## Dear Authors,

I am happy to say that all three referees see substantial improvements in your manuscript. They are also clear in that your study is covering a challenging topic that is of great interest to the community. However, the referees also state that the manuscript would profit from a number of improvements and clarifications and have made some very constructive comments. In the light of providing the community with a clear and convincing publication on this topic I recommend to make another effort in revising your manuscript according to the referees' suggestions and by providing answers to the still open questions identified by the referees.

I am looking forward to your revised manuscript. Best regards, Theresa Blume

Anonymous during peer-review: Yes No Anonymous in acknowledgements of published article: Yes No

#### **Recommendation to the Editor**

1) Scientific Significance Does the manuscript represent a substantial contribution to scientific progress within the scope of this journal (substantial new concepts, ideas, methods, or data)?	Excellent Good Fair Poor
2) Scientific Quality Are the scientific approach and applied methods valid? Are the results discussed in an appropriate and balanced way (consideration of related work, including appropriate references)?	Excellent Good Fair Poor
3) Presentation Quality Are the scientific results and conclusions presented in a clear, concise, and well structured way (number and quality of figures/tables, appropriate use of English language)?	Excellent Good Fair Poor

For final publication, the manuscript should be

## accepted as is

accepted subject to **technical corrections** accepted subject to **minor revisions** 

reconsidered after major revisions

I am willing to review the revised paper.

I am **not** willing to review the revised paper.

## Rejected

Suggestions for revision or reasons for rejection (will be published if the paper is

## accepted for final publication)

The manuscript introduces a challenging research topic still unsolved.

The manuscript is well organized and authors have put great effort on the review of the manuscript. I had the opportunity to read both the manuscript, the rebuttal letter and also the manuscript with track of changes. I have to admit that the manuscript has been improved significantly, but according to my perspective there are still a number of open questions.

I have some comments that have been written with the aim to improve the final quality of the manuscript:

1. The authors use the relationship between relative saturation and evapotranspiration to derive an estimate of the available water content. I would like to stress this point because the ET can certainly provide good indications on the available water content, but when the relative saturation exceeds the field capacity, this method is unable to properly identify the state of the soil. Therefore, ALEXI SM is an estimate of the available water content not soil moisture.

**Response:** We agree with the reviewer that the relationship between fractional ET and available water content has limitations. It can only effectively provide SM information between wilting point and field capacity. However, since ALEXI senses the moisture content of the entire root-zone (~0-100 cm), it would require a very large rain event for the entire soil column to experience a moisture content greater than field capacity, or a prolonged drought to produce SM less than wilting point. Further, if conditions above field capacity are underestimated, then the root zone may dry out faster than observed, but theoretically that would be corrected with the next available retrieval. Therefore if ALEXI retrieval is available within next few (~2-4) days the errors would be rather small (page 7 lines 11-15).

2. Given the above consideration I wonder if such limitation may be reasonable of some of the errors observed may be due to such an assumption.

**Response:** We agree with the reviewer that the empirical relationship between fraction ET and available water content has some limitations and may be responsible for some errors in the POME profiles. This point is further clarified in the revised MS page 7 lines 12-15.

3. Looking at the results, it seems that the proposed model leads to results similar to those by Noah LSM. The argument of the authors is that POME tends to be better in the lower soil layer, but this result is imposed by calibrating the lower limit of relative saturation profile. As stated by the authors the lower boundary condition is imposed equal to 0.55. In fact, all time series in the lower layer (40-100cm) show a similar dynamics with small variability around a relative value close to 0.55. Therefore, this is not an evidence of model reliability in my personal opinion.

**Response:** We agree with the reviewer that the POME profiles are affected by the lower boundary condition which in this case is set to 50% of available water content. First, this approximation is soil type dependent (and therefore not strictly constant), and secondly, it is based on experience that soil moisture in the deeper soil zones varies less dramatically throughout the year due to lower root density (resulting in minimal root water uptake) and dampened connectivity to variations in the surface layer. Since in many ways this is a proof-of-concept study, we felt this was appropriate for an initial appraisal of the technique. The POME implementation was not based on any prior knowledge of specific SM in the bottom layers, and in fact one can argue that its use actually weakened the results in this case. It certainly impacted the correlations, as a simple assumption like this would not be expected to correlate with actual observed soil moisture. As discussed in comment 5 below, a few

stations did exhibit considerable variability in the lower layers in contrast to our assumption. So we do not see how our lower boundary assumption unfairly biased the results in our favor, as implied. On the contrary, we feel that our selection of a lower boundary without any prior knowledge, and that even this assumption led to fairly good results, demonstrates the strength of the approach. These points are discussed in the MS page 9 line 27-30 and page 10 lines 1-4.

However, we have mentioned in the manuscript (page 16 line 2-4) that the lower boundary can be parameterized (as done here) or used as a calibration factor. Since the ultimate purpose of the profiles is to be assimilated into a Land Surface Model (LSM) or agricultural model, the lower boundary can also serve as an ideal point to tie the remotely sensed profile to the climatology of the model. In fact, we have done this in a companion paper and found that the POME profile is greatly improved.

- 4. Referee 2 comment 3. I think that the discrepancies between soil moisture measurements in the top layer and the POME predictions may be due to the ALEXI SM estimates that are probably rescaled according to the relative soil porosity. **Response:** We appreciate this observation and the referee is correct in that the ALEXI data are functions of the soil properties as stated above. However, in this case, the SM in the top layer of the POME model is a result of the MW estimates used as the surface boundary, not the ALEXI model.
- 5. In my experience, the soil moisture signal tend to be smoothed moving to the lower layers (see Manfreda et al., HESS 2014), but the time series 2115, 2113, 2013 (figure 5) show an amplification of soil moisture changes over time. This may be due to the presence of a phreatic surface interfering with the unsaturated zone. I suspect that these point are not coherent with the modeling scheme adopted.

**Response:** We thank the referee for this observation and we too were struck by the behavior of these particular stations. We agree that in our experience too most SM profiles show a damping effect with depth and, in fact, that was the reasoning behind our selection of the lower boundary condition as discussed in Number 3 above. We have investigated these particular stations extensively and have concluded that the SM behavior is site specific. We note that these stations are located in cropland/short vegetation areas and thus we do not believe that perched water would be located within 1-m of the surface. Two sites (2013 and 2115) have very porous soils near the surface (2115 even classified as gravel) with clay layers beneath and the other site (2113) is located very near a stream and is probably influenced by surface water intrusion. Of course, we had this information available beforehand but did not want it to influence our selection of the lower boundary on the profile as discussed in our response to Comment 3 above.

6. In general, I admit that the authors are working on a challenging topic, but the overall presentation of the results does not fully convince about the advantages and potential of the proposed method. The fact that POME is superior to Noah LSM only on 50% of the stations and the fact that the better performances in the lower layers, claimed by the authors as an advantage of the proposed method, may be an outcome of a calibration is a bit weak to justify its use in future applications. I would like to have more arguments about the potential of these model, how and where it can be used.

**Response:** We appreciate the reviewer's comment and acknowledgement of the challenges involved in this study. We also appreciate the opportunity to articulate the positive aspects of the recommended approach.

First, it is true that the POME profiles were clearly superior to the Noah LSM in about half of the cases in terms of Bias and RMSE. However, the results were very comparable in the other 50% of the cases. Only in terms of correlation was the LSM significantly better

and the results clearly indicate that this was a function of the two boundary conditions, and particularly the parameterization of the lower boundary. The Noah LSM is executed within NASA LIS operated by the SPoRT team at Marshall Space Flight Center. Noah is driven by the best high resolution climatological and energy data available in the U.S. and possibly the world. On the other hand, the POME model requires only three inputs, two of which are readily available from RS, while the third can be parameterized as done here or used to tie the profile to the climatology of a LSM or to field conditions if known. We would like to reiterate that we did not calibrate the lower boundary to field conditions in this case, and in fact, merely assumed that 50% of available water capacity remained in the spirit of the Maximum Entropy concept of relying on a minimum of a-prior information. So we feel that the fact that the POME profiles were superior to the LSM at half the instances, and were comparable everywhere, is a strong positive for the approach. Second, since the POME model can be used with remote sensing observations, it can be applied anywhere on Earth where vegetation is active, which would be particularly useful in data scarce regions of the world. The POME model is also computationally inexpensive whereas LSM models (such as Noah, VIC etc.), which require multiple inputs (ranging from static inputs like soil type, landcover to dynamic inputs such as weather information etc.). These LSMs also often need local inputs for regional calibration and can be computationally expensive over large regions and at finer scales.

However, if we can achieve accuracies similar to LSMs with significantly fewer input parameters, at large spatial scales with negligible computational resource requirements using the POME model (as shown in this study), then we believe the POME model concept has huge potential. Further, the LSMs usually don't take irrigation activities into account (unless grid scale irrigation maps are available), while the POME model, which is based on satellite SM retrievals of surface as well as root-zone, contains the signals from irrigated fields. Therefore, as discussed in the manuscript several times, POME seems to represent both irrigated and non-irrigated fields and provide more realistic estimations.

Anonymous during peer-review: Yes No Anonymous in acknowledgements of published article: Yes No

## **Recommendation to the Editor**

1) Scientific Significance  Does the manuscript represent a substantial contribution to scientific progress within the scope of this journal (substantial new concepts, ideas, methods, or data)?	Excellent Good Fair Poor
2) Scientific Quality Are the scientific approach and applied methods valid? Are the results discussed in an appropriate and balanced way (consideration of related work, including appropriate references)?	Excellent Good Fair Poor
3) Presentation Quality Are the scientific results and conclusions presented in a clear, concise, and well structured way (number and quality of figures/tables, appropriate use of English language)?	Excellent Good Fair Poor

For final publication, the manuscript should be

## accepted as is

accepted subject to **technical corrections** 

accepted subject to minor revisions

reconsidered after major revisions

I am willing to review the revised paper.

