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Five Year Comparison of Mixing Height Determinations at the Savannah River Site

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EXECUTIVE SUMMARY

Air quality dispersion modeling is performed for the Savannah River Site (SRS) to demonstrate compliance with applicable regulations. The AMS/EPA Regulatory Model (AERMOD) modeling system is an EPA recommended model for air quality applications with a data processor (AERMET) to incorporate meteorological data collected on site. AERMET parameterizes or calculates meteorological variables that are not directly measured onsite. One of the parameters estimated by AERMET is the atmospheric mixing height. While the mixing height is not currently a measurement input into AERMET, SRS has the capability to measure the local mixing height. The Savannah River National Laboratory (SRNL) operates a Vaisala CL31 Lidar Ceilometer which estimates mixing height from aerosol backscatter. This study compares the parameterized mixing height from AERMET to the ceilometer estimated mixing height for the current regulatory period at SRS incorporating data from 2015-2019. Results from this study showed the average daily minimum values (morning) from AERMET were an order of magnitude lower than the commonly used Holzworth (1972) method and the ceilometer estimated mixing heights. Additionally, on average, the ceilometer exhibited a daily maximum mixing height value that occurred 1-3 hours later than the AERMET estimated maximum. This difference is likely due to the nighttime atmospheric mixing height assumptions and calculations used by AERMET. The AERMET algorithm cuts off mixing height growth at sunset while the ceilometer data show ongoing evening convection typical of the southeastern United States. These results suggest that the AERMET parametrization scheme assumptions may not be representative of a forested landscape and evening convection which could account for more mixing overnight. The results obtained in this study are significant for air dispersion modeling applications for regulatory purposes and worker safety. Mixing height can impact model estimated pollutant concentrations. A greater mixing height will provide more volume for pollutant dispersion. This report documents efforts to quantify the dependence of mixing height inputs toward a conservative estimated pollutant concentration.

TABLE OF CONTENTS

LIST OF TABLES.....	viii
LIST OF FIGURES	viii
LIST OF ABBREVIATIONS.....	ix
1.0 Introduction.....	1
2.0 Experimental Procedure.....	1
2.1 Onsite Data.....	1
2.2 Mixing Height	2
2.2.1 Ceilometer Data.....	2
2.2.2 AERMET.....	2
3.0 Results and Discussion	3
4.0 Conclusions.....	7
5.0 Funding	8
6.0 References.....	8

LIST OF TABLES

Table 3-1. Average daily maximum mixing height from Holzworth, AERMET (Z_i), and ceilometer (MLH1, MLH2, MLH3) estimates.	3
Table 3-2. Average daily minimum mixing height from Holzworth, AERMET (Z_i), and ceilometer (MLH1, MLH2, MLH3) estimates.	3

LIST OF FIGURES

Figure 3-1. Monthly average of mixing height by season for MLH1 and AERMET.....	5
Figure 3-2. Monthly average of mixing height by season for MLH2 and AERMET.....	6
Figure 3-3. Monthly average of mixing height by season for MLH3 and AERMET.....	7

LIST OF ABBREVIATIONS

AERMOD	AMS/EPA Regulatory Model
AERMET	AERMOD Meteorological Preprocessor
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
DOE	Department of Energy
EPA	Environmental Protection Agency
CCF	Central Climatology Facility
NWS	National Weather Service
USGS	United States Geological Survey
PBL	Planetary Boundary Layer
MLH1	Mixing Height of the Largest Gradient
MLH2	Mixing Height of the Second Largest Gradient
MLH3	Mixing Height of the Third Largest Gradient
Z_i	AERMET Mixing Height
LST	Local Standard Time

