbulence production at the top of the stable boundary layer and therefore Ri_b exceeds its critical value at the top of the boundary layer (Seibert et al., 2000). Several different critical thresholds of Ri_b, are provided in the literature

based on resolution of sondes, location, etc. The ARM PBL VAP includes z_i estimates based on two critical thresholds (0.25 and 0.5). Liu and Liang (2010) provide different thresholds for estimating convective and stable boundary layer depths using potential temperature profiles. The inversion strength thresholds used in the method varies for given stability regime and land type classification (land, ocean, or ice). We note that the various estimates can differ considerably. More details about the ARM PBL VAP are provided by Sivaraman et al. (2013).

2.1 Preliminary Data Analysis

Boundary-layer height estimation algorithms (Tucker et al., 2009, Berg et al., 2017, Bonin et al., 2018) purely using the Doppler lidars are limited by the range of the Doppler lidars at the ARM SGP facility, which may or may not reach the top of the boundary layer. The data availability of the ARM Doppler lidar SGP C1 systems is typically less than 1-2 km (Newsom and Krishnamurthy, 2020), and the data availability of the Doppler lidar vertical stares and velocity azimuth display scans for the study period are shown in Appendix A. The Tucker method z_i is used for inter-comparison with the RF model in this study, primarily due to its ease in application to the multi-year dataset, known performance, including its established usage in studies using the ARM Doppler lidar and other locations and instruments (Träumner et al., 2011, Shukla et al., 2014, Schween et al., 2014, Berg et al., 2017, Lareau et al., 2018, Lareau 2020). Vertical velocity variance profiles provided in the sgpdlprofwstats4newsC1.c1 VAP and a variance threshold of 0.04 m^2s^{-2} is used to determine z_i, following Tucker et al., 2009. The results are somewhat sensitive to the choice of threshold such that the z_i estimates decrease as the threshold is increased (Berg et al., 2017).

Figure 2 shows a typical example of vertical velocity variance during the warm season at SGP. Also shown are estimates of z_i from the Tucker method. We find that the Tucker method generally works well at tracking the height of the convective mixed layer during its initial development phase and can be made to match the radiosonde observations by changing the vertical velocity variance threshold (Schween et al., 2014). In that case, there is sufficient SNR for the lidar to see both the developing convection and the overlying residual layer. However, as the mixed layer continues to deepen, at some point the SNR becomes too small to enable reliable estimates of the vertical velocity variance. This problem is sometimes compounded by a slight reduction in sensitivity during the hottest portion of the day, which we suspect is the result of strong refractive turbulence in the surface layer. Although this effect has not been thoroughly analysed due to lack of refractive turbulence profiles and concurrent radiosonde data, there could be instances when the Doppler lidar is indeed measuring the top of the boundary layer. In any event, the loss of signal near the CBL top could result in z_i estimates from the Tucker method to be low biased.
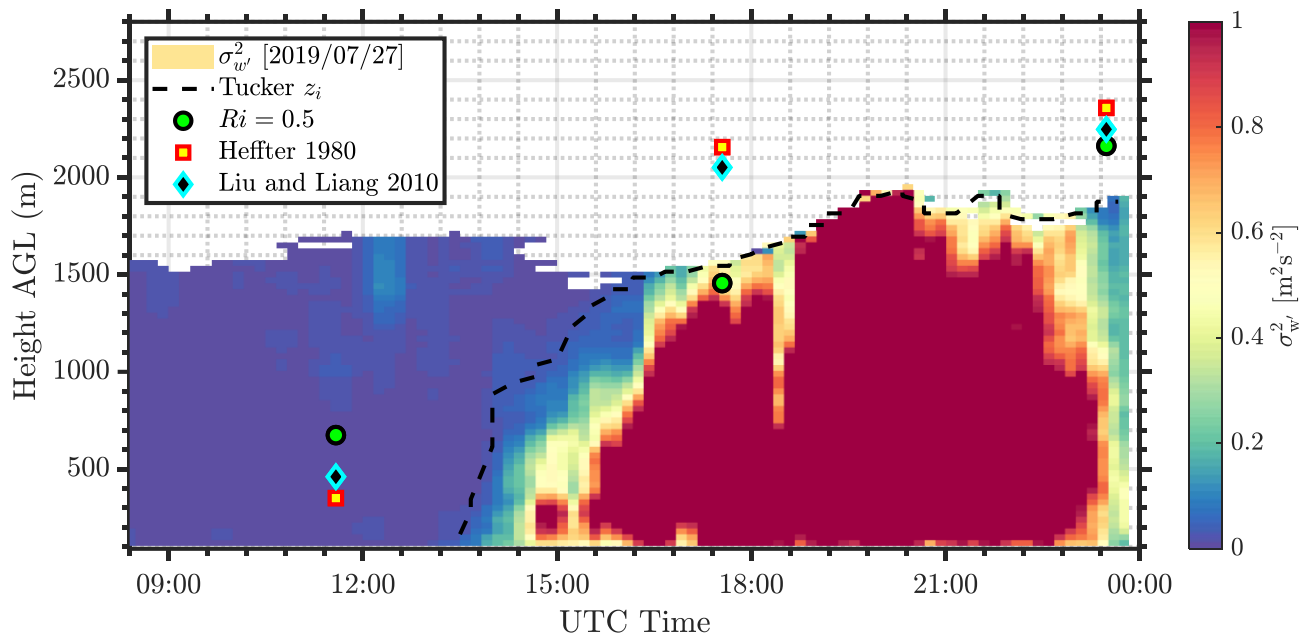
Figure 2: Typical CBL showing lidar variance (colours), Tucker z_i (black line), and radiosonde z_i (three methods; symbols). The horizontal axis shows the number of hours after 00:00 UTC on 27 July 2019.

180   For this study, radiosonde-derived z_i estimates are used to calibrate the RF algorithm. Figure 3 shows comparisons between lidar-derived CBL (using the Tucker method) and simultaneous estimates from the ARM PBL VAP. These comparisons were performed using 1785 cases with radiosonde data and daytime clear (identified as periods when surface heat flux is positive from sunrise to sunset and cloud base height is zero) or shallow cumulus conditions (identified as cloud base height less than 5 km from Doppler lidar and cloud fraction less than 0.1) for the years 2016 through 2019. From these results,

185   we found that the Liu and Liang (2010) technique resulted in the best overall agreement with the Tucker method z_i, in terms of the correlation coefficients (r = 0.75) and slope (0.70). Thus, z_i estimates from the Liu-Liang technique in the ARM PBL VAP (pblhtsonde1mcfarl.c) are used as a reference to calibrate the RF model in this study. It should be noted that any of the above three model outputs can be used to calibrate the ML model, if needed, and the choice could vary with each site. For a different site, we would recommend conducting a similar correlation analysis as shown above with various radiosonde models

190   and lidar data to determine the optimal model for RF calibration. It is important to note that during stable conditions, the determination of z_i from radiosondes is very uncertain, as the turbulence can result from either buoyancy forcing or wind shear and radiosonde rapidly rises through the relatively thin stable boundary layer. At SGP C1, the nose of the low-level jet can also be used to define the height of the boundary layer (Sivaraman et al., 2013). Therefore, the focus of this study is to only demonstrate the ability of the RF model to replicate nighttime z_i estimates compared to radiosonde-derived values. We hope

195   this framework developed in this article can be adapted easily to future research in estimating the true stable boundary layer

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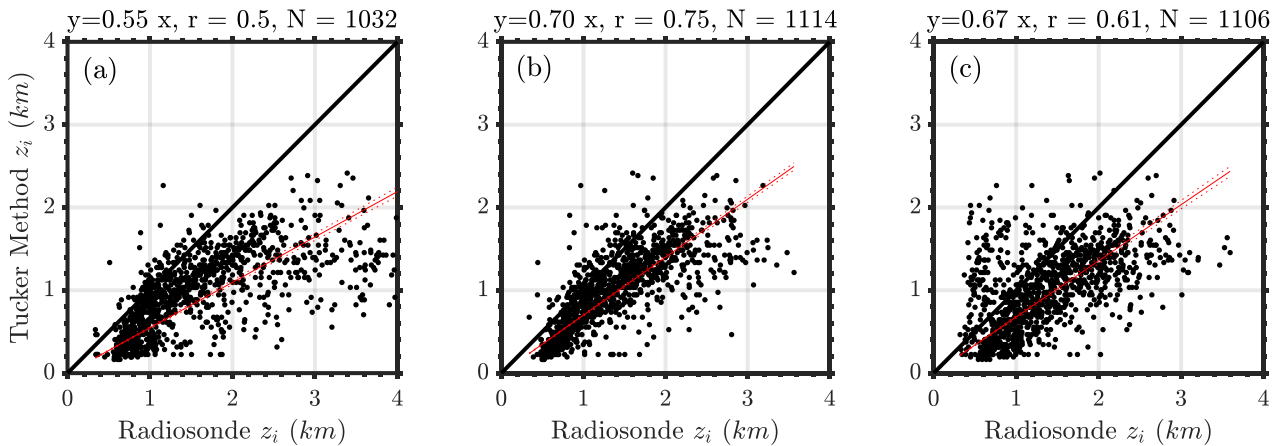
Figure 3: Comparisons between Tucker method and three different z_i estimates from radiosondes a) Heffter 1986, b) Liu and Liang 2010 and c) Bulk Richardson number method using a threshold of 0.5. The red line is the best fit with the fit y = mx shown above. r is the correlation coefficient and N is the total number of radiosonde and Tucker method observations used in each scatter plot.

3 Machine Learning

In this study, an RF algorithm was used to predict PBL heights. RF regression (Breiman, 2001) is an ensemble method that is made up of a population of decision or decorrelated trees. Figure 4 provides a graphical illustration of the RF bootstrapping process. Bootstrap aggregation (bagging) is used so that each RF tree (a sample is shown in Appendix B) can randomly sample from an entire feature set, while only a subset of the total feature set is given to each individual tree. For example, if the entire feature set contains say M different features, an individual RF tree can contain a fraction of those M features. The premise behind RF is to improve the variance reduction of bagging by reducing the correlation between the trees without increasing the variance. The trees can be truncated to add further diversification. After construction, the population's individual predictions are averaged to give a final prediction of the target variable. Ideally, this process results in a diversified and decorrelated set of trees whose predictive errors cancel out, producing a more robust final prediction.