I am **not** willing to review the revised paper.

## rejected

# Suggestions for revision or reasons for rejection (will be published if the paper is accepted for final publication)

The manuscript entitled "Development of Soil Moisture Profiles Through Coupled Microwave-Thermal Infrared Observations in the Southeastern United States" presents interesting and relevant research on the development of vertical soil moisture profiles using POME using remote sensing data. The manuscript is well structured and concise. It has already undergone one round of reviews. My comments are mostly addressing some points which need further clarification. In my opinion these are mostly minor issues and therefore I hope to see this article soon published in HESS.

1) The ALEXI SM is calculated using a linear function based on the available water. Can you argue why you use only one equation for the entire domain and should this not be vegetation depended. For example forest which intercepts the rainfall may require another relationship than grassland which has a lower interception.

**Response:** This is an excellent point, and we thank the referee for bringing this into discussion. We agree that there are multiple possible relations between fractional PET and AWC that could be used (linear, piece-wise linear, logarithmic etc.). These relationships are usually dependent on vegetation (tall tree vs medium vs crop vs grassland), soil texture and location type (water limited vs well-watered) (Anderson et al., 2007). An earlier study by Hain et al. (2009) considered four such relationships and found that the hybrid relationship (linear and non-linear merged) provided the best results for Oklahoma region. However, for large scale applications, linear functions are generally used because: a) less detailed soil and vegetation inputs are required for implementation; and b) their sensitivity to soil moisture is constant (Song et al., 2000). Therefore, a linear model was used in this study as well. This point is mentioned in the MS page 7 lines 1-5.

2) If I am not mistaken you do not mention the penetration depth of the AMSR-E microwave instrument. To my knowledge this can vary depending on the soil moisture conditions. How does this affect your methodology and results?

**Response:** The MW penetration depth is a function of its sensors wavelength, penetration depth increases with wavelength. L-band sensors such as SMAP or SMOS with higher wavelength have penetration depths of 3-5 cm while X and C band sensors like AMSR-E have 0-2 cm penetration depths. For this study, the POME model is applied at 5 cm layer depth therefore the surface observations from AMSR-E (0-2cm) were assumed to be representing 0-5cm. We understand there is a mismatch in depths, although the integral function within the POME model which couples boundary conditions from mean moisture content can compensate for the surface layer depth mismatch. The MW sensing depth is mentioned in MS page 17 line 4.

3) The LST data used in ALEXI is constrained to cloud free conditions. However Figure 5 presents complete timeseries of the POME model. I guess this is described in section 3.4,

but I am surprised that you can gap fill the days with cloud cover by using a simple moving window. Please clarify your method and its limitations.

**Response:** Figure 5 actually shows the SM conditions after every 8-day interval. We have updated the caption to clarify this representation. This was done for simplification/figure clarity and to represent the general trends (instead of daily variabilities). Even though we use data from every 8<sup>th</sup> day, still some data gaps can be seen with POME time series (blue) few sites (e.g. end of 2006 in sites 2009, 2053, 2078 or mid-2009 for sites 2115 and 2027 etc.).

The gap filling method is more effective in root-zone where SM variabilities are relatively less compared to the surface at daily time-step. Earlier studies such as by (Leng et al., 2017a, 2017b) explored the vegetation and aerodynamic coefficient based gap filling algorithm for satellite derived SM estimations. Despite showing promises, the proposed algorithm requires ancillary datasets that are not part of this study. Further, there is a strong correlation between surface and SM dynamics at lower layers for temporal lags of less than 5-days (Alfieri et al., 2017; Penna et al., 2013). Therefore a 3-day moving window can be used to fill in some of the gaps in ALEXI retrievals. This point is further clarified in the revised MS (page-10 lines 9-14)

4) As I understand POME, it is a statistical model not a physically based approach. How can POME account for different soil types which will affect the vertical SM profile? **Response:** The POME integrals are applied over effective SM conditions. At the time of application, both mean and lower boundary condition data are available in effective SM state (with no prior information regarding soil type), only the surface volumetric SM conditions are known which are converted to effective. After the model application the effective SM profile distribution is then converted to volumetric by mapping the layers soil characteristics information available (Page 9 line 12).

monymous during peer review. Tes 100	
Anonymous in acknowledgements of published article: Yes No	
Recommendation to the Editor	
1) Scientific Significance Does the manuscript represent a substantial contribution to scientific progress within the scope of this journal (substantial new concepts, ideas, methods, or data)?	Excellent Good Fair Poor
2) Scientific Quality Are the scientific approach and applied methods valid? Are the results discussed in an appropriate and balanced way (consideration of related work, including appropriate references)?	Excellent Good Fair Poor
3) Presentation Quality Are the scientific results and conclusions presented in a clear, concise, and well	Excellent Good Fair Poor

Anonymous during peer-review: Yes No

structured way (number and quality of figures/tables, appropriate use of English

For final publication, the manuscript should be

## accepted as is

language)?

accepted subject to **technical corrections accepted subject to minor revisions** 

## reconsidered after major revisions

I am willing to review the revised paper.

I am **not** willing to review the revised paper.

## Rejected

# Suggestions for revision or reasons for rejection (will be published if the paper is accepted for final publication)

Review HESS-2017-351

First of all I would like to make clear that I have not been a reviewer on this manuscript before. I studied the response to the reviewers and the revised manuscript and I think the authors responded well to most of these comments, but being a new reviewer for this manuscript I cannot avoid having some questions. I found the manuscript extremely interesting, and the approach without a-priori assumptions at the scale of LSM models is very useful to the community of HESS. At present however, the manuscript is somewhat impenetrable to me, and therefore I assume to other readers of HESS as well (comments below). Which readership did the authors have in mind: the well-informed LSM or remote sensing community that is certainly present in HESS, or the broader hydrologic community with an interest in remotely sensed applications?

1. The objective of the paper evolves around the POME model by using SM profiles developed from remotely sensed data only. Although I am sure everyone knows about entropy, the explanation of POME is rather short, as mentioned by one other reviewer as well. The reader is referred to several previous publications that employ the POME model. I suggest to include a more extensive description of the POME results instead of referring to whom applied it. This would help out the interested non-expert HESS readership to get to a level of insight that helps to appreciate this manuscript.

**Response:** We thank the reviewer for the comment. In the earlier revision, we included more details on the POME model and its applications. However, given the length of the paper we were little conservative in the model description. But in the current revision we have added an appendix-A detailing the POME model description. We agree with the reviewer that having a detailed POME model description will definitely add more value to the manuscript and will be more interesting to the readers.

2. For ALEXI field capacity and wilting point are employed in Eq. 1. Which values were used for the different soil types?

**Response:** We thank the reviewer for raising this point. We have added a table listing all the major soil types of the region with their characteristics values used in this study as an appendix B.

3. Line 250-253: Can the authors explain a bit more about the varying spatial scales and locations instead of only giving r and RMSE/RMSD/ubRMSD for various authors? For scientists unfamiliar with SEE disaggregation this part could be more informative, also because it is important for the approach used in this study.

**Response:** We agree with the reviewer, adding information about spatial resolutions will provide the reader with a more complete description of the downscaling approach. We have revised the MS to add the spatial resolution information as well as included the citation of our recent publication solely on downscaling approach using ALEXI surface evaporation over Continental U.S. Please refer to page-7 lines 22-25; page-8 lines 29-30 and page-9 lines 1-2 of the revised MS.

4. What was the rationale/advantage for using surface and potential evaporation instead of

the SEE definition given in line 275? Not clear now, only clear it changes the definition. Would be good to know as the change in definition seems to limit its applicability to water rich environments?

**Response:** We thank the reviewer for raising this point. The SEE definition provided in Line 275 (MS rev1) refers to the original approach used by Merlin et al. (2013, 2012) where SEE is computed using MODIS land surface temperature, vegetation index and albedo information. This was an indirect approach to estimate the ratio of surface evaporation to potential surface evaporation (i.e. SEE). In this study, however, the SEE is computed directly from actual surface evaporation and potential surface evaporation data. Conceptually, the SEE employed by Merlin, et al and in this study is the same. The surface evaporation and potential surface evaporation data were available relatively easily since the former is coming from the ALEXI model, which is already an important part of this study. Furthermore, for consistency purposes the utilization of same data source (ALEXI) for surface SM disaggregation and root-zone mean moisture content seems a better approach.

The issue of water rich vs dry environment arises with the selection of  $\frac{\partial SM_{mod}}{\partial SEE}$  model. Earlier studies e.g. Djamai et al. (2015), Mishra et al. (2018) etc. suggest that the linear model is better suited for dry conditions whereas non-linear models outperform the linear approach under water rich environments (such as Southeast U.S. in this study).

5. One of the assumptions needed for POME is due to non-monotonic behavior of SM. This necessitates the assumption of an inflection point. In the present study, only for 9% of the profiles generated such an assumption was needed. So, although POME is assumption free, the application of POME may not be (still better than LSM regarding number of assumptions). Can the authors reflect on the applicability of POME for other studies? If POME was not applied on SM but instead on the soil water potential (SWP) non-monotonic behaviour across a profile is no longer a concern. This would of course require a relation between SWP and SM, but increasingly assumption free relations are being developed to do so, they only at present take a lot of computational time.