1.0 Introduction

The Savannah River Site (SRS) is a 310 square mile Department of Energy (DOE) site located in Aiken, South Carolina. To comply with regulatory requirements, the AMS/EPA Regulatory Model (AERMOD) is the preferred modeling system for air dispersion modeling to estimate pollutant transport that could impact worker safety. AERMOD uses the AERMOD Meteorological preprocessor (AERMET) to process meteorological measurements as input to the model (EPA, 2019). AERMET also produces estimates of meteorological parameters that are not directly measured, using parametrization schemes. AERMET incorporates meteorological data collected by the onsite meteorological monitoring program (Weinbeck et al., 2020) to create an AERMOD ready dataset for use in air quality modeling and permitting applications. The onsite meteorological data from 2015-2019 is the current regulatory data period used at SRS. Besides the typical regulatory use of AERMOD (air permits), it is used to determine the worst case (bounding) pollutant concentrations associated with the most restrictive dispersion conditions within the 5-year period. Since the 5-year period contains a wide range of meteorological conditions, this approach is preferred over simplified extreme conditions (F stability and 1 m/s wind speed), which are often used to depict extreme dispersion conditions (Pontiggia et al., 2009; Zoras et al., 2006).

One of the parameters estimated by AERMET is atmospheric mixing height. Mixing height is an important parameter for air pollution modeling which has a large impact on the concentration of pollutants at ground level (Lena & Desiato, 1999). A greater mixing layer provides more volume for pollutant dispersal, whereas a smaller volume of air has less space to mix resulting in a higher pollutant concentration. Since mixing layer height is an important parameter in air dispersion modeling, it is important to ensure the mixing layer used as input into air dispersion modeling is representative of local conditions.

There are several methods to estimate mixing height, three of which are included in this study. The parcel method (referred to as the Holzworth Method) estimates mixing height from a sounding temperature profile using radiosonde data. A second method consists of using remote sensing techniques to estimate the height of the mixing layer. For this method, we use a Vaisala CL31 Lidar Ceilometer operated by the Savannah River National Laboratory (SRNL). Lastly, the mixing height estimated from the AERMET parametrization scheme is included. The purpose of this study is to evaluate local mixing heights calculated from the ceilometer backscatter compared to the AERMET parameterized mixing height and the parcel method which relies on geographically displaced atmospheric soundings. The comparison was conducted using a 5-year dataset for 2015-2019. As previously mentioned, this is the latest approved 5-year dataset and is currently used for safety and regulatory modeling at SRS. The average daily maximum and minimum mixing heights from the ceilometer and AERMET estimates were obtained for each season and compared against the widely used Holzworth (1972) estimates. Additionally, average hourly values were obtained for each season using the 5-year dataset to illustrate the average daytime progression of the mixing height as estimated by the ceilometer and by AERMET. Comparing these three methods for estimating mixing height will determine which method is the most representative and should be used as an input for future air dispersion modeling.

2.0 Experimental Procedure

2.1 Onsite Data

SRNL maintains the SRS onsite meteorological program to aid with emergency response, air quality monitoring, and support engineering analysis. The meteorological program includes 9 towers onsite (Weinbeck et al., 2020). Each of the meteorological towers are equipped with temperature, relative humidity, and wind instrumentation at 61 m above ground level. The Central Climatology Facility (CCF) near the center of SRS has instrumentation at four levels: surface conditions measuring temperature at 2 m and wind at 4 m; and three elevated levels (18 m, 36 m, and 61 m) measuring temperature and winds.

Additional surface measurements at CCF include solar radiation, precipitation, and barometric pressure recorded every 15 minutes.