An advantage of RFs is their ability to determine the importance of all input features for the predictive process. This is done by calculating the mean decrease in impurity, or the decrease in variance that is achieved during a given split in each decision tree. The decrease in impurity for each input feature can be averaged over the entire forest, providing an approximation of the feature's importance for the prediction (feature importance estimates sum to 100% to ease interpretability). A sample regression tree developed by real data used in this article is shown in Appendix B (Figure B1). The statistics and ML toolbox in MATLAB contain all the functions needed to build the RF algorithm used in this study.
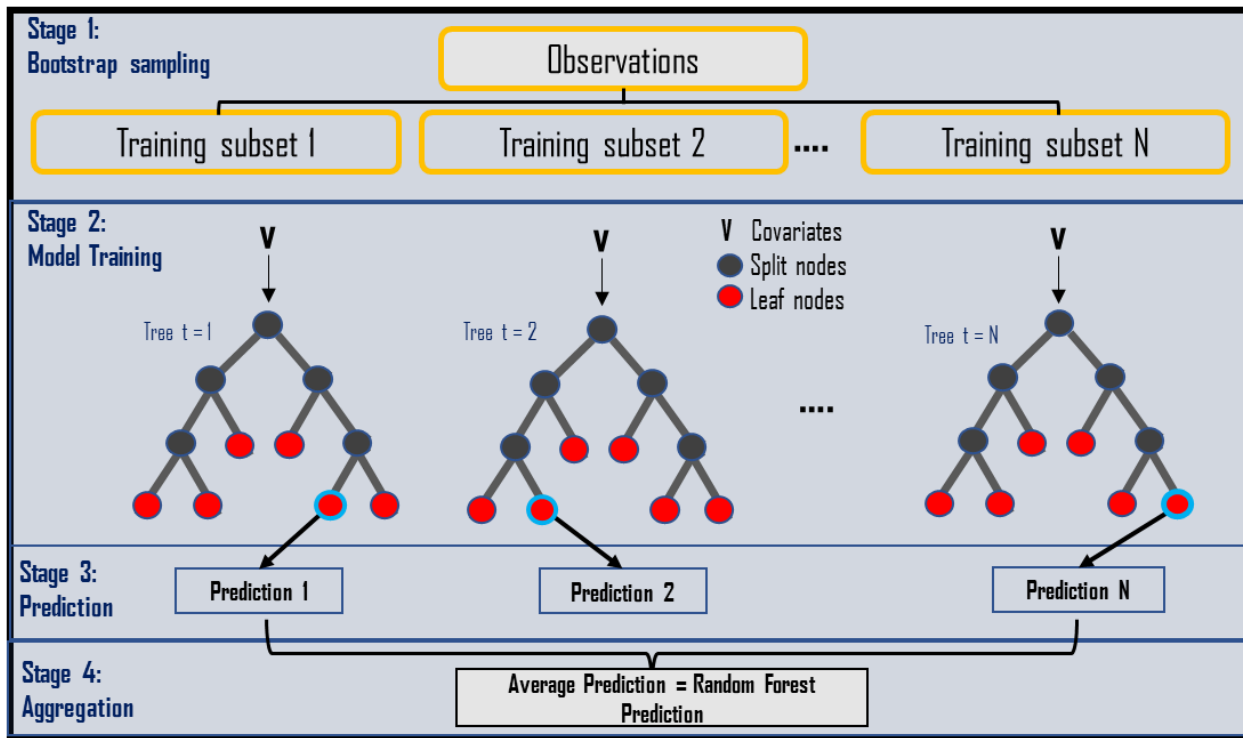
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Figure 4: Graphical representation of a standard RF algorithm (adapted from online sources and Figure A1).

3.1 Model Hyperparameters

225   In this study, a least-squares boosting regression (LSboost) ensemble RF model (Breiman 2001) is built based on observational data listed in Table 1. At every iteration, the ensemble fits a new decision tree to minimize the mean-squared error between the observed response and the aggregated prediction of all decision trees developed previously. The MATLAB function *fitrensemble* is used to develop the RF model. The algorithm creates several regression trees using a subset of input features and radiosonde observations. The RF model creates a learning process to map the reference data to input features.

230   Hyperparameters are used to control the learning process in the RF model. It is good practice to tune hyperparameters such as the maximum number of decision splits per tree (see Figure 4), learn rate for shrinkage and the number of iterations for reducing the generalization error (Breiman, 2001). In this article, hyperparameters for the RF model are chosen by performing a Bayesian optimization on the data, which minimizes the k-fold cross validation loss function for select hyperparameters (MATLAB function *bayesopt*). For this study, three hyperparameters were optimized: the number of tree splits, number of

235   learning cycles or iterations, and learn rate for the model. Based on the optimization results, the number of iterations was set to 460, number of tree splits to 11 and the learning rate was set to 0.25 for the current model.

Regularization techniques are used to prevent statistical overfitting in a predictive model (Hastie et al., 2008), by reducing the magnitude of the coefficients of the RF model for certain parameters that do not contribute to the target variable. In general, regularization algorithms can treat issues such as multicollinearity and redundant predictors and make the model more precise. The MATLAB function *regularize* is used for the regularization process, which is based on the Lasso regularization algorithm (Tibshirani, 1996). This regularization algorithm optimizes the number of trees and avoids data overfitting.

3.2 Data Preprocessing

Surface and lidar data from 2016 to 2019 are used in this analysis. ARM VAPs provides processed and quality-controlled data from several atmospheric sensors. Each VAP provides quality control thresholds that are used to filter the data. For example, the lidar VAPs (DLWSTATS and DLWIND) provide quality control flags based on the system noise and SNR (Newsom and Krishnamurthy, 2020). For this analysis, thresholds specified in the VAPs are used to remove any erroneous data. Similarly, quality control flags for all variables mentioned in Table 1 above are used to filter bad data (Tang et al., 2019). Because the temporal resolution of the surface data are variable, measurements are interpolated or averaged to the lidar 15-minute resolution time stamps. The frequency of radiosondes is generally 6 hours at SGP but can be in intervals of 3 hours during select field campaigns (Mather et al., 2018). For training purposes, surface and lidar data to the nearest radiosonde observations within 15-minutes are chosen.

Normalizing/standardizing/scaling processes are used to scale the variables in an ML model, such that they have the same order of magnitude in their value. Standardizing involves aligning the features to have a zero mean and scaled to have standard deviation of one. Typically, RF models do not need standardizing or normalizing features due to the inherent bagging process (Breiman, 2001). At SGP C1, large diurnal variability was observed for certain parameters (like TKE, dissipation rate, etc.), leading to a large distribution of values between daytime and nighttime. This skewed the number of trees the RF model builds for daytime and nighttime estimates. Standardizing the features showed improvements while estimating nocturnal z_i estimates from the RF model. Therefore, to improve nocturnal z_i estimates, standardized datasets will be used in the following analysis for all conditions.

All the features, listed in Table 1, are filtered based on ARM mentor guidelines for each instrument and then normalized. These measurements are fed into an ensemble RF model using the hyperparameters described above. Once the RF model is built, a Lasso regularization approach is used on the RF model to limit the effect of collinearity on the target variable. Similar to a least-squares regression, collinear columns tend to deteriorate the accuracy of the output (Krishnamurthy et al., 2013, Yoo et al., 2014). Once the RF model is built, it can be used to estimate z_i for time periods that are not being used to train the model. In MATLAB, this is typically done using the *predict* function.

The RF model is trained using sub-surface, surface, lidar and concurrent radiosonde z_i data from 2016, 2017 and 2018. Hereon, these data are referred to as training-input features. A total of 3919 radiosonde z_i measurements were used in the training process. The 2019 sub-surface, surface and lidar data are referred to as future-input features and are used to provide

an independent dataset to evaluate the trained RF method. From an operational perspective, missing input features are quite common. The most common approach is to fill in (impute) the missing features (Hastie et al., 2008). Surrogate data using a local median of the nearest 10 data points are used in the analysis (Hastie et al., 2008). Other imputation algorithms such as k-nearest neighbour was also tested, and similar results were observed. It is critical for the RF model to deal with missing values in its training phase. In some cases, the added noise in the system can help improve the stability of the RF model. But too much noise is also detrimental in the training process, and the imputed data may no longer be useful and can cause erroneous results. The imputation process is done inherently during the RF bagging process. The effect of data imputation on model performance was evaluated by training the RF model with and without data imputation. Four different possibilities in evaluating the performance of the RF model with and without imputation are evaluated, as shown in Table 2 below. In the case of no imputation (no missing data), only time periods when all features/parameters are available are used in the RF regression. In the case of 50% missing data, approximately 50% of the time series data were missing (at random) due to say issues with data quality and surrogate data were used. The choice of 50% was to mimic a worst-case real-world scenario based on experience, where either one or two instruments from the feature set of 20 odd variables have data quality issues. Other combinations, such as no missing data used in the RF regression during training process and 50% future-input feature missing data and vice versa were evaluated.