**Response:** We thank the referee for this observation and it is an excellent point. In the dynamic case an additional assumption is required to employ the POME method correctly. This case is clearly identified when the mass balance constraint cannot be met and thus equation 4 has no solution. The assumption is then that the inflexion point is located in the soil layer with the greatest ability to retain water (i.e., field capacity) and thus the SM would be less both above and below that point. In an earlier study Mishra et al. (2015) the authors used a detailed model of soil moisture movement to verify this assumption, and it has generally been verified by the results shown here and elsewhere. As the referee points out, if soil water characteristics are used that are known to be monotonic, then that particular problem is solved, but as stated, assumptions relating actual SM to the variable being modeled (such as SWP) are necessary. So we feel that our approach, based as it is on well known properties of SM, is appropriate at this time.

6. Restricting ALEXI and POME by soil moisture at field capacity means that comparison with in situ data misses out on the field capacity to saturated soil moisture range, especially in the water rich environments of the present study. Can the authors reflect on this? **Response:** We agree with the reviewer that the relationship between fractional ET and available water content has limitations. It can only effectively provide SM information between wilting point and field capacity. Since ALEXI sense the moisture content of the entire root-zone (~0-100 cm), it is highly unlikely that the entire soil column would experience moisture content greater than field capacity or less than wilting point. Further, if we underestimate conditions above field capacity we may dry out the root zone faster than observed, but theoretically that would be corrected with the next available retrieval. Therefore if ALEXI retrieval is available within next few (~2-4) days the errors would be

## rather small (Page 7 lines 11-15).

7. Looking at Fig 4 the correlation for 6 out of 10 sites decreases with depth. What could cause this? The most dynamic SM can be expected at the soil surface if no preferential flow path are present in the profile. In figure 5 most dynamics can be seen at the 40-100 layer at some sites, indicating preferential flow paths (unless a dynamic shallow groundwater table is present). Some of the sites have a clay type soil which may form cracks and thus provide preferential flow conduits. This might perhaps also explain the decrease in correlation at greater depth, because such flow conduits will only be active under very wet conditions. These may are not accounted for in the POME approach as this is limited to field capacity or is this the result of the overpass time?

**Response:** This is an excellent observation. As the referee has deduced, there are several issues at work here. First, our simple assumption of the lower boundary condition at 50% of available SM is the main factor causing the decrease in correlation with depth. As the referee states, several sites showed unusually dynamic SM behavior in the lower layers which is not consistent with our assumption. We made this assumption at this point in order to stay within the spirit of the Principle of Maximum Entropy, i.e. that a minimum of a-prior information should be used in construction of the profile. However, we note that the lower boundary provides an ideal point to link the profile with model climatology or field conditions if they are known. In this case, because this is somewhat a proof-of-concept study, we did not want to do that and we do note that bias and RMSD generally improved with depth in the POME model. Now, as to the cause of the dynamic behavior noted at certain sites, we have conducted an extensive investigation of this dynamical behavior of SM time series at lower depths and have concluded that this behavior is site specific. Two sites (2013 and 2115) have very porous soils near the surface (2115 even classified as gravel) with clay layers beneath and the other site (2113) is located very near a stream and is probably influenced by surface water intrusion. As the referee states, cracked clay soils could also result in the behavior but we do not think that was the case in these instances. As also noted, the cloud constraints on the ALEXI data impacts its availability and for that reason 3 day composites were employed for both the ALEXI and observed data. So it is unlikely that the ALEXI data availability is the cause of the poor correlation in the lower layers of the SM profile.

8. The conclusions puzzle me regarding the comparison between Noah, POME and SCAN. I have fig 5 and 6 for Noah, and fig 4, 5 and 6 for POME. Why is there only one general Noah/Scan comparison for Noah in fig 6?

**Response:** Thanks for the comment; one of the main purposes of this study is to evaluate the performance of the POME profiles. To that end we used two approaches: one to evaluate the POME profiles against in-situ observations from SCAN sites for ground validations. But there is a scale mismatch issues when comparing gridded product with point observations; second, to avoid scale mismatch issue, we used another gridded SM product from Noah LSM to further evaluate the POME profiles. Here we do not assume that Noah is free from any error, rather its errors are independent of the errors of either POME or in-situ profiles. Through this study, our intension are not to perform an inter-comparison between the three SM products, rather it is to evaluate the POME model performance against two separate and independent data sources. Therefore, we did not focus on the extensive comparison of SCAN with Noah SM product in this study but limited our analysis to general trend as shown in fig. 6.

Specific comments:

Line 44-46: Very confusing line: In general, in-situ SM profile data are only available at a few locations in the US for any given period of time. Why the focus on the US? I am sure globally there will only be a few in situ, but this line somehow seems to suggest there are only US data.

**Response:** We thank the reviewer for pointing this out. We have revised the sentence in the revised manuscript to avoid any confusion regarding data availabilities. (Page-2 lines 15-16)

Equation 2: for consistency please define SMmod as well.

**Response:** The model that defines the relationship between soil moisture and soil evaporative efficiency is defined in the manuscript. Please refer to Page-8 eq. (3).

Table 1: Soil type for site 2037 and 2038 unknown? Also site 2037 typo in Shrubland. **Response:** We again thank referee for point the type out. We have rectified the type in the revised manuscript.

As for the soil types for sites 2037 and 2038 (both in SC), the soil information is indeed unavailable on SCAN website for those two sites. Therefore it was intentionally left blank. In the revised MS we have added this information in table caption as well for clarity.

#### References:

- Alfieri, J.G., Anderson, M.C., Kustas, W.P., Cammalleri, C., 2017. Effect of the revisit interval and temporal upscaling methods on the accuracy of remotely sensed evapotranspiration estimates. Hydrol. Earth Syst. Sci 21, 83–98. doi:10.5194/hess-21-83-2017
- Anderson, M.C., Norman, J.M., Mecikalski, J.R., Otkin, J.A., Kustas, W.P., 2007. A climatological study of evaportranspiration and moisture stress across the continental United States based on thermal remote sensing: 1. Model formulation. J. Geophys. Res. 112, doi:10.1029/2006JD007506.
- Djamai, N., Magagi, R., Goita, K., Merlin, O., Kerr, Y., Walker, A., 2015. Disaggregation of SMOS soil moisture over the Canadian Prairies. Remote Sens. Environ. 170, 255–268. doi:10.1016/j.rse.2015.09.013
- Hain, C.R., Mecikalski, J.R., Anderson, M.C., 2009. Retrieval of an Available Water-Based Soil Moisture Proxy from Thermal Infrared Remote Sensing. Part I: Methodology and Validation. J. Hydrometeorol. doi:10.1175/2008JHM1024.1
- Leng, P., Li, Z.-L., Duan, S.-B., Gao, M.-F., Huo, H.-Y., 2017a. A practical approach for deriving all-weather soil moisture content using combined satellite and meteorological data. ISPRS J. Photogramm. Remote Sens. 131, 40–51. doi:10.1016/j.isprsjprs.2017.07.013
- Leng, P., Li, Z.-L., Duan, S.-B., Tang, R., Gao, M.-F., 2017b. A Method for Deriving All-Sky Evapotranspiration From the Synergistic Use of Remotely Sensed Images and Meteorological Data. J. Geophys. Res. Atmos. 1–15. doi:10.1002/2017JD027880
- Merlin, O., Escorihuela, M.J., Mayoral, M.A., Hagolle, O., Al Bitar, A., Kerr, Y., 2013. Self-calibrated evaporation-based disaggregation of SMOS soil moisture: An evaluation study at 3km and 100m resolution in Catalunya, Spain. Remote Sens. Environ. 130, 25–38. doi:10.1016/j.rse.2012.11.008
- Merlin, O., Rudiger, C., Al Bitar, A., Richaume, P., Walker, J.P., Kerr, Y.H., 2012. Disaggregation of SMOS Soil Moisture in Southeastern Australia. IEEE Trans. Geosci. Remote Sens. 50, 1556–1571.

## doi:10.1109/TGRS.2011.2175000

- Mishra, V., Ellenburg, W., Al-Hamdan, O., Bruce, J., Cruise, J., 2015. Modeling Soil Moisture Profiles in Irrigated Fields by the Principle of Maximum Entropy. Entropy 17, 4454–4484. doi:10.3390/e17064454
- Mishra, V., Ellenburg, W.L., Griffin, R.E., Mecikalski, J.R., Cruise, J.F., Hain, C.R., Anderson, M.C., 2018. An initial assessment of a SMAP soil moisture disaggregation scheme using TIR surface evaporation data over the continental United States. Int J Appl Earth Obs Geoinf. 68, 92–104. doi:10.1016/j.jag.2018.02.005
- Penna, D., Brocca, L., Borga, M., Dalla Fontana, G., 2013. Soil moisture temporal stability at different depths on two alpine hillslopes during wet and dry periods. J. Hydrol. 477, 55–71. doi:10.1016/j.jhydrol.2012.10.052
- Song, J., Wesely, M.L., LeMone, M.A., Grossman, R.L., 2000. Estimating Watershed Evapotranspiration with PASS. Part II: Moisture Budgets during Drydown Periods. J. Hydrometeorol. 1, 462–473. doi:10.1175/1525-7541(2000)001<0462:EWEWPP>2.0.CO;2

## Development of Soil Moisture Profiles Through Coupled Microwave-Thermal Infrared Observations in the Southeastern United States

Vikalp Mishra<sup>1</sup>, James F. Cruise<sup>1</sup>, Christopher R. Hain<sup>2</sup>, John R. Mecikalski<sup>3</sup>, and Martha C. Anderson<sup>4</sup>

<sup>1</sup>Earth System Science Center, The University of Alabama in Huntsville, 320 Sparkman Drive, Huntsville, AL 35805, USA

<sup>2</sup>NASA Marshall Space Flight Center, Earth Science Branch, Huntsville, AL, 35805, USA

<sup>3</sup>Atmospheric Science Department, University of Alabama in Huntsville, 320 Sparkman Drive, Huntsville, AL 35805, USA

<sup>4</sup>Hydrology and Remote Sensing Laboratory, USDA Agricultural Research Service, Beltsville, MD 20705, USA