Meteorological data files were prepared using AERMET, which incorporates the National Weather Service's (NWS) hourly observations from Bush Field in Augusta, GA, upper air soundings from the NWS Atlanta, GA (Peachtree airport) radiosonde station, and quality-assured 15-minute values of wind and temperature at four levels (2/4 m, 18 m, 36 m and 61m AGL) from CCF. The five-year period used includes the years 2015-2019. Data that did not meet quality control criteria was not included in the text file, and a value indicative of 'missing data' was assigned to the empty timestep consistent with AERMET input data requirements. Quality assurance procedures for SRS meteorological data are described in Weinbeck et al. (2020). A more detailed description on the five-year quality assured dataset for the site and the process to create this is provided in Weinbeck (2022) and Rivera-Giboyeaux (2022). Values used by AERMET for roughness length, Bowen ratio, and albedo were determined from EPA's AERSURFACE algorithm (build 20060). Input to the algorithm consisted of a United States Geological Survey (USGS) National Land Cover Data image for 2016 (Wickham et al., 2021). These images were analyzed for the area around CCF and the Bush Field station in Augusta, GA (which is the alternate site used for data substitution when data is missing from CCF). Monthly wind sector values of surface parameters were generated and imported into AERMET to then generate the meteorological files used by AERMOD (Weinbeck, 2022).

2.2 Mixing Height

2.2.1 Ceilometer Data

A Vaisala CL31 ceilometer is located at SRS to support aviation operations. Additionally, it is used to make measurements to estimate mixing height. The ceilometer transmits 910 nm laser pulses vertically. These pulses are scattered by aerosol, clouds, precipitation, fog, mist, and haze; the ceilometer subsequently detects the pulse backscatter strength and timing. The two-way attenuated backscatter profile from aerosols in the boundary layer is used to observe the planetary boundary layer (PBL) structures (e.g. sea breezes (Viner et al., 2021), fire plumes). The strength of the backscatter signal indicates where particle concentrations are higher, usually within the PBL, and a weaker signal where fewer particles exist, i.e., in the free atmosphere (Brooks, 2003). A gradient in backscatter signal is used as a proxy for the mixing layer height, as regions with uniform aerosol loading indicate regions where aerosol are well-mixed due to constant mechanical or convective turbulence, whereas large differences in aerosol loading indicate a drastic change in mixing conditions and are characteristic of a boundary between layers in the lower atmosphere.

The Vaisala CL31 ceilometer integrates data to obtain backscatter profiles (Weinbeck et al., 2020). Ceilometer data collected prior to February 5, 2019 was configured for 30 second reporting intervals and 20 meter resolution. After February 5, 2019 the ceilometer was configured for 15 second reporting intervals and 5 meter resolution. An automated algorithm following the method outlined by Brooks (2003) identifies strong gradients in the two-way attenuated backscatter and the respective height where the gradient is found as the mixing layer height. Using this method, three estimates of the mixing layer height are determined corresponding to the height of the largest gradient (MLH1), the height of the second largest gradient (MLH2), and the height of the third largest gradient (MLH3). The ceilometer was considered the ground truth for determining the mixing height at SRS.

2.2.2 AERMET

Two mixing height values are calculated in AERMET: mechanical mixing layer height and convective mixing layer height. The convective boundary layer is characterized by a warm surface, common during daytime over land, when compared to the air directly above results in strong surface heat fluxes (Honnert et al., 2020). The mechanical boundary layer is formed from friction exerted by the wind against the surface

which causes the wind to be sheared creating turbulence (Cushman-Roisin, 2014). The final mixing height used in AERMOD is dependent on the condition of the boundary layer. AERMOD determines whether convective or stable conditions are present using the Monin-Obukhov length (L). For $L < 0$, convective conditions are assumed and AERMOD uses the larger of calculated the mechanical mixing height and convective mixing height. In turn, when $L > 0$ stable conditions are assumed and the mixing height is considered exclusively a result of mechanical turbulence and is therefore equal to mechanical mixing height (Cimorelli et al., 2005). For more details and technical description of AERMET calculations, see Cimorelli et al. (2005).