Table 2. Data imputation evaluation and performance on boundary layer heights for year 2019

Case	Training-Input Features	Future-Input Features	R^2 (%)	RMSE (m)	$Y_{RF} = m\,X_{RS} + C$
No Imputation	No missing data	No missing data	76.86%	324	$Y_{RF} = 0.912\,X_{RS} + 211$
Future-Input Imputation	No missing data	50% missing data imputed	65.28%	366	$Y_{RF} = 0.789\,X_{RS} + 288$
Training-Input Imputation	50% missing data imputed	No missing data	76.15%	328	$Y_{RF} = 0.876\,X_{RS} + 258$
Training and Future-Input Imputation	50% missing data imputed	50% missing data imputed	66.50%	357	$Y_{RF} = 0.792\,X_{RS} + 324$

* RF – Random forest, RS – Radiosondes

As can be seen from Table 2, data imputation overall reduces the accuracy of RF model performance. Missing future-input features seems to have the highest effect on the RF model z_i estimates, regardless of training the model based on missing training-input features. This could be due to several reasons, such as the median value does not represent the current state of the missing data, the same input features are not missing in both training and future input features as the combinations to test are near infinite (as the data in real-world can be missing in random as in the case above), etc. Assessing the performance of the RF algorithm using data imputation creates an additional level of complexity when one of the features is missing for a given time step compared to others. For example, if relative humidity feature is missing for a given time step and lidar

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300 this analysis, the model is trained with no missing data, and no imputation is done on the data (either input or future features) to accurately test the efficacy of the RF model. The authors would like to note that the results in Section 4 are in some sense optimistic due to the treatment of missing data, and the worst-case performance of such an algorithm must be thoroughly evaluated. Future studies are planned to implement a better imputation model based on data from past trends for a given feature and to test RF model performance.

305   RF models are generally site specific; initial tests (not shown) show the possibility to develop a generalized RF model to estimate z_i for all sites around SGP (C1 and other satellite sites) with good accuracy under all atmospheric conditions. A round-robin type analysis, where a model developed at a given site is tested at every other site and vice versa, would be a valuable exercise (Bodini and Optis, 2020).

310 **4 Performance of RF z_i**

Boundary layer height predictions from the RF model and Tucker method were compared to radiosonde estimates. Mean absolute error (MAE) is defined as:

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left|z_{iRS} - z_{i\gamma}\right| \tag{1}$$

315

Where, z_{iRS} is the boundary layer height estimated from the radiosondes (Liu and Liang, 2010), $z_{i\gamma}$ is the boundary layer height estimated from either the Tucker method or RF model. The root mean square error (RMSE) is defined as

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(z_{iRS} - z_{i\gamma}\right)^2} \tag{2}$$

320

Similarly, the linear correlation coefficient (R) is defined as

$$R = \frac{1}{\sigma_{RS}\sigma_{\gamma}(N-1)}\sum_{i=1}^{N}(z_{iRS} - z_{RS})(z_{i\gamma} - z_{\gamma}) \tag{3}$$

325 Where, z_{RS} and z_γ denote the mean of radiosonde and RF/Tucker method boundary layer heights, respectively, σ_{RS} and σ_γ denote their standard deviations, and N denotes the number of samples.

MAE and RMSE for the daytime atmospheric conditions from Tucker and RF methods are shown in Table 3. Daytime is defined as the period when surface heat flux is positive (i.e., sunrise to sunset), clear sky is defined as time periods when no clouds are observed from the Doppler lidar (with an hourly cloud fraction less than 0.1) and cloudy conditions are defined as

330 time periods when clouds below 5 km are observed from the Doppler lidar (with an hourly cloud fraction greater than 0.1). It can be observed that the RF method shows considerable improvements compared to the Tucker method for all three categories. Improvements of 40-50% in MAE and RMSE are observed under various conditions. The least improvement in RF z_i estimates is observed during cloudy conditions, with a MAE improvement of 45% compared to the Tucker method. Correlation coefficients are also observed to improve significantly during all daytime conditions.

335 Due to the presence of a nocturnal low-level jet (LLJ) at SGP, all seasons, the radiosonde nighttime z_i estimates are generally below the LLJ height and are well tracked by the RF model (see Section 4.1). A comparison of nocturnal RF model z_i estimates with other remote sensing devices that continuously monitor the boundary layer height needs to be conducted (e.g., Raman lidar) and is a part of future work.

340 Table 3. Systematic mean absolute errors, root mean square error and correlation coefficient (R^2) between RF, Tucker method, and radiosonde z_i estimates in 2019.

Observed atmospheric conditions	MAE (m)			RMSE (m)			R^2	
	RF	Tucker Method	% Improvement	RF	Tucker Method	% Improvement	RF	Tucker Method
Daytime Only	167	311	46%	249	441	43%	0.845	0.545
Daytime Clear sky	165	336	51%	235	479	51%	0.857	0.520
Daytime Cloudy	141	255	45%	208	363	43%	0.878	0.725

Nocturnal estimates of z_i from radiosondes at SGP are much more uncertain (Sivaraman et al., 2013). Regardless of the accuracy of the z_i estimate from radiosondes, the ability of the RF model to predict the input data is evaluated.

345 Consequently, the data were split into five atmospheric conditions: 1) daytime and clear sky (26%), 2) day and night clear sky (60%), 3) day and night cloudy (40%), 4) daytime only (53%), and 5) nighttime only (46%). Although some cases overlap in the above situations, the idea was to evaluate the RF model performance reasonably during both daytime, nighttime, cloudy, and clear-sky condition combinations. These five atmospheric conditions were chosen, because these are commonly observed atmospheric conditions at SGP and have been observed to have an impact on z_i (e.g., variations in cloud base height varies z_i).

350 The associated correlation plots between RF z_i estimates and corresponding radiosonde z_i estimates are shown in Figure 5. Overall, the RF model z_i estimates correlate well with radiosonde z_i, with an R^2 of greater than 0.85 during all the above conditions. During clear sky conditions (including both daytime and nighttime), RF z_i estimates show the highest correlation

of 0.88. Although the sample size varied for five categories, the correlation coefficients are overall high for the RF z_i estimates (compared to Tucker method in Figure 3). During the night, the z_i values from the radiosondes are relatively constant, and the

355 RF estimates are consistent with these values. However, due to the small dynamic range of the nighttime z_i values, the correlation between the radiosonde and RF methods is relatively poor (0.54). Based on the slopes of the regression lines in Figure 5, the RF model tends to overestimate z_i when it is small and slightly underestimate z_i when it is large. Possible reasons for this trend are under further investigation.

Overall, a uniform improvement in z_i can be obtained using RF techniques. Reducing or increasing the training data

360 had an impact on the RF model performance, but the increase in the magnitude of the correlation coefficient was negligible using at least two years of data. In this analysis, three years of data were used for training the RF model.
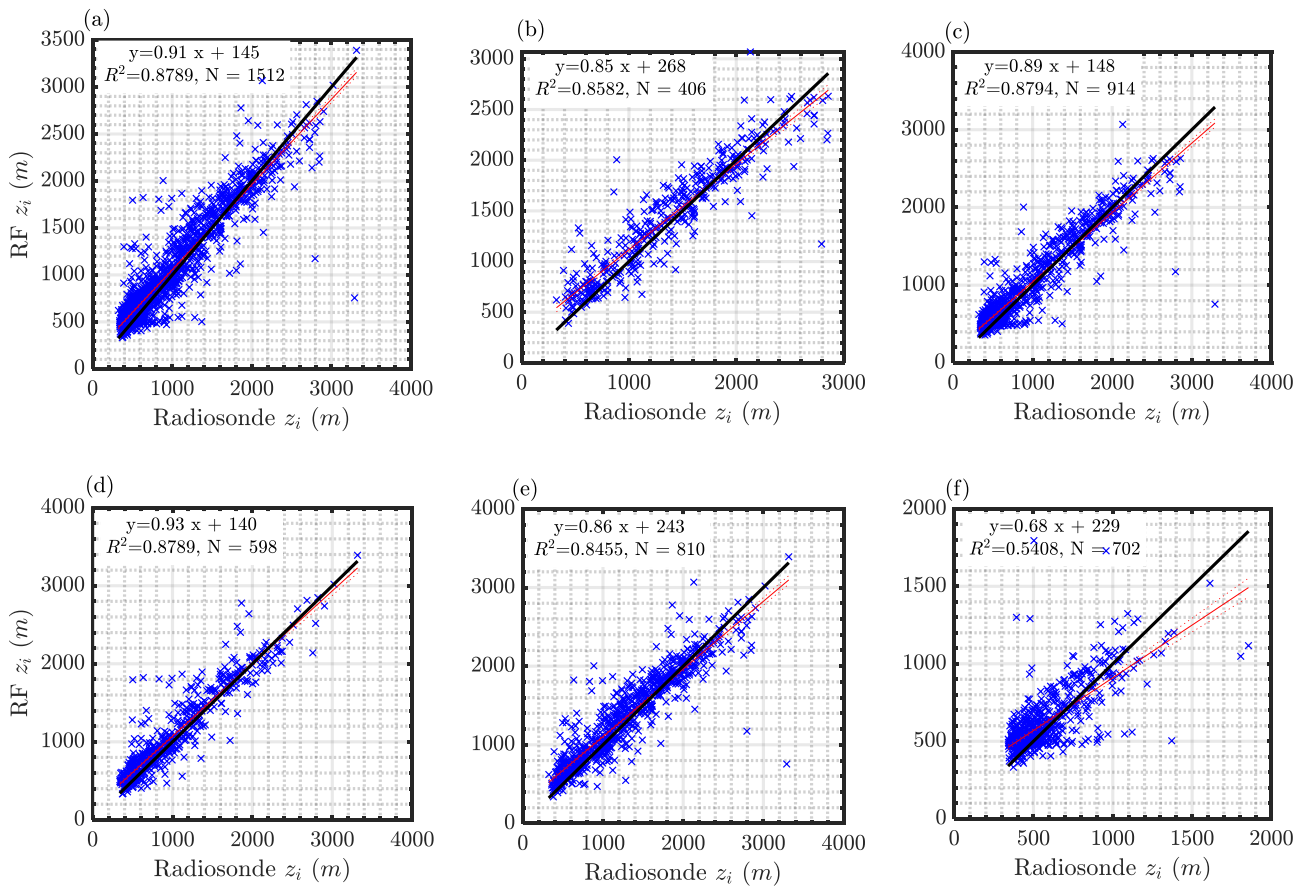

Figure 5: Correlations between RF PBL height and radiosonde PBL height for a) all data in 2019, b) daytime clear sky, c) clear sky