**Correspondence:** James F. Cruise james.cruise@nsstc.uah.edu

**Abstract.** The principle of maximum entropy (POME) can be used to develop vertical soil moisture profiles. The minimal inputs required by the POME model make it an excellent choice for remote sensing applications. Two of the major input requirements of the POME model are the surface boundary condition and profile-mean moisture content. Microwave-based soil moisture estimates from Advanced Microwave Scanning Radiometer (AMSR-E) can supply the surface boundary condition whereas thermal infrared-based moisture estimated from the Atmospheric Land EXchange Inverse (ALEXI) surface energy balance model can provide the mean moisture condition. A disaggregation approach was followed to downscale coarse resolution ( $\sim$ 25 km) microwave soil moisture estimates to match the finer resolution ( $\sim$ 5 km) thermal data. The study was conducted over multiple years (2006-2010) in the southeastern United States. Disaggregated soil moisture estimates along with the developed profiles were compared with the Noah land surface model (Noah LSM) within the framework of NASA Land Information System (LIS), as well as in-situ measurements from 10 Natural Resource Conservation Services (NRCS) Soil Climate Analysis Network (SCAN) sites spatially distributed within the study region. The overall disaggregation results at the SCAN sites indicated that in most cases disaggregation improved the temporal correlations with unbiased root mean square differences (ubRMSD) in the range of 0.01-0.09  $\mathrm{m}^3\mathrm{m}^{-3}$ . The profile results at SCAN sites showed a mean bias of 0.03 and 0.05 ( $\mathrm{m}^3\mathrm{m}^{-3}$ ); unbiased RMSD ubRMSD of 0.05 and 0.06 (m<sup>3</sup>m<sup>-3</sup>); and correlation coefficient of 0.44 and 0.48 against SCAN observations and Noah LSM, respectively. Correlations were generally highest in agricultural areas where values in the 0.6-0.7 range were achieved.

#### 1 Introduction

Although soil moisture (SM) represents a relatively small part of the overall hydrologic cycle, it is perhaps the most important part to human survival. SM is the source of water for all vegetation on Earth. It also plays an important role in water and energy exchanges between the land surface and atmosphere. Hydrologically, SM is an indicator of drought or lack thereof, and

antecedent moisture conditions are important determinants of runoff response to rainfall events. Thus, SM is a vital part of any terrestrial ecosystem analysis as well as land surface and climate models.

Much of the recent efforts particularly in remote sensing of SM estimation have been focused on surface or near surface observations (0-5 cm); however, moisture throughout the root zone can be just as important. The moisture within the root zone exerts a controlling influence on land-atmospheric fluxes of energy and water under vegetated condition. The actual distribution of root zone moisture is a function of vegetation canopy root density and distribution (Mishra et al., 2013). For this reason, SM at shallow depths (< 100 cm) is known to be extremely variable both as functions of time (Starks et al., 2003) and depth (Scott et al., 2003).

Although several approaches have been proposed for determining SM profiles, most require either observed profile data so that a regression or inversion model can be developed (Arya and Richter, 1983; Kondratyev et al., 1977; Kostov and Jackson, 1993; Srivastava et al., 1997; Singh, 1988). Another common approach is to estimate surface or total root zone moisture using remote sensing and then assimilate those observations into a land surface model (LSM) to determine root zone SM distributions. The NASA Land Information System [LIS, (Kumar et al., 2006)] contains a suite of land surface models and data assimilation tools for this purpose that are commonly utilized as a source of SM data.

15

However, LSMs have their own issues (e.g., bias, ancillary data requirements, computational expense) so it would be advantageous if SM profiles could be deduced directly from satellite observations without the use of a LSM or the availability of *in-situ* profile data. *In-situ* SM profile data are only available generally at a few locations over the continental United States (CONUS) for any given period of timespatially sparse locations (Aghakouchak et al., 2015). In addition, a number of field campaigns over the years have produced high-density observations globally, but only for very short time periods over limited domains. *In-situ* data suffer from the fact that they are site specific and may not be representative of wider surrounding regions. Thus, they are of limited value for modeling or operational purposes. These deficiencies have led to the increased reliance on remote sensing to retrieve SM. However, remotely sensing SM estimates alone cannot deduce the distribution of moisture within a soil column.

Due to the inherent complexities involved with the movement of SM in the column, several studies have argued that SM uncertainties and complexities can be best described through the description of its entropy (Mays et al., 2002; Pachepsky et al., 2006; Singh, 2010) The maximization of entropy characterizes the diffusion of moisture through the soil column over a period of time. The principle of maximum entropy (POME) states that if the inferences had to be drawn from incomplete information then they should be based on the probability distribution with maximum entropy allowed by the *a-priori* information. Al-Hamdan and Cruise (2010) used the maximum entropy formulation of Jaynes (Jaynes, 1957a, b) based on the Shannon entropy (Shannon, 1948) to formulate the POME-based SM profile development algorithm. Unlike other methods, the entropy approach suffers from no *a-priori* assumptions about the nature or shape of the moisture profiles in real space. The method is a statistical approach and guarantees the minimum variance unbiased profile subject to the boundary and initial conditions specified. This could be an improvement over other analytical methods that do presuppose a functional form of the SM distribution. Singh (2010) provides a full explanation of the theory of entropy of moisture movement in porous media.

Subsequent to its introduction the POME method has been adopted and extended by several authors e.g., Mishra et al. (2013, 2015); Pan et al. (2011); Singh (2010). Initial studies by Al-Hamdan and Cruise (2010) and Singh (2010) compared their results against experimental data under laboratory settings. However studies by Pan et al. (2011) and Mishra et al. (2013) involved application and validation of the POME model outside laboratory environment. More recently Later, Mishra et al. (2015) provided extensive validation of the profiles developed using the POME approach against a U.S. Department of Agriculture Soil Climate Analysis Network (SCAN) site located in northern Alabama, as well as with a detailed mathematical model of moisture movement in the soil profile.

The objective of this study is to develop SM profiles from remotely sensed data over the southeastern U.S without the aid of observed profile data or the use of a LSM. The approach utilizes both microwave (MW) data (to supply surface estimates) and thermal infrared (TIR) estimates (for total root zone moisture) within the POME profile methodology. The POME model requires only the upper and lower boundary conditions, as well as the mean moisture content, as input. The surface and mean moisture contents can be supplied by satellite estimates, whereas the lower boundary condition ( $\sim$ 100-200 cm) is often fairly stable and can be parameterized. Therefore, the POME model is ideal for the integration of remotely sensed data from multiple sensors such as MW and TIR to develop a unified SM profile.

15

25

The goal of this research is to provide SM profiles at operational or near operational (1-5 km) spatial resolutions to be consistent with other fine scale hydrologic and agricultural modelling work taking place in the study region (Mishra et al., 2013; McNider et al., 2015). Consequently, before the SM profiles can be calculated, the disparity in spatial resolution between the MW and TIR data must be resolved. MW data are available at much coarser spatial resolutions (25-40 km) than are TIR data (1-10 km). The approach selected here is to downscale (or disaggregate) the coarse MW data to the resolution of the TIR data. This is accomplished via an evaporative efficiency method proposed by Merlin et al. (2013, 2012, 2015). The spatial resolution selected is 4.7 km (~5 km hereafter) that corresponds to the operational scale of the NWS Multisensor Stage IV precipitation product (Lin and Mitchell, 2005). This facilitates the future integration of the profiles into operational land surface, hydrologic, or agricultural models that are currently operating in the region. It is quite possible that these models could be improved through assimilation of observed SM profiles, especially in regions of the world where climate information is sparse.

As stated earlier, the overall objective of the study is to determine the efficacy of SM profiles developed directly from remotely sensed data only, without the use of a LSM or ancillary data. The study consists of four parts: (a) a multiyear disaggregation of the coarse resolution MW surface SM to the 5-km spatial resolution; (b) calculation of SM profiles for each 5-km grid using the POME approach with the downscaled MW data serving as the surface boundary condition and TIR estimates providing mean SM; (c) validation of the SM profiles against a gridded LSM and *in-situ* data; and (d) error analyses including evaluation of downscaled MW surface SM estimates against LSM and *in-situ* data. Two independent data sources are used for comparison and validation purposes, using ground observations from 10 available NRCS SCAN sites and gridded 3-km Noah LSM SM data aggregated to the 5-km spatial resolution.

## 2 Study Area and Data Sources

#### 2.1 Study Area

The study area for this research is the southeastern U.S consisting of four states including Alabama, Georgia, Florida and South Carolina (Fig. 1). The region is home to a significant amount of current hydrologic and agricultural research activity where accurate SM modeling is a premium (McNider et al., 2011, 2015; Mishra et al., 2013). The southeastern U.S. represents a subtropical humid climate that typically has relatively hot and humid summers and precipitation that is generally evenly 100 distributed throughout the year. The mean annual precipitation is 1250-1500 mm based on the 1981-2010 period. Mean annual temperature ranges from  $14^{\circ}C$  in Northern Alabama to nearly  $24^{\circ}C$  in southern Florida. The region is roughly 31% forested; 54% shrubs; 12% agricultural land and rest of the area is covered by urban (1.9%), savanna (1.8%), water etc. according to Moderate Resolution Infrared Spectroradiometer (MODIS) 2008 land cover data aggregated to 5-km spatial resolution. The majority of the soils (nearly 80%) at the surface are classified as sand with loamy sand and sandy loam, as determined from the Soil Information for Environmental Modeling and Ecosystem Management (Miller and White, 1998). These soils are known to have relatively low water holding capacity that can lead to great temporal variation in upper level (1-10 cm) SM conditions and relatively frequent short-term droughts (1-4 week period) during growing seasons in various parts of the region MeNider et al., 2014) (McNider et al., 2015). Although the study region is overwhelmingly represented by a forest and shrub landscape. vegetation that are known to adversely affect the accuracy of MW signals, the study does present an opportunity to evaluate the performance of the merged MW/TIR profiles in a challenging environment and may provide greater confidence in the robustness of the system. Further, the Southeastern U.S. is one of the more data rich regions of the world (climate and soils data) providing ample opportunity for calibration as well as validation of results.