3.0 Results and Discussion

Comparing the results of the 5-year period of mixing height data illustrates that there are significant differences between mixing height estimates obtained from the ceilometer and those obtained through the AERMET parametrization scheme. The seasons have been defined using astronomical seasons. A look at seasonal average maximum values (Table 3-1) shows that values estimated by AERMET (Z_i) agree well with those obtained by Holzworth (1972) while estimates of the mixing height obtained with the ceilometer indicate a deeper mixing layer on average. All three ceilometer estimates of mixing height (MLH1, MLH2, and MLH3) result in a mixing layer that is approximately 1 km higher than Holzworth and AERMET estimates. The average daily maximum values generally correspond to the mixing height observed during the afternoon hours, at the peak of convective turbulence. In turn, the minimum mixing heights are generally observed during the overnight period when turbulence is reduced and generally associated with mechanical effects. Table 3-2 shows the minimum mixing height estimates from Holzworth (1972), AERMET, and the ceilometer. AERMET estimates of the minimum mixing height are an order of magnitude smaller than Holzworth (1972) estimates. On average, minimum mixing height estimates obtained from the ceilometer have better agreement with Holzworth estimates, in particular those obtained using the strongest backscatter gradient (MLH1). These results are of interest because restrictive dispersion conditions are associated with lower mixing height values and low wind speeds. Dispersion models generally estimate the maximum pollutant concentrations downwind during the overnight period when mixing layer heights are low. Table 3-2 suggests that although on average ceilometer estimates agree with the well accepted Holzworth method, dispersion model estimates using the ceilometer mixing height estimates would produce lower pollutant concentration estimates than those obtained using the default AERMET values. However, the average minimum mixing height values obtained by AERMET are significantly low – no higher than 10 meters in height which is below the surrounding canopy height. This can also have implications on preventing mixing to the surface.

Table 3-1. Average daily maximum mixing height from Holzworth, AERMET (Z_i), and ceilometer (MLH1, MLH2, MLH3) estimates.

Season	Holzworth Afternoon (meters)	Z_i Average Maximum (meters)	MLH1 Average Maximum (meters)	MLH2 Average Maximum (meters)	MLH3 Average Maximum (meters)
Winter	1050	1245	2725	2179	2205
Spring	1700	1810	2989	2509	2427
Summer	1800	2184	2899	2556	2485
Fall	1400	1551	2696	2316	2169

Table 3-2. Average daily minimum mixing height from Holzworth, AERMET (Z_i), and ceilometer (MLH1, MLH2, MLH3) estimates.

Season	Holzworth Morning (meters)	Z_i Average Minimum (meters)	MLH1 Average Minimum (meters)	MLH2 Average Minimum (meters)	MLH3 Average Minimum (meters)
Winter	200	9	144	87	50
Spring	250	11	174	139	93
Summer	300	10	174	186	185
Fall	250	10	183	127	93

An evaluation of the average progression by time of day for the mixing layer height by season was conducted to see how the estimates depict the growth of the mixing layer through the day. Average hourly values of mixing layer height were obtained for each month using the 5-year dataset for both the ceilometer data and AERMET estimates. Figure 3-1 illustrates the results of this comparison for the ceilometer estimated MLH1, which corresponds to the largest gradient in backscatter signal. The months are separated by astronomical season: winter – Figure 3-1a, spring – Figure 3-1b, summer – Figure 3-1c, and fall – Figure 3-1d. Afternoon estimates of the mixing layer height generally agree with different months of the year showing better agreement than others.