365 **daytime and nighttime, d) cloudy daytime and nighttime, e) daytime only, and f) nighttime only.**

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4.1 Time series, diurnal, and seasonal performance

The RF model was trained using data from 2016 to 2018, and z_i estimates for 2019 were estimated using the parameters listed in Table 1. The temporal resolution of the RF model z_i estimates is 15 minutes. Figure 6 and Figure 7 show lidar z_i estimates from the Tucker method, radiosondes and RF model on June 20 and June 22, 2019, respectively. Cloud base height and vertical velocity variance profiles from Doppler lidar are also overlaid. Due to an ongoing field campaign, the micropulse differential absorption lidar demonstration project, these days observed a higher frequency of radiosonde observations (Weckwerth et al., 2020). It is clear that the RF model z_i closely follows radiosonde z_i estimates and the Tucker method underestimates z_i as estimated from radiosondes. Although, the Tucker method is observed to track the convective boundary layer height effectively, a bias is observed when compared to the radiosonde z_i. Optimizing the vertical velocity variance thresholds could potentially reduce the bias in certain conditions, but the bias is not uniform across all time periods (see Figure 7). Because aerosol concentration decreases with altitude, signal availability reduces as a function of height. During peak convection, when the aerosol concentration above the boundary layer is minimal, lidar measurements sometimes do not reach the top of the boundary layer with sufficient SNR to be detected. The lidar beam also attenuates considerably when it encounters clouds or fog due to increased atmospheric scattering or attenuation. In Figure 6, it can also be seen that lack of aerosols limits the Doppler lidars' ability to measure above the boundary layer height during peak convective periods. During nighttime conditions, vertical velocity variance is low and is not effective in estimating z_i. In this study, the lowest range-gate is used as the stable boundary layer height from the lidar as a first guess. As mentioned earlier, nocturnal conditions during summer months are dominated by southerly winds where in the nocturnal boundary layer is capped by a low-level jet (Krishnamurthy et al., 2020). During these conditions, the RF model shows near constant z_i which is observed to be well correlated with radiosonde z_i (just below the LLJ height).
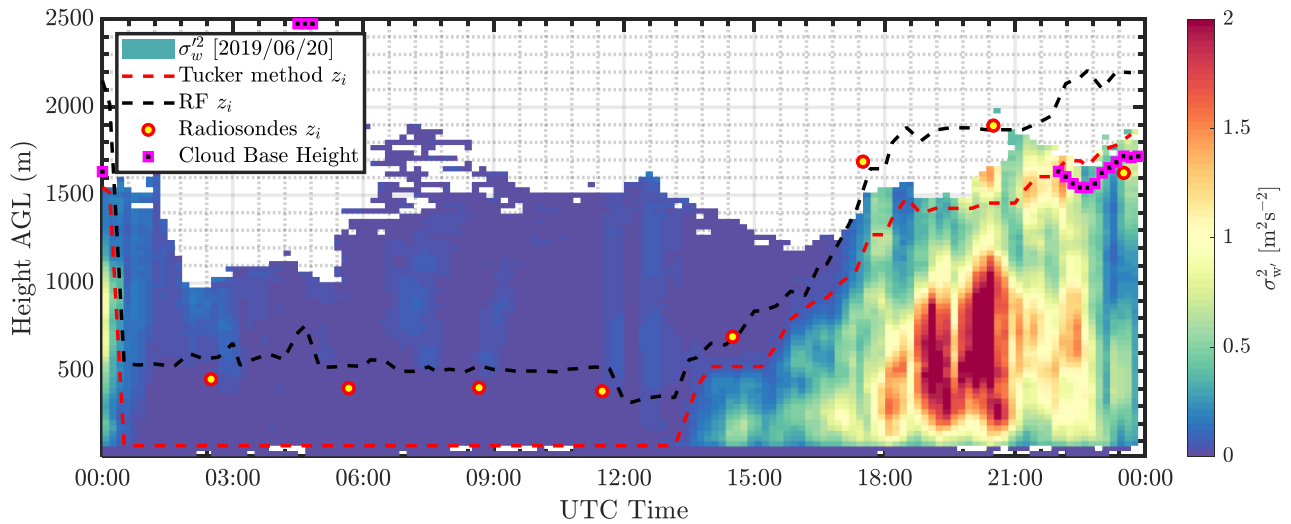
Figure 6: Boundary layer height estimates at the SGP central facility on June 20, 2019 from Tucker method (Tucker et al., 2009), RF model z_i, radiosondes z_i (Sivaraman et al., 2013), cloud base height estimates from lidar (Newsom et al., 2019), and the background colours represent vertical velocity variance measurements from Doppler lidar.

In Figure 7, the effectiveness of the RF model can clearly be observed. At 0300 hours and 0600 hours UTC, during stable nocturnal conditions, the RF model matches the radiosonde estimates very well. At 0900 hours UTC, a possible nocturnal convection initiation event results in high vertical velocity variance for several hours (Reif et al., 2017). Convection initiation refers to the process in which an air parcel is successfully lifted to its level of free convection and produces a precipitating updraft (Markowski and Richardson, 2010). The RF model is observed to detect that burst of convection and provide coherent boundary layer heights past 1200 UTC until daytime transition at ~1400 UTC. The correlation between RF model and radiosonde z_i estimates is very high. Therefore, various atmospheric interaction effects are aptly characterized by the parameters in the RF model. Hourly averaged z_i and daily maximum z_i averaged for each season in 2019 from Tucker method, RF model, and radiosondes are shown in Figure 8a. Although, the number of samples between the radiosondes and RF model estimates are vastly different, the generic trend in the hourly and seasonal boundary layer height variability is well captured by the RF model. Although the Tucker method captures the average boundary layer height trend, it shows a clear bias in convective boundary layer height estimates compared to radiosonde and RF model derived z_i values. As observed earlier from the time series analysis, a standard bias correction would not always improve z_i estimates from the Tucker method. Daily daytime maximum z_i estimates averaged over four seasons in 2019 from all three methods are shown in Figure 8b. Summer months (May through August) show high boundary layer heights. During these months, the peak convective period occurs during the daytime at around 2000 hours UTC, and the average boundary layer height as observed from the RF model is ~2100 m above ground level, which correlates well with radiosondes released during the same time period. During winter and fall months, the peak convective period does not always occur at 2000 hours UTC and therefore the maximum z_i estimates

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from radiosondes do not coincide with RF estimates. The Tucker method invariably underestimates maximum z_i during all seasons.
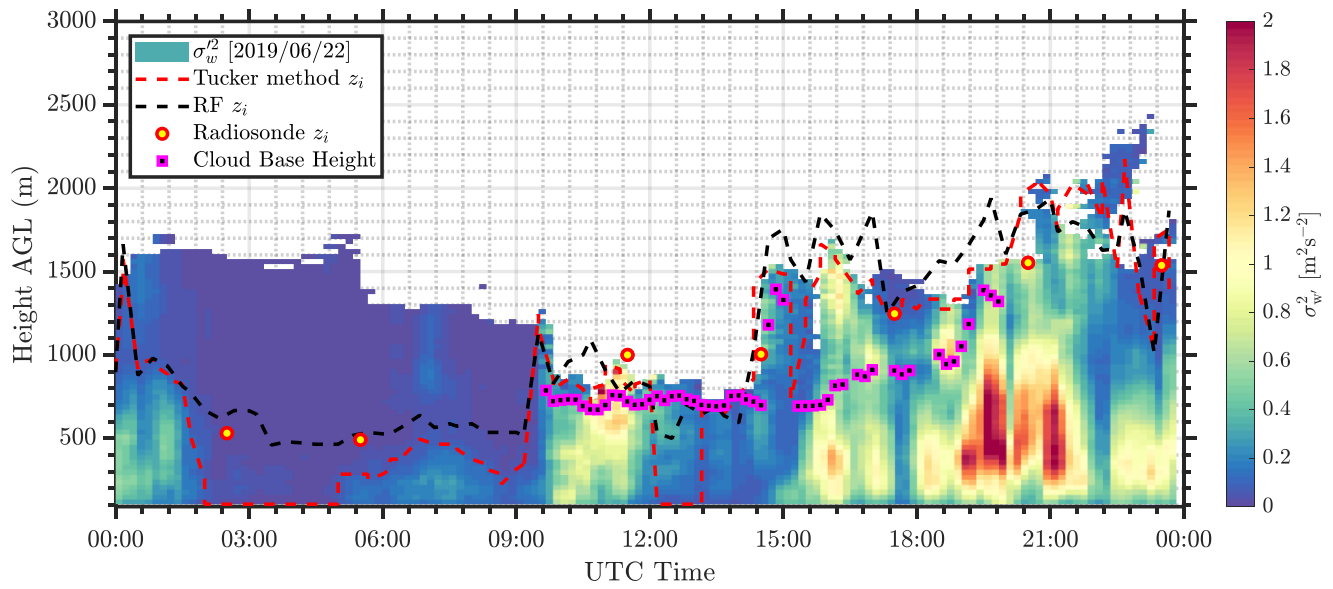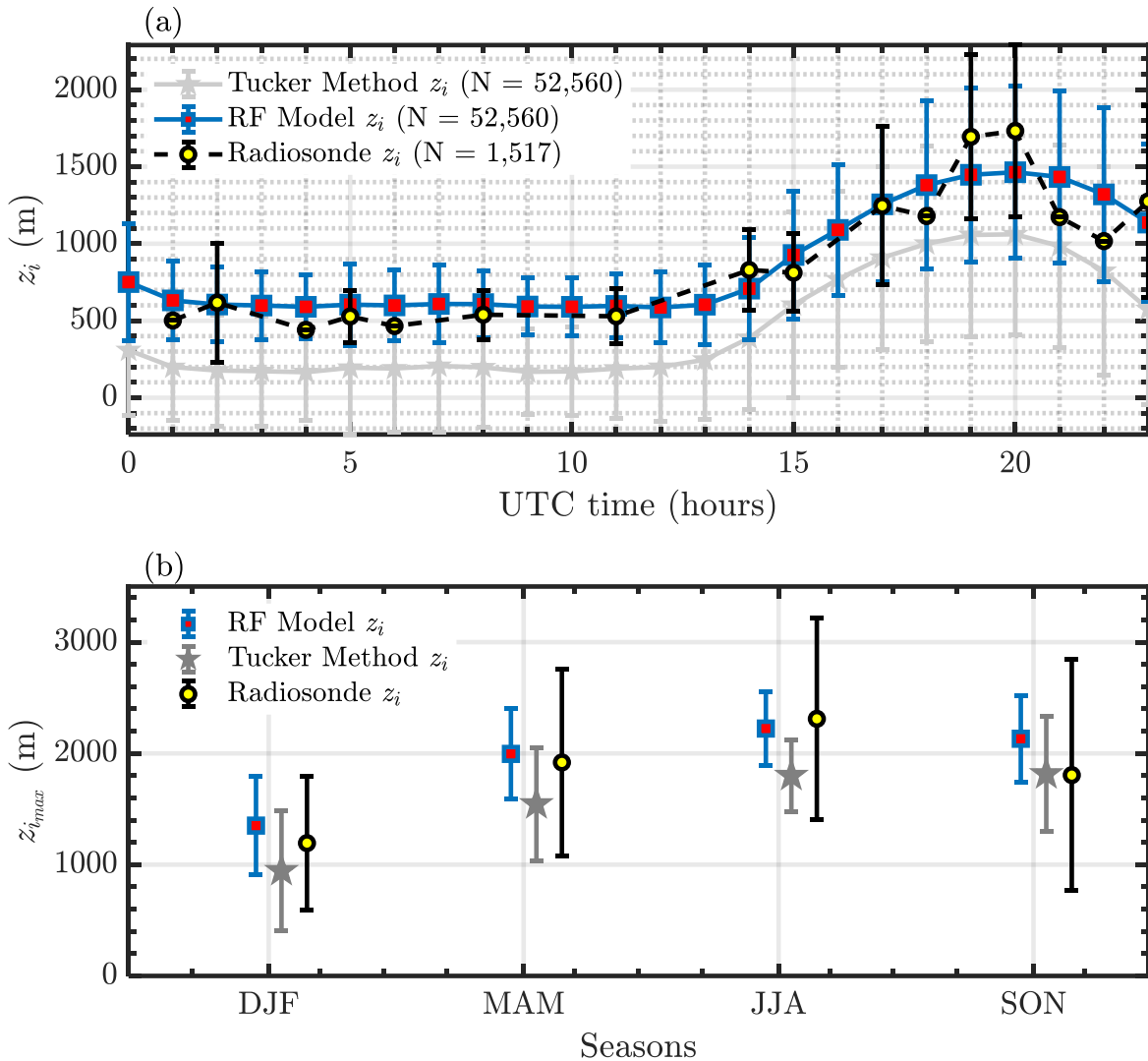
415