#### 20 2.2 Data Sources

## 2.2.1 Microwave Surface SM

Moisture Active Passive (SMAP); the Special Sensor Microwave Imager (SSM/I) etc. (Kerr et al., 2010; Entekhabi et al., 2010a; Njoku et al., 1977; Schmugge et al., 1992). Furthermore, due to their all-weather and day/night capabilities, MW sensors are widely used globally and offer high temporal data availability. This study employs one of the more extensively used and validated MW based SM data sets from the Advanced Microwave Scanning Radiometer (AMSR-E) mission operating in the X-band frequency from the National Snow and Ice Data Center (NSIDC) and employs the standard NASA retrieval algorithm (Njoku et al., 2003). The NSIDC is one of two AMSR-E data sets supported by NASA with the other being the Vrije Universiteit Amsterdam - Land Parameter Retrieval Model (VUA-LPRM) data. The LPRM uses a single dual polarized channel (X- or C- band) to deduce relationships between geophysical variables such as soil-moisture-SM and vegetation characteristics and

Over the past several years, much attention has been given to the use of MW sensors to measure surface SM remotely -e.g. Soil Moisture Ocean Salinity (SMOS); the Advanced Microwave Scanning Radiometer for Earth Observation (AMSR-E); Soil

brightness temperatures (Cho et al., 2015). Several studies such as Wagner et al. (2007); Draper et al. (2011); Jackson et al. (2010); Gruhier et al. (2008) etc. have compared the two data sets and the general conclusion has been that the VUA-LPRM algorithm may be slightly superior in terms of correlation to *in-situ* data, especially at lower latitudes and sparse vegetation (Brocca et al., 2011). However, Jackson et al. (2010) found that for the southeast U.S, the NASA retrieval algorithm outperformed the LPRM in terms of bias and RMSE. Furthermore, as pointed out by Njoku et al. (2005) and Jackson et al. (2010) the effects of radio frequency interference (RFI) on C-band signals are more pronounced over countries such as the United States and Japan, therefore X-band retrievals are preferred over such regions. Hence X-band based on the standard NASA (or NSIDC) data set was selected for this study. The daily Level-3 AMSR-E SM X-band product (AELand3) (Njoku, 2004) from the ascending (1:30 pm local time) overpass was collected for this study. The ascending overpass was selected to be consistent with the ALEXI-timings of the TIR retrievals, which are forced with morning and local noon skin temperatures obtained from the Geostationary Operational Environmental Satellite (GOES) Imager instrument. The Level-3 AMSR-E SM estimate is a 25-km gridded data product.

## 2.2.2 Thermal Infrared - ALEXI

Techniques to retrieve root-zone moisture that rely upon TIR data are inferred from surface energy fluxes typically retrieved at relatively high spatial resolutions. TIR-based evapotranspiration (ET) estimates are generally related to LST and vegetation cover fraction. Models such as the Surface Energy Balance System [SEBS: (Su, 2002)]; the Surface Energy Balance Algorithm for Land [SEBAL: (Bastiaanssen et al., 1998)]; and the Two Source Energy Balance [TSEB: (Norman et al., 1995)] exploit this relationship with varying degrees of complexities. A two-source based ALEXI Atmospheric Land Exchange Inverse (ALEXI) (Anderson et al., 1997, 2007; Hain et al., 2011) model has been implemented over the continental U.S. and used as a source of surface energy fluxes (Anderson et al., 1997; Norman et al., 2003); evapotranspiration (ET) ET (Anderson et al., 2011b, 2012); SM (Hain et al., 2009; Mishra et al., 2013); and an Evaporative Stress Index (Anderson et al., 2011a, 2013). A continental-scale implementation of the ALEXI model was used in this study to estimate instantaneous energy fluxes. ALEXI fluxes are available at approximately 4.7 km  $(0.04^o)$  spatial resolution on a daily time-step since the year 2000 over the CONUS continental U.S., generated using 15-min resolution GOES 10.7  $\mu$ m channel TIR data. ALEXI estimates of actual ET and SM are used in this study. A known drawback of TIR-based methods is that they are limited to cloud-free conditions.

#### 2.2.3 *In-situ* Observations

The study area contains 25 operational U.S. Department of Agriculture SCAN (Schaefer et al., 2007) monitoring stations. In addition to meteorological observations such as precipitation, air temperature, relative humidity etc. these monitoring stations measure soil temperature and moisture content primarily at depths of 5, 10, 20, 50 and 100 cm at hourly and daily time steps. The SCAN sites use Hydra Probes (Stevens) to observe SM conditions (Schaefer et al., 2007). Most of these 25 SCAN sites are located in northern and central Alabama. Ten sites with the most consistent data availability and with good geographical distribution across the study area were employed for the comparison. The SM data were obtained from

http://www.wcc.nrcs.usda.gov/scan/. Table 1 lists the major land cover type (at 5 km 5 km scale) along with soil characteristics at these ten sites.

## 2.2.4 Noah Soil Moisture

The Noah SM product generated with the NASA LIS (Kumar et al., 2006) framework was selected as a comparison dataset. The Noah model SM product used in this study is provided by the NASA Short-Term Prediction Research and Transition Center (SPoRT). The model is driven by actual meteorological forcings from the North American Land Data Assimilation system-Phase 2 (NLDAS2) (Xia et al., 2012), and thus serves as a valuable comparison dataset by which to measure the MW downscaling and profile results. While Noah SM also has biases and uncertainties, the comparisons reveal regional patterns of agreement (disagreement) with the remote sensing estimates. In the event that the POME profiles prove to be superior to the LSM in certain instances, this would indicate that the LSM (or other hydrologic or agricultural models) might be improved through assimilation of the remotely sensed SM profiles. The comparison assumes that errors in the Noah model are independent from the errors associated with MW and TIR based estimates. Noah SM estimates are available in four layers: 0-10; 10-40; 40-100 and 100-200 cm depths. It should be noted that there are inconsistencies in the surface layer depths between Noah and MW data: The surface layer in the Noah model is the top 10 cm of the soil column, while the downscaled MW represents the top 0-2 cm. The Noah 3-km Noah SM products were aggregated to 5-km to be product scale to be consistent with the downscaled MW-productTIR products.

Additionally, the NLDAS2 gridded temperature forcing data (0.125° resolution) were also utilized for computing of potential ET (PET). The NLDAS2 forcing data was available from NASA land data assimilation portal, (https://ldas.gsfc.nasa.gov/nldas/NLDAS2forcing.php). The GTOPO30 digital elevation model (DEM) was used as source of elevation information for the study area. The GTOPO30 product was made available by the U.S. Geological Survey's EROS Data Center (https://lta.cr.usgs.gov/GTOP30). The 1-km gridded soil characteristic data for the study area was available from the Soil Information for Environmental Modeling and Ecosystem Management (Miller and White, 1998).

#### 3 Methodology

## 3.1 ALEXI Retrievals

#### 5 3.1.1 Surface Evaporation

A time differential application of the ALEXI model was performed to monitor the rise in land surface temperature (LST) from morning to local noon. The early rise in LST is used to diagnose the partitioning of net radiation into sensible, latent and soil heat fluxes. The rise in LST from morning to near-noon is known to be correlated with the moisture content of the soil: compared to a dry land surface, wetter surfaces warm slowly, thus requiring more energy for evaporating surface moisture (Hain et al., 2011; Kustas et al., 2001). The soil heat conduction flux is parameterized as a function of net radiation following (Santanello and Friedl, 2003); latent heat from the canopy (transpiration) is estimated assuming a non-stressed modified

Priestley-Taylor (Priestley and Taylor, 1972) approach. Finally, the soil (surface) latent heat is the residual of the canopy latent heat and latent heat of the soil and canopy system  $LE_s = LE_{sys} - LE_c$ . Here  $LE_s$ ,  $LE_{sys}$  and  $LE_c$  represent the latent energy of surface, system and canopy, respectively. Detailed model description and derivation is provided in earlier studies (Anderson et al., 2007; Hain et al., 2011). If the residual is negative [an indicator of condensation, an unlikely process during daytime (Hain et al., 2011)] then the canopy transpiration is relaxed iteratively until it reaches zero. The surface evaporation from ALEXI is used to compute the soil evaporative efficiency (SEE) function required for the disaggregation (described in section 3.2).

#### 3.1.2 Mean Root Zone Moisture Retrieval

The ratio of actual to potential ET ( $f_{PET}$ ) is functionally related to the fraction of available water ( $f_{AW}$ ). Multiple relationships between the ratios of PET and available water have been proposed with varying degrees of success including linear; non-linear; piecewise linear or threshold (Hain et al., 2009). Large-scale applications prefer simpler linear functions as sensitivity to SM is constant and thus relatively less detailed soil characteristics are required (Song et al., 2000). In this study a linear relationship proposed by Wetzel and Chang (1987) is employed:  $f_{PET} = 0.85 * f_{AW}$ . The resulting ALEXI SM estimation is given as:

$$\theta_{ALEXI} = (\theta_{fc} - \theta_{wp})(0.85 * f_{AW}) + \theta_{wp} \tag{1}$$

Here θ<sub>fc</sub> and θ<sub>wp</sub> represent the field capacity and wilting point of the soil, respectively. It is argued that the SM retrieval from diagnosed evaporative fluxes is reasonable when the SM content is within the limits of wilting point and field capacity (Hain et al., 2011). ALEXI retrievals can be interpreted based on fraction of vegetation cover (f<sub>c</sub>) as either surface moisture content (f<sub>c</sub> < 0.3); predominantly root-zone moisture (f<sub>c</sub> > 0.75) or a composite of both surface and root-zone moisture for f<sub>c</sub> between these limits. In this study Priestly-Taylor PET was used with ALEXI actual ET to compute f<sub>AW</sub>. It is argued that the
 SM retrieval from diagnosed evaporative fluxes is reasonable when the SM content is within the limits of wilting point and field capacity (Hain et al., 2011). Since in this study we are concerned with root zone SM content, it is not anticipated that the limitation mentioned will lead to significant error as conditions resulting on entire soil column through the root zone be above field capacity (or less than wilting point) would be rare.