Overall, Figure 3-1 illustrates that there are differences in the average progression of the mixing height for each estimated method. A particularly large difference is observed during the overnight hours where the ceilometer values suggest a deeper mixing layer is present. The minimum in mixing height estimated from the ceilometer is generally observed around 0700 LST followed by the daytime transition to the convective boundary layer. A notable feature most apparent in the months of April-August is the delay or flattening of the ceilometer mixing layer height estimate between 0700-1300 LST which results from the development of boundary layer shallow cumulus clouds which are common in the humid conditions typical during spring and summer in the SRS region. In turn, AERMET estimated values reach the minimum values after 2000 LST and remain constant until sunrise. During daytime hours, particularly during the spring and summer, agreement is observed between the mixing layer height estimate. However, Figure 3-1 shows that the ceilometer suggests the mixing layer continues to grow and reaches its maximum value later than the AERMET estimated mixing height. A difference of 1-3 hours is observed for the time on which the maximum mixing height is reached on each method (Figure 3-1). AERMET's mixing height reaches the maximum value around 1500 – 1800 LST (depending on the season) and then drops immediately after sunset. Contrastingly, the ceilometer mixing height (MLH1) does not reach the maximum value until around 1700 – 2000 LST and then exhibits a slight decrease before reaching a near constant value overnight.

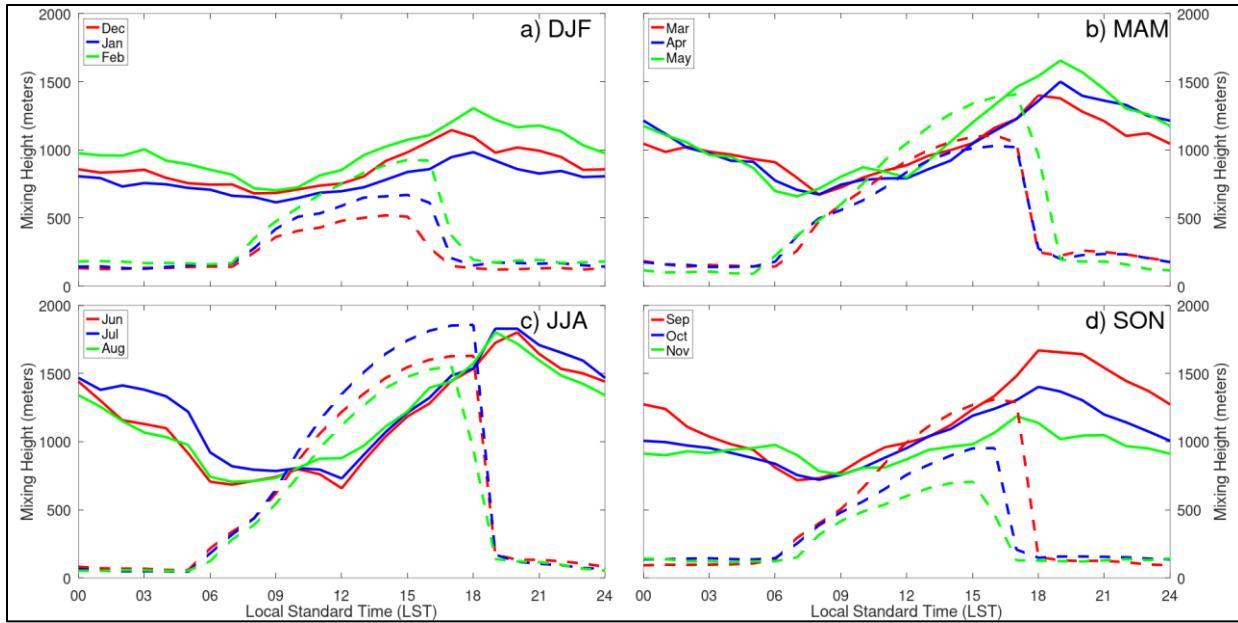


Figure 3-1. Monthly average of mixing height by season for MLH1 and AERMET. a) shows winter months (December, January, and February), b) shows spring months (March, April, and May), c) shows summer months (June, July, and August), and d) shows fall months (September, October, and November). The solid lines show mixing height estimated from the ceilometer at the largest gradient (MLH1) and the dashed lines show the mixing height estimated from AERMET.