Figure 7: As in Fig. 6, but for June 22, 2019.

Figure 8: **a) Hourly averaged z_i estimates at SGP central facility for 2019 from RF, Tucker method, and radiosondes. Total number of samples (N) for each dataset is also shown in the legend. b) Daily daytime maximum z_i estimates for four seasons (DJF, MAM, JJA, SON) from RF, radiosonde, and Tucker method. The bars in both plots represent one standard deviation.**

4.2 Input Feature Importance

All the input features within the RF model explain approximately 82% of the total variance in the data. Table 4 provides the unbiased predictor importance estimates, which is computed by permuting or shuffling a variable in the model and estimating its mean square error (Breiman, 2001). If a predictor is significant in prediction, then permuting its values will affect the model error and vice versa. However, if two input variables are highly correlated (as is expected when testing

atmospheric forcing), it is highly unlikely that the reported importance values will accurately represent each variable's significance (Breiman, 2001). Based on this analysis, the most important parameter is the initial z_i guess from the Tucker method. This provides a very good first guess to the RF model, especially during convective conditions. Although the RF model is sensitive to the initial guess from the Tucker method, it is observed to be robust enough to ignore uneven spikes in z_i estimates due to noise in the lidar vertical velocity variance data (Figure 7). The second most important feature observed to have high correlation with z_i estimate is the hour of the day. A clear diurnal pattern in z_i, i.e., higher values in the daytime and near constant values during the nighttime, estimates are observed at SGP. Therefore, hour of the day can effectively classify the data, which is beneficial in the RF bagging process. Relative humidity also shows higher importance ($> 5\%$), where drier conditions are observed to have higher correlations with boundary layer height. Deep convection and larger z_i is generally a consequence of greater sensible heat flux and lower latent heat flux, which are primarily due to higher surface temperature and lower relative humidity. Based on an evaluation of z_i over Europe, it was also observed that relative humidity had a strong negative correlation with z_i, and surface temperature had a positive correlation (Zhang et al., 2013). Other features such as lidar attenuated backscatter, surface air temperature, Monin-Obukhov length, soil temperature, surface wind direction, and TKE all are observed to be important for accurately characterizing the boundary layer height at SGP. Other surface features such as surface friction velocity, sensible heat flux, longwave radiation, etc., have lower correlations with z_i within the RF model framework. Therefore, the model can be reduced to the list of parameters defined in Table 4 for optimal estimation of the boundary layer height at SGP.

Table 4: Key parameter/feature unbiased importance estimates during all conditions

Parameters/Features	% Importance
Tucker method z_i	58.67%
Hour of the day	10.05%
Surface Relative Humidity	6.82%
Attenuated Backscatter	2.90%
Surface Air Temperature	2.77%
Monin-Obukhov Length	2.77%
Soil Temperature	1.92%
Surface Wind Direction	1.78%
Turbulence Kinetic Energy	1.32%
Others	$< 11\%$

To assess the key features during nighttime, a similar RF model was built by conditionally sampling nighttime data. During nighttime, the key parameters that affect the RF model predictions are shown in Table 5. It is interesting to note that the key features deemed important during nighttime are significantly different compared to all conditions, and the percent importance is more evenly distributed across many features. This result alludes to the fact that nocturnal stable boundary layers are indeed complex to model and several processes are at play (Fernando and Weil, 2010). Monin-Obukhov length is

observed to have the highest impact on the nighttime RF model estimates and is consistent with theory on stable boundary
455   layers (Zilitinkevich, 1972, Zilitinkevich and Baklanov, 2002). Although nighttime z_i initial guesses are generally a constant
(lowest lidar range-gate if no high vertical velocity variance is observed), the initial guess has shown to be effective in adjusting
the RF model z_i estimates. Other local parameters such as soil temperature, surface air temperature, dew point temperature,
longwave radiation and turbulence kinetic energy are observed to be correlated with nighttime z_i estimates. One of the stable
boundary layer models by Brost and Wyngaard 1978 is given by:

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$$z_i = 0.4 \left(\frac{u_* L}{|f|} \right)^{1/2}$$
(4)

Where u_* is the friction velocity, L is the Monin-Obukhov length, and f is the Coriolis parameter. As shown in Table 5, the
nighttime parameters deemed important by the RF model include both Monin-Obukhov length and friction velocity. As
465   discussed earlier, the dominant feature of nocturnal boundary layer at SGP is the presence of the LLJ. The turbulence
production at SGP is not only influenced by surface characteristics but also heavily influenced by the presence of the LLJ. A
preliminary comparison with the above model to RF model z_i estimates at SGP was very poor, as the radiosondes (from all
three methods) invariably pick up the nocturnal LLJ at SGP as the height of the boundary layer. Although the height of the
nocturnal boundary layer height could be debatable at SGP, the premise of this paper is to show the effectiveness of the RF
470   model in tracking and detecting the boundary layer height and the input boundary layer height provided to the model. Further
research needs to be conducted on providing widely acceptable nocturnal boundary layer height at SGP, and a trained RF
model can provide continuous boundary layer height estimates even in nocturnal conditions with acceptable levels of accuracy.

Table 5: Key parameter/feature unbiased importance estimates during nighttime conditions

| Parameters/Features	% Importance
Monin-Obukhov Length	19.12%
Tucker Method z_i	11.49%
Soil Temperature	7.81%
Surface Air Temperature	7.56%
Dew Point Temperature	6.31%
Longwave Radiation	6.24%
Turbulence Kinetic Energy	5.21%
Net radiation	4.72%
Surface wind speed	4.28%
Surface wind direction	3.76%
Lidar Dissipation rate variance	3.54%
Surface friction velocity	3.45%
Cloud base height	3.40%
Shortwave radiation	3.26%

Others	< 10%

475

The partial dependence of key features on z_i during all conditions is shown in Figure 9. Partial dependence estimates show the marginal effect of features on the predicted outcome of an ML model. Therefore, a higher partial dependence estimate corresponds to higher sensitivity to the predicted outcome, in our case the boundary layer height and vice versa. From Figure 9, we see that RF model z_i is sensitive to warmer soil temperatures, lower relative humidity conditions, daytime hours, higher

480 z_i from Tucker method, northerly wind directions, and stable atmospheric conditions. Most of these conditions would mimic dry convective conditions, with increased turbulence activity within the boundary layer. Monin-Obukhov length is observed to effectively categorize the training data into stable and unstable atmospheric conditions, with high partial dependence estimates during stable boundary layer conditions. Similar relationships can be derived for other parameters. It is important to note that the parameters shown to be important with respect to the RF model are features that successfully aid in the RF

485 bagging process. Santenello et al., 2007 and Tang et al., 2018 showed parameters such as soil moisture and evaporative flux to be key variables in warm seasons, in a 2-parameteric regression framework, to affect boundary layer properties. Within the RF model, although those parameters are deemed important, soil temperature, lidar backscatter, and relative humidity were shown to have a higher impact on boundary layer height at each site.