## 3.2 Surface Disaggregation

The spatial resolution of the TIR- based ALEXI SM estimates are roughly 5 x 5 km. Thus, in order to utilize them in conjunction with the AMSR-E MW data, the coarse resolution MW surface estimates must be downscaled to match the ALEXI spatial scale. A physically based, semi-empirical soil evaporative efficiency (SEE) model in combination with a first order Taylor series expansion around the coarse resolution SM was used to map surface evaporative fluxes to SM content at finer resolutions. The SEE disaggregation approach has become very popular recently and has been employed by several investigators at varying spatial scales and locations such as: Chen et al. (2017) disaggregated SMAP SM to 250-m [r: -0.3-0.72, RMSE: 0.06-0.27]; Malbéteau et al. (2016) used the algorithm to downscale coarse scale SM to 1-km resolution [r: 0.70-0.94, RMSD: 0.07-0.09]; Merlin et al. (2015) downscaled SMOS SM to 1-km scale [r: -0.22-0.64, RMSD:0.05-0.32]; Molero et al. (2016) also

downscaled coarse resolution SMOS SM to 1-km scale [r: 0.35-0.47, ubRMSD:0.04-0.12]. In general, the disaggregation improves agreement with *in-situ* observations in comparison with coarse-scale estimates.

The disaggregation approach decouples the soil evaporation from the top few centimeters of the soil and the vegetation transpiration through ET partitioning. The disaggregation algorithm used in this study follows the concept of the DISaggregation based on Physical and Theoretical scale CHange [DISPATCH: (Merlin et al., 2012, 2013, 2010)] model. The model accounts for aerodynamic resistance over bare soil in addition to soil parameters such as field capacity via the SEE. Detailed DISPATCH algorithm derivation and description is presented by Merlin et al. (2012). Here we represent the prominent disaggregation equation as:

$$SM_{HR} = SM_{LR} + \frac{\partial SM_{mod}}{\partial SEE} \left[ SEE_{HR} - \left\langle SEE_{HR} \right\rangle_{LR} \right] \tag{2}$$

HR and LR refer to the high and low-resolution variables, respectively. There have been multiple linear and non-linear relationships proposed between SEE and surface SM in the past (Budyko, 1961; Komatsu, 2003; Lee and Pielke, 1992; Manabe, 1969; Noilhan and Planton, 1989). A recent study by Djamai et al. (2015) suggest that the non-linear model performs better in humid climatic condition. Therefore non-linear model suggested by Noilhan and Planton was used in this study to guide the DISPATCH algorithm—:

$$\frac{\partial SM_{mod}}{\partial SEE} = \frac{SM_{LR}}{\cos^{-1}(1 - 2SEE_{LR}\sqrt{SEE_{LR}(1 - SEE_{LR})})}$$
(3)

## 3.2.1 Modified SEE Computation

The SEE, which can be defined as the ratio of actual to potential surface soil evaporation (Fang and Lakshmi, 2014; Merlin et al., 2010), is computed at the high resolution first, and then the SEE results are aggregated to the respective low resolution 25-km MW scale. The studies by Merlin et al. (2010, 2012) demonstrated the use of MODIS LST, Normalized Difference Vegetation Index (NDVI) and albedo to determine surface and vegetation temperature and evaporation. The SEE was defined as:  $\frac{T_{s,max}-T_{s,HR}}{T_{s,max}-T_{s,min}}$ , where  $T_{s,max}$  is the soil temperature at SEE = 0;  $T_{s,min}$  is soil temperature at SEE = 1, and  $T_{s,HR}$  represents soil temperature at the high resolution grid scale.

However, in this study we employed the ratio of the estimated surface evaporation from ALEXI to the potential evaporation to compute SEE directly at the 5-km ALEXI resolution. As mentioned earlier, the two-source land surface representation in ALEXI separates surface evaporation and canopy transpiration. The potential surface evaporation is calculated using the Hamon PET (Hamon, 1963). Hamon PET estimates are completely dependent upon atmospheric demand irrespective of soil and vegetation characteristics and can act as a proxy of potential surface evaporation (PE). This represents a subtle change in the definition of SEE from the Merlin formulation in that in our case all land cover/soil matrix combinations are weighted equally as opposed to being weighted by their assumed PE value as in Merlin (approximated as function of surface temperature). Since the Southeastern U.S. is an energy limited, water rich environment (Ellenburg et al., 2016), evaporation is controlled primarily

by water availability and atmospheric demand; therefore, the effects of this change are not expected to be large. Hamon PET estimates have been found to be comparable to radiation based methods (e.g., Priestly-Taylor) to observed ET in the Southeastern U.S. at monthly or longer time scales (Lu et al., 2005), and are computed using air temperatures from the NLDAS2 forcing data subject to terrain adjustment. Terrain adjustment of coarse resolution temperature data was performed using a 30 m digital elevation map of the region and constant lapse rate of -6.5  $K.km^{-1}$  (Cosgrove, 2003). Recently, Mishra et al. (2018) utilized the DISPATCH algorithm with modified SEE computation to disaggregate the coarse resolution SMAP SM over continental U.S. to 9 and 3-km resolutions with mean correlation of 0.47 and ubRMSD of 0.064 ( $m^3m^{-3}$ ) against SCAN observations.

## 3.3 Profile Development

A multi-year vertical SM profile was developed for each ALEXI grid cell using the POME model developed by Al-Hamdan and Cruise (2010) over the study area. The application of POME to develop a one-dimensional SM profile requires two constraints; total probability:  $\int_{\Theta_L}^{\Theta_0} f(\Theta) d\Theta = 1$ ; and the mass balance constraint:  $\int_{\Theta_L}^{\Theta_0} \Theta f(\Theta) d\Theta = \overline{\Theta}$ . Here  $\Theta$  is effective saturation and  $\overline{\Theta}$  is the mean moisture of the soil column; whereas  $\Theta_0$  and  $\Theta_L$  are the upper (surface) and lower (bottom) effective saturation. The effective SM is given as:  $\frac{(\theta - \theta_{wp})}{(\theta_{fc} - \theta_{wp})}$ . The second constraint serves to connect the first moment in probability space to the mean water content of the soil column in physical space. The Shannon entropy is given by (Shannon, 1948):

15 
$$I = -\int_{0}^{\infty} f(x)ln(f(x))dx$$

20

where f(x) is the probability density function (pdf) of the variable. Maximizing I in Eq. (3) for the uniform pdf subject to the constraints, Chiu (1987) developed Maximizing the Shannon entropy, they developed a model to create monotonic profiles using boundary conditions and mean moisture content information via the 1-D profile of a variable decreasing monotonically from the surface down using the method of Lagrange multipliers. Al-Hamdan and Cruise (2010) applied the same technique to develop vertical SM profiles either increasing or decreasing with depth from the surface:

$$\Theta(z) = \frac{ln[exp(\lambda_2\Theta_0) \pm exp(1-\lambda_1)(\frac{z}{L})]}{\lambda_2}$$
(4)

The Lagrange multipliers  $(\lambda' s)$  can be determined from application of the constraints and boundary conditions (surface effective saturation, $\Theta_0$ ) and mean effective saturation value of the soil column  $(\overline{\Theta})$ , z is calculation depth, and L is total depth of the column. Eq. (4) is a monotonically increasing (+ sign) or decreasing (- sign) function, representing dry (increasing from the top boundary) and wet (increasing from the bottom boundary) case profiles. For details of the POME model please see the appendix A. Effective saturation values are mapped back to volumetric water content using soil water characteristics from Rawls et al. (1982) (see appendix B).

## Handling Dynamic Cases:

Experience has shown that not all SM profiles are monotonic as given by Eq. (4). In fact, it is clear that some profiles can be parabolic in shape (i.e., demonstrate an inflection point), especially immediately subsequent to rain events (dynamic case), or due to sharp changes in soil characteristics (Al-Hamdan and Cruise, 2010; Mishra et al., 2015) —(see Fig. Al). Such cases are identified when mass balance cannot be kept by the monotonic assumption and thus Eq. (4) has no solution. In these cases, it is assumed that the inflection point is located in the soil layer with the greatest field capacity (Mishra et al., 2015). The POME model is then applied twice; from the surface to the inflection point, and then from the inflection point to the bottom boundary. This procedure was only required in 9% of the profiles generated in the study.