Figure 3-2 illustrates the results comparing the ceilometer estimated MLH2, which has the second strongest backscatter gradient, to the AERMET estimate of mixing height (same values as those depicted on Figure 3-1). The maximum values of mixing layer height during the daytime hours are lower when using MLH2 (than MLH1), but the overnight estimates remain similar. MLH2 shows better agreement in the maximum mixing layer value reached for the winter and fall seasons (than MLH1). The ceilometer estimates of overnight mixing height using the second strongest backscatter gradient continue to suggest a deeper mixing layer than AERMET estimates, resembling results obtained using the strongest backscatter gradient (MLH1). The ceilometer estimates did not reach the maximum value until around 1800 – 2000 LST and then seemed to reach a constant value overnight after exhibiting a slight decrease. A difference of 1-3 hours is observed for the time on which the maximum mixing height is reached. After reaching the minimum mixing height there is a time difference of 3-6 hours before the ceilometer and AERMET mixing heights begin to increase.

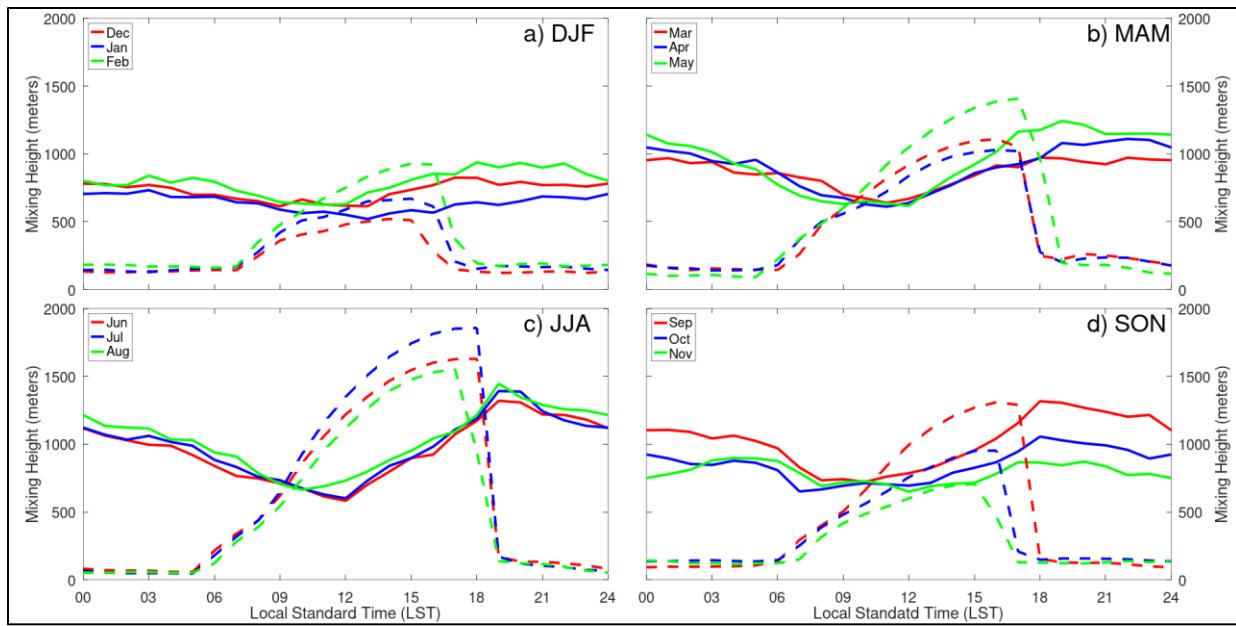


Figure 3-2. Monthly average of mixing height by season for MLH2 and AERMET. a) shows winter months (December, January, and February), b) shows spring months (March, April, and May), c) shows summer months (June, July, and August), and d) shows fall months (September, October, and November). The solid lines show mixing height estimated from the ceilometer at the second largest gradient (MLH2) and the dashed lines show the mixing height estimated from AERMET.