In this research, the input features into the RF model are standard atmospheric parameters (such as wind speed,
490 temperature etc.). An alternate approach to this effort would be to provide several non-dimensional inputs (such as Bulk Richardson number, Froud Number, etc) as inputs because they capture multiple dimensions of the data with a single variable (Vassallo et al., 2020). Because non-dimensional scaling is a common approach in atmospheric fluid dynamics to detect patterns in the data, a similar approach would provide the RF model with various relations and be helpful in classifying the data better. But further research needs to be conducted in defining the key nondimensional parameters that affect z_i and is a
495 part of future work.
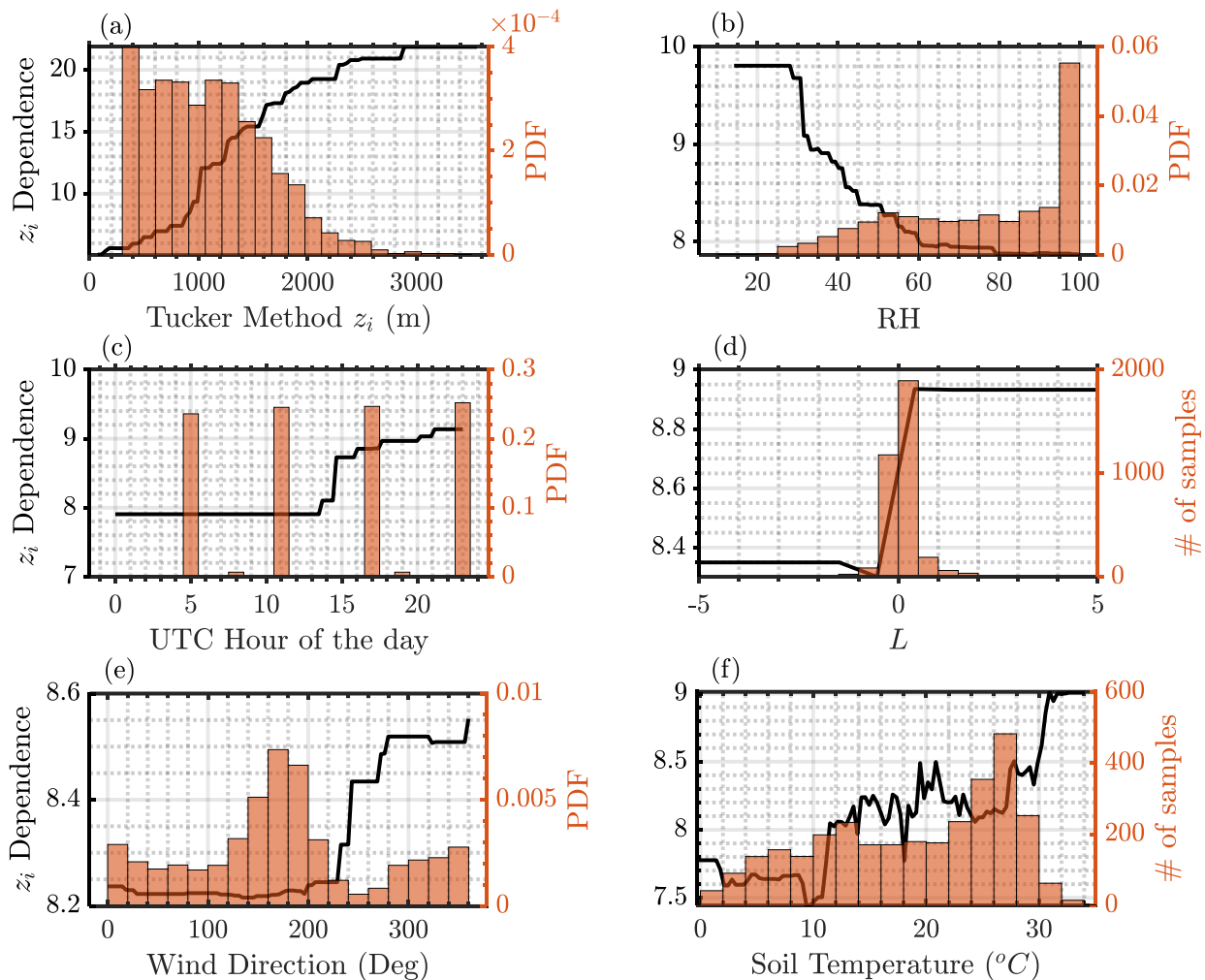
Figure 9: RF partial dependence during all conditions from a) Tucker method z_i, b) relative humidity c) hour of the day, d) Monin-Obukhov Length, e) surface wind direction, and f) soil temperature to boundary layer height at the central facility. High dependence shows more sensitivity of the RF model to the bin of feature values.

5 Normalized vertical velocity variance profiles

Within a convective boundary layer, vertical velocity variance profiles are often scaled by the convective velocity scale (w*), which is a function of z_i (Lenschow et al., 1980) for analysis. Therefore, any error in z_i estimates can result in altering the vertical velocity variance profiles. Herein, we attempt to estimate the effect of z_i on normalized vertical velocity variance profiles and convective velocity estimates, often used to compare results in boundary-layer studies and in the functional relationships used in atmospheric models. The convective velocity scale is given as

23

$$w^* = \left[\frac{gz_i\overline{w'\theta'}}{\theta}\right]^{1/3} \tag{5}$$

510

where, g is the gravitational constant, θ is potential temperature, and $\overline{w'\theta'}$ is heat flux. The heat flux is obtained from the surface Eddy Covariance system at SGP C1 (Cook 2016) and potential temperature is measured at 4-m. An uncertainty in z_i will cause a non-linear effect in the convective velocity scale estimates. Assuming the uncertainty in z_i can be given as z_i', and the mean is given as $\overline{z_i}$. The error caused in the convective velocity scale due to uncertainty in z_i can be formulated as

515 shown below:

$$w^* = \left[\frac{g(\overline{z_i} + z_i')\overline{w'\theta'}}{\theta}\right]^{1/3} \tag{6}$$

This can also be written as

520 $$w^* = \left[\frac{g\overline{z_i}\overline{w'\theta'}}{\theta}\right]^{1/3}\left(1 + \frac{z_i'}{\overline{z_i}}\right)^{1/3} \tag{7}$$

Therefore, the convective velocity scale error due to uncertainty in z_i can be estimated using the term $(1 + x)^{1/3}$, where $x = \frac{z_i'}{\overline{z_i}}$. Based on observations at SGP C1, z_i from Tucker method is observed to be negatively biased to radiosonde estimates. The ratio, $(\frac{z_i'}{\overline{z_1}})$, is calculated using the median error between Tucker method and RF model z_i by the median z_i using the RF model.

525 The ratio is calculated to be approximately -0.28 for data from 2016 to 2019. This would result in an uncertainty of approximately 10% in the convective velocity estimates when Tucker method z_i values are used in the calculations. Although this is an average, during certain conditions (e.g., during transition time periods) the effect of poor characterization of z_i can be even larger. Figure 10 shows average vertical velocity variance profiles during convective time periods at SGP from 2015 to 2019 using z_i estimates from Tucker method and RF model. Higher z_i values result in lower scaled vertical velocity variance

530 estimates. Differences in variance profiles are observed to be smaller during daytime transition (1500 hours UTC or 0900 hours local time), as the Tucker method generally provides reliable z_i estimates. While during peak convective conditions (2000 hours UTC) and evening transition (2300 hours UTC), as observed earlier, the Tucker method z_i estimates tend to diverge from radiosonde z_i depending on the scenario and are negatively biased. Overall, the error introduced in the scaled vertical velocity variance profiles due to Tucker method z_i are above 15%.

535 As per definition, the turbulence at the top of the boundary layer is expected to be near zero, except during cloudy conditions. As shown in Figure 10, during morning transition periods, when the lidar does measure above the boundary layer, the scaled vertical velocity variance profiles do converge to zero. In contrast, during peak convective conditions the scaled profiles do not converge to zero and are observed to have an offset of generally around 0.1 at z_i (also observed in Lareau et al.,

24

2018). This could be due to higher uncertainty in lidar vertical velocity variance estimates near z_i, ineffective filtering of the
540   lidar false alarm rates (Bouquet et al., 2016), uncertainty in surface in situ measurements, and the possibility of residual
turbulence above the boundary layer during downdrafts/updrafts.
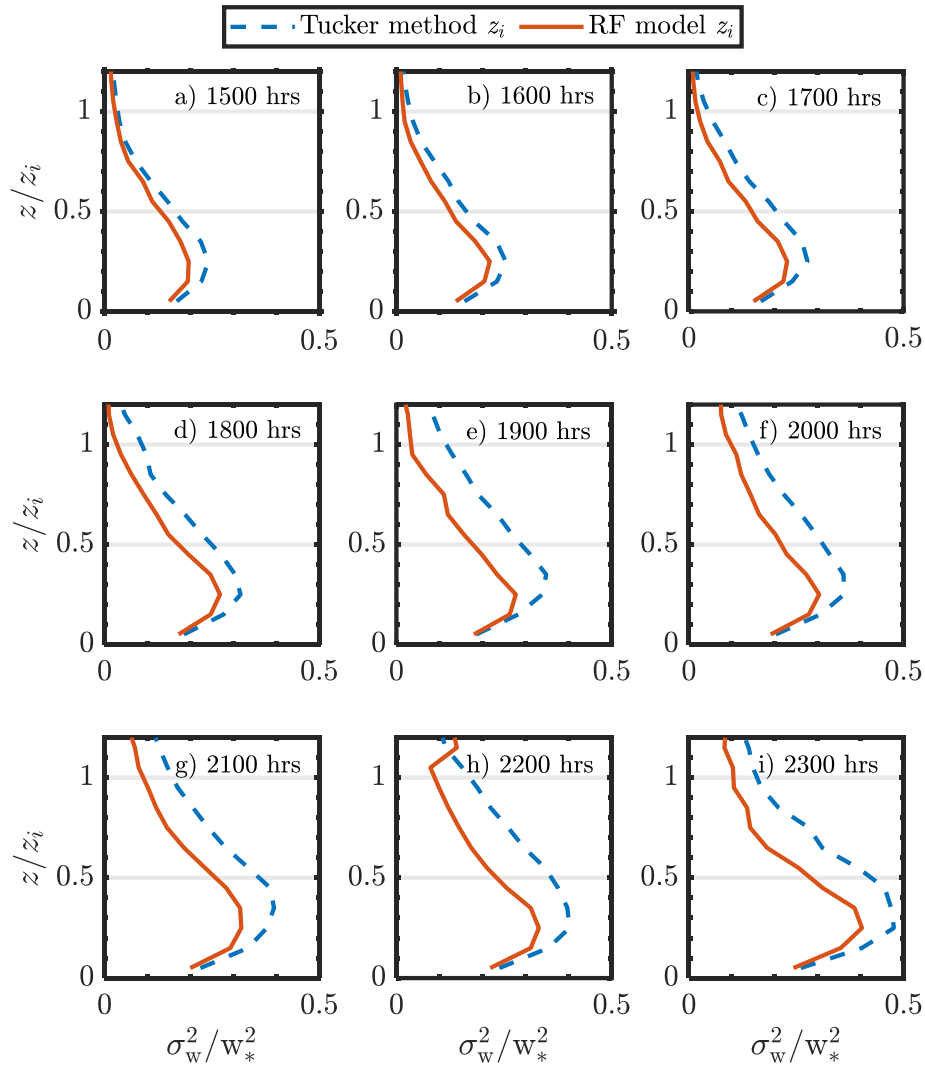
Figure 10: Average normalized vertical velocity variance profiles during convection periods [1500 UTC to 2300 UTC (a-i)] at SGP
545   **from 2015 to 2019 versus non-dimensional height using Tucker method and RF model estimated** z_i**. Appropriate** z_i **(RF model or**
Tucker method) was used in both X and Y axis scaling.