As mentioned previously, POME is a statistical approach that begins with the assumption of a uniform soil moisture-SM distribution initially and envisions the profile as either monotonically increasing or decreasing, or possessing one prominent inflection point. The final profile will then be the optimal one subject to the given boundary and initial conditions. Of course, this is a simplification of the true behavior of soil moisture-SM in the field; however, numerous previous studies have demonstrated that if given accurate input data, the error in the profiles will generally be less than three percent (Al-Hamdan and Cruise, 2010; ?; Mishra et al., 2015)(Al-Hamdan and Cruise, 2010; Singh, 2010; Mishra et al., 2015). In the present application, the surface boundary condition is supplied by the downscaled AMSR-E estimates, the mean moisture content from the ALEXI model, and the lower boundary is parameterized as 50% of available water content. The lower boundary was selected so as to maintain the idea of Experience has shown that SM behavior becomes less dynamic deeper into the soil column and thus selection of a constant value (in terms of effective moisture content) might serve as a useful first approximation. Since in many ways, this is a proof-of-concept study, it was felt that this would be appropriate and would remain in the spirit of the Maximum Entropy concept that a minimum of a-priori information available and experience has shown that the moisture content at lower depths (100-200 cm) is usually not highly variable should be used in the calculation of the profiles. Of course this assumption serves to introduce error into the analysis as all profiles do not exhibit this behavior (see Fig. Al) (depending on soil characteristics) and even those that do may not stabilize around the particular SM state selected.

#### 3.4 Temporal Compositing

The ALEXI data are available from 2000 to present and AMSR-E from 2002-2011. For this study, the years 2006-2010 were selected for analysis as the NRCS SCAN data was most consistently available during this period (nearly 92%). The ascending AMSR-E SM estimates were available 64.5% of the days on an average for all scan site locations while ALEXI retrievals were available on only 36% of the days due to cloud cover limitations. Earlier studies such as by Leng et al. (2017a, b) explored a vegetation and aerodynamic coefficient based gap filling algorithm for satellite derived SM estimations. Despite showing promise, the proposed algorithm requires ancillary datasets that are not part of this study (e.g. wind speed) which might add additional error to the analysis. Whereas, temporal compositing can be used for gap filling, it further tends to reduce the day-to-day noise associated with the satellite retrievals (Anderson et al., 2011a). Further, there is a strong correlation between surface SM and moisture dynamics at lower layers for temporal lags of less than 5-days (Penna et al., 2013; Alfieri et al., 2017).

Therefore, a three day moving window un-weighted mean was used on AMSR-E and ALEXI retrievals to develop a composite datasetthat serves as gap filling and also tends to reduce day-to-day noise in satellite retrievals (Anderson et al., 2011a). Compositing of the ALEXI surface ET increased the mean data availability from 36 to nearly 63% over all scan sites and in the case of AMSR-E compositing ensured close to 100% data availability. The availability of pixels with intersection of AMSR-E and ALEXI data more than doubled from 22.5% to 58.7% for the study period over all sites.

#### 3.5 Evaluation Metrics

The remote sensing derived SM profiles developed using the POME model were compared and validated against *in-situ* observations from 10 NRCS SCAN sites along with the gridded Noah LSM SM products over the study area. The LSM was used as a basis of comparison since the long term goal of the project is to develop remotely sensed SM profiles that can be assimilated into hydrologic and other land surface models. The data gaps in all three datasets restrict the possibility of time series analysis; therefore, pair-wise temporal statistical comparisons were performed using traditional matrices such as correlation coefficient (*r*), root mean square difference (RMSD) and bias. It has been argued that in cases with either the model or reference dataset being biased in mean or amplitude of fluctuations, the traditional RMSD tends to be an overestimation of true unbiased data (Entekhabi et al., 2010b). Therefore an unbiased RMSD in addition to traditional RMSD was also computed. The unbiased RMSD can easily be computed by removing the bias term form the definition as:

$$ubRMSD = \sqrt{(RMSD^2 - Bias^2)} \tag{5}$$

To assess the quantitative error between three datasets against an unknown true observation, the triple collocation (TC) error estimation method was employed (Stoffelen, 1998). TC has become a very popular technique for simultaneous error analysis of three data sets since its adaptation to SM states by Scipal et al. (2008). The procedure is based on the assumption of linear relationships between the three estimates of the SM at a specific location and the unknown true value. The unknown truth is eliminated from the linear error equations through subtraction and then cross multiplied to determine the error variances of the datasets relative to each other (Gruber et al., 2016). The assumption is that the errors in the three datasets are independent and random. Multiple recent studies have used the triple collocation method for error estimation [such as Crow et al. (2015); Yilmaz et al. (2014); Su et al. (2014); McColl et al. (2014) etc.]. A detailed review of method derivations and application to SM error estimation and analysis is presented by Gruber et al. (2016). In this study, the TC errors were computed using variances and covariances of the datasets (McColl et al., 2014; Stoffelen, 1998; Su et al., 2014). The covariance based approach enables us to compute unscaled error variances directly. Further, the covariance notation also computes the sensitivity of the datasets  $(\beta_i^2 \sigma_{\Theta}^2)$  against true SM signal. Here  $\beta$  is the scaling parameter, i is the dataset and  $\sigma_{\Theta}^2$  is the variance of the true jointly observed SM signal. Sensitivity estimates can be used to further validate and inter-compare the datasets. Recently, McColl

et al. (2014) proposed a methodology to compute the correlation coefficient between the involved datasets (referred as X,Y,Z) and underlying true SM signal as:

$$R_i^2 = \frac{\beta_i^2 \sigma_{\Theta}^2}{\beta_i^2 \sigma_{\Theta}^2 + \beta_i^2 \sigma_{\epsilon_i}^2} \tag{6}$$

Here  $\sigma_{\epsilon_i}^2$  is the error variance if of the dataset where  $i \in [X,Y,Z]$ . The sensitivity of individual dataset is estimated as:

$$5 \quad \beta_X^2 \sigma_{\Theta}^2 = \frac{\sigma_{XY} \sigma_{XZ}}{\sigma_{YZ}} \qquad \beta_Y^2 \sigma_{\Theta}^2 = \frac{\sigma_{YX} \sigma_{YZ}}{\sigma_{XZ}} \qquad \beta_Z^2 \sigma_{\Theta}^2 = \frac{\sigma_{ZX} \sigma_{ZY}}{\sigma_{XY}} \tag{7}$$

## 4 Results and Discussions

#### 4.1 Comparison with Noah LSM

For comparing SM profiles, 0-100 cm POME based profiles at 5 cm layer depth intervals were aggregated using the unweighted simple mean to the depths consistent with the Noah LSM: 0-10; 10-40; and 40-100 cm. The analysis can be approached from three perspectives: the surface values represent the MW downscaling; the bias represents the ALEXI model performance as it is providing the total SM content in the root zone; and the RMSD is representative of the entropy model as it measures the moisture distribution within the soil column.

Figure 2 shows the statistics of multi-year temporal SM profile comparisons between the POME and the Noah LSM for the study region. The figure shows the mean RMSD and ubRMSD tend to be relatively stable with depth over the entire region, an indication of relative stability for the profile developed using the POME model. As depth increased, pixel bias ranged from 0.05-0.13 m<sup>3</sup>m<sup>-3</sup> indicating that the mean SM data from the ALEXI model is positively biased compared to the Noah LSM, although the mean bias was  $\ge < 0.05$  m<sup>3</sup>m<sup>-3</sup> for all layers. The overall RMSD at all layers was found to be under 0.085 in volumetric SM. Moreover  $\ge$  more than 97% pixels across the study area showed ubRMSD of less than 0.06 m<sup>3</sup>m<sup>-3</sup> across all layers, indicating good agreement between the POME model and the Noah SM estimates (Jackson et al., 2010). Comparing Fig. 2 with the landcover map (Fig. 1), it seems that the higher correlations (r > 0.6) occur more prominently in the agricultural dominant portions of the study area for the top two layers (0-40 cm). The overall correlations in the range of 0.46-0.54 across layer depths suggest that the temporal variabilities from remotely sensed driven POME model compared fairly well against Noah SM.

Comparison between POME and Noah SM profiles by land cover type (Fig. 3) indicate that the absolute bias tends to increase with depth in the savannah, shrub, and forest land covers while the reverse is evident for the urban, grass and crop coverages. It appears that overall bias is lowest in the savannah, forest, and agricultural land classes and since those classes (particularly forest) dominate the region, this naturally leads the relatively low overall region-wide bias shown in Fig. 2.

The RMSD (and ubRMSD) present an opportunity to judge the overall profile development process. It is clear from Fig. 3 that the RMSD improves from the surface to the middle layer and then increases again in the bottom layer in every land

cover class except shrub. The top and bottom layer RMSD is being impacted by the boundary conditions placed on the POME integral by the MW and the parameterized lower boundary. Clearly, the POME process tends to improve the imprecise surface boundary as depth increases until the assumed lower boundary condition is encountered and results in deterioration of the profile RMSD.

In terms of correlation, the mid layer (10-40 cm) has the highest correlation (overall mean r = 0.54) for all land cover types with the highest mean correlation of 0.7 for crop dominated landcover. This further demonstrates the capabilities of the ALEXI model to estimate root-zone mean SM content in comparison to the Noah LSM. Incidentally, for most crops, the majority of the root mass is distributed in the top 60 cm of the soils column (Wu et al., 1999). The higher root density ensures the strong coupling of the land-plant-atmosphere system which tends to improve the accuracy of ALEXI in that zone. Increased correlations in the 10-40 cm layer indicate the ability of ALEXI to mimic the temporal patterns in the root-zone consistently relative to Noah. As depth increases, the root density is reduced and thus the coupling between land and atmosphere is also reduced. This fact, along with the relatively coarse parameterization of the lower boundary on the POME profile, leads to a relative decrease in correlation at layer 3 (40-100 cm) at all land covers except for trees (forest). The cropland showed the highest correlations with the Noah profile while keeping the RMSD and bias consistent with other land types. Agricultural areas demonstrated correlations ranging from 0.5 to 0.7 with a mean correlation of 0.62.

The overall analysis by layer depths appear to indicate that the profiles developed through the POME model using the disaggregated MW and the ALEXI derived mean SM content is in good agreement with the Noah LSM in the southeastern U. S. and in very good agreement in agricultural areas of the region.