Figure 3-3 illustrates the results comparing the AERMET estimated mixing height to the ceilometer estimated MLH3, similar to Figure 3-1 but with the third strongest backscatter gradient. Reasonable agreement is observed for some of the months on average but as with the other two ceilometer estimates (MLH1 and MLH2), the ceilometer suggests a deeper mixing layer height overnight and there are timing differences in the progression of the mixing layer. The minimum in mixing height estimated from the ceilometer varies from 1000-1200 LST, after this time the mixing height begins to increase. After reaching the minimum mixing height there is a time difference of 3-6 hours before the ceilometer and AERMET mixing heights begin to increase. The ceilometer estimates did not reach the maximum value until around 1800 – 2000 LST and then slightly decreased before reaching a nearly constant value overnight.

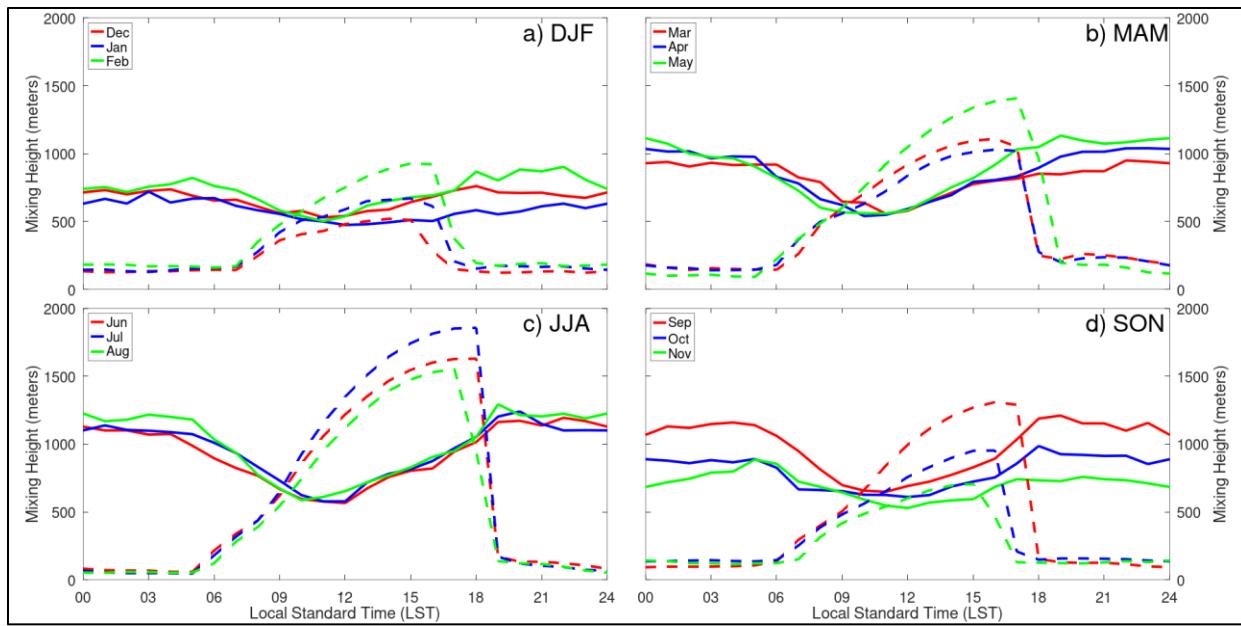


Figure 3-3. Monthly average of mixing height by season for MLH3 and AERMET. a) shows winter months (December, January, and February), b) shows spring months (March, April, and May), c) shows summer months (June, July, and August), and d) shows fall months (September, October, and November). The solid lines show mixing height estimated from the ceilometer at the third largest gradient (MLH3) and the dashed lines show the mixing height estimated from AERMET.