6 Case Study: Preliminary Model Comparisons

We expect the RF model z_i outputs to be developed into a VAP that will be easily accessible and can be used by
researchers across the community. Therefore, the motivation for this case study is to provide a preliminary comparison
between model estimated z_i and the RF model z_i. These types of comparisons will help understand the impact of boundary-
layer properties on model physics and guide further in improving parameterizations used to represent boundary-layer
turbulence.

The surface and sub-surface layer measurements are key for understanding land-atmosphere interactions. Land–
atmosphere interactions drive Earth's surface water and energy budgets. They can alter clouds and precipitation around a
region, affect the growth of the planetary boundary layer height, and influence the persistence of extremes such as droughts.
In view to better understand land-atmosphere interactions, a field campaign, Holistic Interactions of Shallow Clouds, Aerosols
and Land Ecosystems (HI-SCALE), was conducted at the SGP site in Oklahoma (Fast et al., 2019). The field campaign was
conducted from April to September of 2016, with two four-week intensive observational periods in May and September.
Simulations were conducted on select clear sky days during the HI-SCALE filed campaign. Two simulations using different
modelling systems were performed: Energy Exascale Earth System Model (E3SM; Golaz et al., 2019) Atmosphere Model
version 1 (EAMv1; Rasch et al. 2019), and a LES model. The Weather Research Forecasting (Skamarock et al. 2008) LES is
set up in the same way as that used in operational LASSO (Gustafson et al., 2017, 2020). The Weather Research Forecasting
model version used is v3.7. The model horizontal domain is square, doubly periodic, and 25.6 km wide with a 100-m horizontal
grid spacing. The model top is set at 14.8 km above the surface. There are 226 vertical levels with a vertical grid spacing of
~30 m in the lowest 5 km. The model is run for 15 hours for each case day starting at 6 AM. The Rapid Radiation Transfer
Model for Global Climate Models parameterization is used for shortwave and longwave radiation (Clough et al. 2005; Iacono
et al. 2008; Mlawer et al. 1997). The Thompson parameterization is used for microphysics (Thompson et al. 2004; 2008). The
Deardorff 1.5-order turbulent kinetic energy approach is used for subgrid-scale parameterization (Deardorff 1980). The model
is initialized with ARM sounding from the SGP site (ARM user facility, 2001). The surface sensible and latent heat fluxes are
horizontally uniform and prescribed from the ARM constrained variational analysis data product (ARM user facility, 2004).
The large-scale forcing is also taken from the ARM variational analysis data product. Due to high computational expense, the
LES model was run for three days while EAMv1 model was run for the entire duration of the HISCALE campaign. The
EAMv1 model is run in the standard coarse-resolution configuration with ~ 1-degree horizontal grid spacing and 72 vertical
levels and a physics timestep of 30 minutes and a cloud and turbulence timestep of 5 minutes. In these models, z_i was estimated
using resolved vertical velocity variance estimates from the LES or the parameterized vertical velocity estimate from the Cloud
Layers Unified by Binormals (CLUBB) boundary-layer parameterization applied in E3SM (Golaz et al., 2002; Larson and
Golaz, 2005; Bogenshutz et al., 2013; Larson, 2017), and like the Tucker method a low threshold was used to estimate the
depth of the convective boundary layer. Estimates of boundary-layer height from E3SM and LASSO were not made during
nocturnal conditions. The LASSO simulations extend only from approximately sunrise to sunset so nocturnal estimates of the

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boundary-layer height are not possible. The E3SM simulations generally have too much nighttime turbulence, making estimates of the boundary-layer height unreliable at night.

Figure 11 shows Doppler lidar vertical velocity variance measurements for three days during the HI-SCALE campaign (September 10 – 12, 2016) and boundary layer height estimates from RF model, radiosondes, LASSO, and E3SM.

585 Because the RF model provides z_i estimates at a much finer temporal resolution than radiosondes, these estimates are ideal for comparing with models and assessing areas where model performance can be improved. Therefore, in this preliminary comparison, the primary motivation is to see if we can identify areas where the models diverge significantly by using near continuous accurate z_i values from the RF model. Due to computational expense, we could evaluate only three days of model results, but further research is needed in performing a thorough evaluation.

590 September 10th was relatively calm with northerly winds and no clouds were observed during daytime. September 11 and 12 had southerly winds and clear sky conditions during both daytime and nighttime. Daytime maximum surface air temperature is observed to increase progressively from September 10 to 12, and as mentioned earlier higher air temperature results in deeper planetary boundary layer due to increased convection (see Figure 11).

Overall, the LES model compares better to RF estimates, while EAMv1 is observed to underestimate z_i. Due to the

595 coarse resolution of EAMv1, ~ 100 km, z_i estimates are averaged over a large domain and do not generally capture the fine scale variability. Although the LES model is observed to pick up morning transition, it diverges from observations during evening transitional periods and does not capture the decay of turbulence accurately. During peak convective conditions, when the vertical velocity variance is large, the LES is observed to correlate very well with the RF model and radiosonde z_i. Although EAMv1 is observed to mostly underestimate z_i compared to RF model estimates, occasionally the model captures the peak

600 convective trends. Like the LES model z_i, the EAMv1 also is not observed to capture evening decay of turbulence accurately but is observed to not track the early morning transition at SGP as well. Such systematic differences between the model and data are crucial for targeting future research directions. Further study is needed to evaluate the reasons why models tend to deviate during early morning and/or evening transition periods.
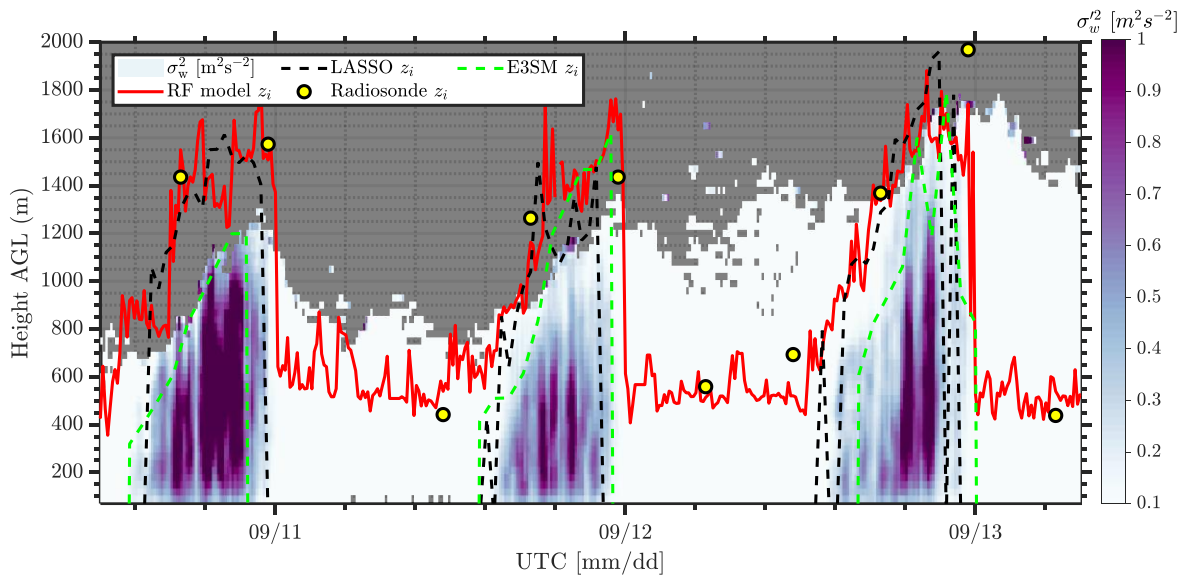
Figure 11: Vertical velocity variance (σ_w^2) estimates from Doppler lidar for three days [September 10, 11, and 12, 2016] with z_i estimates from a) RF model (red solid line), b) radiosondes (yellow circles), c) LASSO model (black dashed line), and d) E3SM model (green dashed line).