In Figures 3-1 to 3-3 the ceilometer estimated mixing height had better agreement with the AERMET estimated mixing height during the day. All three overnight estimates from the ceilometer did not agree with AERMET estimates. It is possible that the ceilometer estimates are accurately representing the mixing height over the heavily forested SRS, rough surface, while AERMET's assumptions on mechanically generated turbulence might not be representative of overnight turbulence conditions at SRS. Differences arise since AERMET does not consider any convective mixing in the absence of surface heating from sunlight. AERMET also does not consider mechanical mixing if wind speeds are low enough. These two assumptions might not truly reflect the local lower boundary layer conditions at SRS. The ceilometer could be measuring a residual mixed layer from the previous day that AERMET is not acknowledging, having already limited the depth of mixing to the radiation inversion. It must be noted that it is also possible that the discrepancies observed are due to instrument/measurement characteristics of the ceilometer. The ceilometer sends out a series of pulses which are measured upon return to the ceilometer. If the mixing height is very low, it could be possible for return laser pulses to arrive at the ceilometer before the last pulse is sent out which would cause the ceilometer to overestimate mixing height (Morris, 2016; Young & Whiteman, 2015). Additionally, fog and clouds can scatter the laser energy and create multipath echoes. Given that fog is common around SRS this could affect the ceilometer measurements by saturating the receiver (de Morales et al., 2024). Given these results and the fact that maximum modeled estimated concentration usually occurs during the overnight/stable hours where the two methods differ, further study of mixing layer estimates and their effects on modeling estimates are important to determining accurate pollution concentrations.

4.0 Conclusions

In this study a 5-year climatology of mixing height values was included to compare the seasonal and diurnal differences between ceilometer and AERMET mixing height estimates. The AERMET average daily minimum values (morning) were an order of magnitude lower than the well accepted Holzworth (1972) method and the ceilometer estimated mixing height for every season. The average daily minimum values

from AERMET were even lower than the height of the surrounding tree canopy. When comparing the ceilometer estimated mixing height to AERMET the ceilometer maximum mixing height occurred 1-3 hours later than the AERMET maximum. This is due to the nighttime atmospheric mixing height assumptions and calculations used by AERMET which cut-off mixing height at sunset since convective mixing is not considered once the sun sets and mechanical mixing is strongly dependent on wind speed (if the wind speed is low the mechanical mixing layer height is very low). These assumptions could be reasonable for a relatively flat surface when there is no wind, clear skies, and low humidity but are not representative of the forested landscape of the southeastern United States. It is unlikely that the nocturnal boundary layer develops that quickly, especially in the summertime, and possibly in the fall and spring when radiative cooling is not immediate. Therefore, we believe that the mixing heights estimated by ceilometer measurements better reflect the early evening conditions in the southeastern United States where convection continues after sunset.

Results from this study showed that in general the AERMET parametrization scheme is conservative in the estimate of mixing layer during periods with a stable boundary layer. The ceilometer seasonally averaged mixing height estimate is more representative of nighttime mechanical mixing conditions at SRS caused by heavily forested areas, while the AERMET mixing height assumptions on mechanically generated turbulence may not be representative of overnight turbulence at SRS. However, the averaged ceilometer mixing height estimates might not be capturing the early morning radiative cooling that create stable conditions that reduce the mixed layer height. Future studies should focus on identifying the conditions and time of day when the ceilometer is more representative and when the AERMET mixing height is more conservative. Currently, SRS uses AERMET to conservatively determine emission source parameters (such as stack height) to ensure potential pollutant concentrations are below industrial hygiene limits. Operationally, measured mixing height from the ceilometer could be used to improve the representativeness in emergency response modeling of dispersion characteristics. If AERMET is providing an overly conservative mixing height that is not representative of mixing height conditions overnight, then resources may be wasted altering emission source parameters to improve dispersion in a model that is not accounting for local mixing conditions. Additionally, air dispersion modeling applications at SRS are used to establish conditions to ensure worker safety, it is important to understand when the inputs are providing a more conservative or less conservative estimate of mixing height which impacts the modeled pollutant concentrations.

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