6 Summary

This study used a range of near surface, sub-surface and Doppler lidar parameters to predict boundary layer heights at the ARM SGP site using an RF model. The RF model was trained using several years of data, and the model was validated with radiosonde estimates of boundary layer height. Because the Tucker method is observed to be low biased during peak convective periods due to low SNR of the Doppler lidars as the boundary layer deepens, the RF model corrects for the bias. Seasonal and diurnal variations of z_i as observed from radiosondes correlate well with RF model z_i. During convective boundary layer conditions, the mean absolute error of boundary layer height estimated by the RF model is reduced by almost 50% compared to the Tucker method. Significant improvement was also observed during clear sky, and cloudy conditions. Nocturnal estimates from the RF model were not well correlated with radiosonde measurements, mostly due to near constant estimates of nocturnal boundary layer height at SGP (due to the presence of the LLJ). Moreover, valuable information on the impact of surface parameters on nocturnal z_i estimates by the RF model provides avenues for further research in accurately estimating stable boundary layer heights at SGP. The key variables that have shown to have the largest impact on the RF model predictions are the initial guess of the boundary layer height from the Tucker method, hour of day, surface relative humidity, soil temperature, and attenuated backscatter (aerosol loading). During nocturnal conditions, several parameters, such as the Monin-Obukhov length, soil temperature, and surface air temperature influence the RF model estimates. These

625 parameters are aligned with theoretical parameterization schemes used to estimate boundary layer heights. The RF model used in this study explains around 82% of the variance in the data at SGP C1.

Uncertainty in convective boundary layer heights results in more than 10% difference in convective velocity scale estimates when the Tucker method is used. The uncertainty results in more than 15% error in scaled velocity variance estimates, which are commonly used in atmospheric models. Limited comparison between microscale model z_i estimates to

630 RF model and radiosonde z_i values show increased correlation during heightened land-air interaction events. Large-eddy simulation estimates are observed to match the convective z_i variability as estimated by the RF model while the global model performance is variable. Neither models capture the evening transitional decay of turbulence accurately.

There are a number of ways to expand on the research presented here. Future will could focus on improved data imputation models to better handle missing data, a RF model z_i uncertainty framework using individual RF tree predictions,

635 and finally a study of the effect of near-by wind farms and surface heterogeneity have on the boundary layer height.

Appendix A

The range availability of the ARM SGP C1 Doppler lidars used in this study is provided below. Figure A1 shows the height range and data availability at SGP C1 for vertical stare scans and Figure A2 for processed VAD scans. The lidar range is consistent across multiple years of operation. The availability of data from the scanning Doppler lidars at SGP C1 is

640 significantly reduced for altitudes greater 1 km (60% availability), which could limit its ability to reach the top of the boundary layer during all conditions.
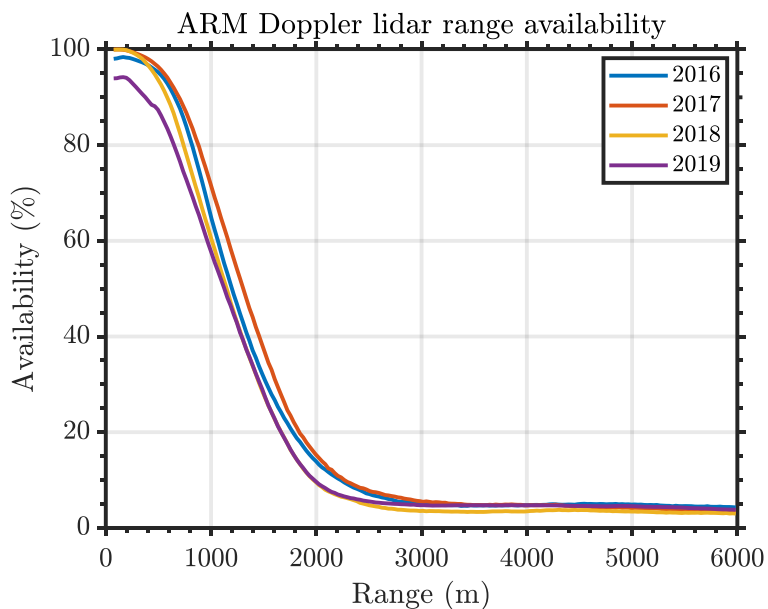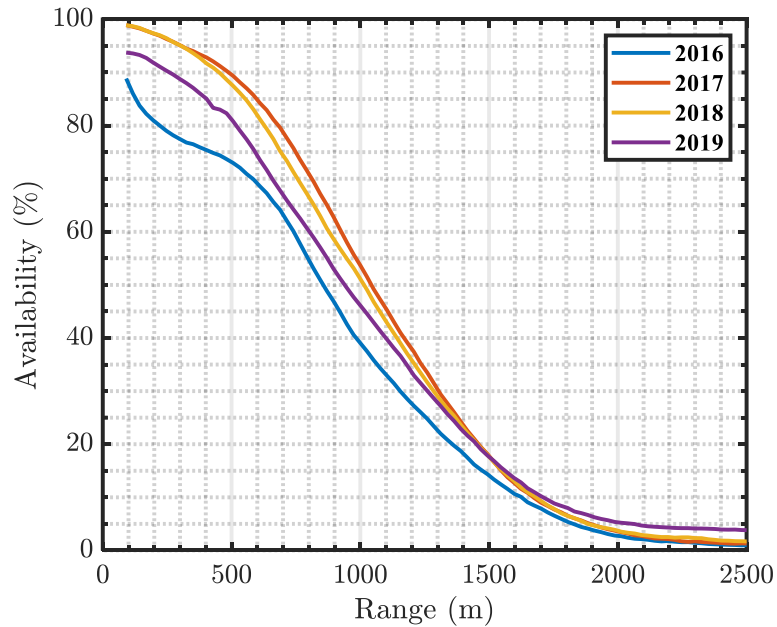

Figure A1: ARM SGP C1 Doppler lidar range availability versus range from vertical stares from 2016 to 2019 after SNR filtering (threshold of 1.008 dB).

645

Figure A2: ARM SGP C1 Doppler lidar wind speed profile range availability versus range using processed VAD scans from 2016 to 2019 after SNR filtering (threshold of 1.008 dB).

650 **Appendix B**

The RF model develops several regression trees by regrouping the data based on several input features. Figure A1 below shows one of the trees developed by the model used in this article. The leaf nodes are the z_i estimates from radiosondes and the split nodes represent the surface and lidar data shown in Table 1. MATLAB built-in functions were used for the development of the RF model.

655
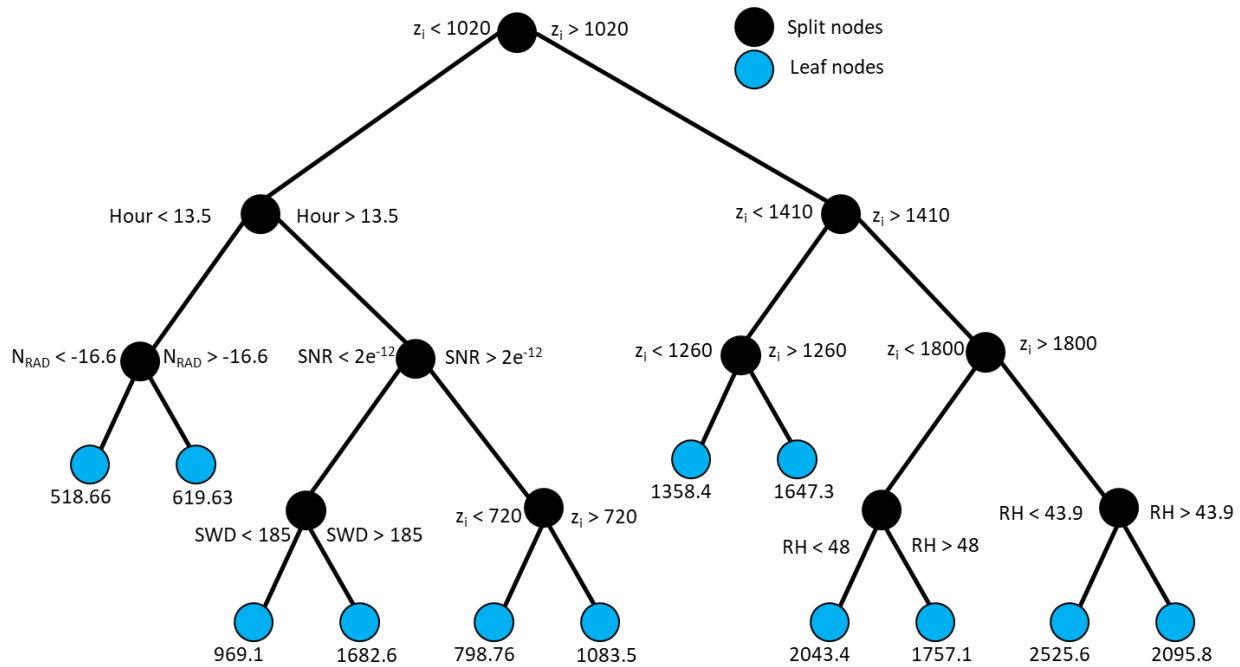
Figure B1: A sample regression tree developed by the RF model. Z_i is the Tucker method boundary layer height estimate, SNR is signal to noise ratio, NRAD is the normal radiation, RH is relative humidity, SWD is surface wind direction, Hour is hour of the day. The black circles represent the split nodes and the cyan circles represent the leaf nodes developed for this regression tree (aka boundary layer height estimates from radiosondes).

Acknowledgements

Data Availability

All data used in this article are publicly available data on the ARM webpage. (https://adc.arm.gov/discovery/#/). Appropriate labels and manual citations for all the data used are provided in the manuscript.

Author Contribution

RK and RN conceptualized the concept, RK, RN, and DDT were involved in the development of the algorithm, RK did the data processing and analysis of the RF algorithm, surface stations, lidar and radiosonde results, HX performed the large-eddy simulation runs, PM performed the E3SM runs, LB calculated the boundary layer height from model outputs, RK wrote the manuscript with contributions from all authors.

680 Competing interests

The authors declare no competing interests.

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