## 4.2 Comparison with *in-situ* Observations

5

The comparison against Noah LSM SM estimates provided useful insights towards the performance of TIR-based SM profiles developed through the POME model. The comparisons against the LSM specifically adds to the analysis of results as a function of land cover, yet as mentioned earlier, the analysis does not assume that Noah is a perfect model - it may have its own errors. Therefore multiple NRCS SCAN site *in-situ* observations are used for further validations. When comparing remotely sensed data to site specific *in-situ* observations, disparities in spatial scale and sensing depth must be considered. Although some authors prefer to remove bias due to the differing scales before comparisons are made (Brocca et al., 2011), it is also quite common to do the comparisons without adjusting for scale, even when only one *in-situ* site is available (McCabe et al., 2005; Sahoo et al., 2008). In this study no bias corrections were performed.

Figure 1 shows the location of each of the sites used for validation along with the underlying land cover map. Table 1 summarizes the SCAN site characteristics, dominant land cover types and soil characteristics at the surface and 100 cm depth. Dominant land cover for sites 2009, 2114 and 2115 are predominantly savannas and forest type (hereafter referred as forest sites), whereas sites 2013, 2037, 2038 and 2113 are a mix of cropland either with savannas or shrubs (hereafter referred as mixed cropland sites). Only sites 2027, 2078 and 2053 (hereafter referred as cropland sites) are predominantly cropland at the 5-km spatial resolution footprint. The crop and mixed crop sites are shown in bold in the following text. The SCAN sites

monitored SM at depths of 5, 10, 20, 50 and 100 cm. The POME based profiles are developed at 5 cm layer depth increments down to 100 cm depth.

The results of the developed profiles in comparison to the SCAN site observations alone are shown in Fig. 4. First, it is evident in all the statistics except the correlation that the pattern demonstrated in the previous comparisons persists in that the statistics often tend to improve with depth with occasional deterioration when the lower boundary is encountered. Considering the performance of ALEXI initially, the bias appears reasonable in most cases where the majority of instances the absolute bias is less than  $0.1 \text{ (m}^3\text{m}^{-3})$ , but it appears to be best in the mixed cropland areas (mean absolute bias of  $0.07 \text{ m}^3\text{m}^{-3}$  across all depths) and worse in forested sites (mean absolute of 0.13 m<sup>3</sup>m<sup>-3</sup>). In fact, at seven of the ten total sites the overall bias is considerably less than the average moisture content at the SCAN site itself. At the two sites with the highest bias (2009) and 2027), the mean moisture content from ALEXI was about twice the observations at all layers, indicating that the satellite estimates showed considerable positive bias (mean bias 0.17 and 0.13 m<sup>3</sup>m<sup>-3</sup>, respectively). Hain et al. (2011) pointed out that sensitivity of the ALEXI model decreases as moisture content nears either the wilting point or the field capacity. Both sites 2009 and 2027 had sandy soils at the SCAN site and exhibited the lowest mean moisture content of all sites. At site 2009 with sandy soil through the column, the mean SM content was 0.05 m<sup>3</sup>m<sup>-3</sup> against the wilting point of 0.033 m<sup>3</sup>m<sup>-3</sup> while 2027 site had sand at the surface and sandy loam (wilting point =  $0.095 \text{ m}^3\text{m}^{-3}$ ) at the 100 cm depth and the mean SM content was 0.12 m<sup>3</sup>m<sup>-3</sup>. Moreover, the site 2009 is located in a forest-dominated region. Whereas for site 2027 (located in southwest Georgia), the higher bias in remotely sensed observations can be attributed to additional SM content due to irrigation. Southwest Georgia is one of the most irrigated regions of the study area. In contrast, the SCAN site observations are primarily governed by precipitation alone.

In the case of RMSD, half the sites showed an average RMSD of 0.1 m<sup>3</sup>m<sup>-3</sup> or less. RMSD tends to be better at the mixed land use sites, while poor performances at sites 2009, 2115 and **2027** skewed the forest and cropland results respectively. As in the bias case, these sites demonstrated the highest mean RMSD values (Fig. 4). However, with the exception of these sites, the average RMSD was less than the SCAN average moisture content in all cases. The ubRMSD, on the other hand, at all sites was better with the overall ubRMSD for all layer depths and land cover types exhibiting an average ubRMSD of 0.07 m<sup>3</sup>m<sup>-3</sup>. The ubRMSD tended to improve with depth for all cases (Fig. 4) up to the depth of 50 cm, but showed a rise at the 100 cm depth as discussed previously. Improvements in ubRMSD with depth indicate the ability of the POME model to converge and correct itself from the effects of the noisy surface boundary condition until the assumed lower boundary affected the performance in that layer.

20

The r results are interesting and do not necessarily track the other two indices. It is clear from Fig. 4 that POME tended to perform better in agricultural land use areas than in other environments. Similar to the bias results, correlation was poorest at forested locations. In all, three sites showed average correlation above 0.5 with four other sites showing a correlation above 0.4. Two sites (2009, 2113) produced average correlations of 0.16 and 0.32 across all depths. As discussed earlier, site 2009 is forested while 2113 is located near a water body (Lake Catoma). Overall, the crop sites showed the highest correlations (0.51) followed by mixed crop sites (0.42), an indication of the ability of the satellite derived surface and mean moisture content estimates to mimic wetting and drying patterns over time across depths.

However, the correlation consistently declined with depth at most of the agriculture and mixed agriculture sites. The decline most often became more pronounced after the second (or sometimes third) layer indicating that the influence of the parameterized lower boundary extends through the lower 50 cm of the profile, at least to some extent. The use of a constant lower boundary condition would not be expected to correlate with variable observation. This phenomenon was not evident in the forest areas where the SM was not as variable in the lower layers.

#### 4.3 Intercomparison of Noah, POME with *In-situ* Observations

The POME profiles have been compared with Noah LSM across the study region and against *in-situ* observations at ten locations. However, as mentioned earlier, both analyses have some limitations either in terms of proxy ground truth (in case of LSM) and spatial representation (*in-situ* observations). Therefore, in this section an intercomparison between the three datasets is performed to assess the relative strength of each SM dataset. Figure 5 shows the time series of the SM state from Noah LSM, SCAN observations and the POME model. Consistent with the layer depths of the Noah, the POME profile and the SCAN observations were aggregated to 0-10; 10-40; and 40-100 cm layer depths.

The figure shows that the three data sets track each other well in some cases and that in others there are significant discrepancies. In general, with the exception of a few cases, it appears that the POME and SCAN profiles track better than the Noah simulations in the lower soil layers. In particular, the Noah model shows a prominent cycling effect in the bottom layer at many sites that is not present in the other two data sets. On the other hand, the POME time series at the sites dominated by agricultural and mixed land uses (e.g., 2027, 2053, 2078, 2037, 2013) exhibit a pronounced cyclic effect in the surface layers in addition to a positive bias compared to the Noah and the SCAN data. The sites in north Alabama (2053 and 2078) and in western Georgia (2027) are located in some of the most highly irrigated regions of the study area. Therefore, the MW derived upper boundary condition for the POME model is likely to sense the irrigation activity in the region compared to the precipitation derived Noah LSM and SCAN observation located in non-irrigated areas. Further, the other two sites (2037 and 2013) are located in areas with close proximity to surface water and hence the MW surface SM estimates can be contaminated and result in the positive bias being observed at those locations. The forest dominated sites (2009, 2114 and 2115) on the other hand showed that the POME model profiles are more comparable overall to the Noah LSM than to the point sourced SCAN observations. The mixed agricultural sites (2113 and 2038) are located in regions hardly experiencing any irrigation activity and not impacted by surface water, and thus showed little to no bias at the surface against Noah and SCAN profiles. The time series observations suggests that the downscaled MW surface SM is able to sense irrigation activity and therefore may provide an accurate surface boundary condition to the POME model. At lower depths (40-100 cm) the POME profile seems to be in better agreement with the SCAN observations than the Noah estimates, which indicate that the parameterization of the lower boundary condition seems to be reasonable in this case, and that the POME profiles actually improve with depth in contrast to the Noah simulations. The dynamic nature is observed at lower depths for few sites (particularly 2013 and 2115). This anomalous behaviour can be attributed to the fact that these sites had porous soils near the surface with clay layers beneath. While site 2113 is located in close proximity to a stream and is potentially influenced by surface water intrusion.

Table-2 shows the detailed statistics of comparison between Noah LSM SM, *in-situ* observations and POME profiles at each SCAN site location. The results are further summarized across all sites in Fig. 6. The overall results show that the satellite-based and LSM SM estimates are reasonably comparable based on error statistics of ubRMSD (0.05 vs 0.04 m³m<sup>-3</sup>) and absolute bias (0.08 vs 0.07 m³m<sup>-3</sup>). For the surface layer (0-10 cm) comparisons, the Noah correlations are superior to the POME model (r = 0.75 vs 0.54), although in several cases the Noah correlations decrease vertically through the soil column to the point that the two approaches are much more comparable (Fig. 6). This case does not show the steep decline in correlation through the POME profiles as before, indicating that amalgamation of the lower layers into one 60 cm layer has dampened that effect. In terms of mean bias across layers, the POME model is superior in four cases, Noah is superior in four cases and in the other two cases (2115 and 2053) the two models perform the same. In terms of ubRMSD, the POME is superior to Noah at three locations while at other six locations the difference is within 0.01 (m³m<sup>-3</sup>). Overall, the average statistics across all depths and all sites, the Noah/SCAN average RMSD was 0.09 m³m<sup>-3</sup> in comparison to the POME RMSD of 0.10 m³m<sup>-3</sup> against ground based SCAN observations. The unbiased RMSD between Noah and SCAN was 0.04 m³m<sup>-3</sup>, and for the POME it was 0.05 in volumetric SM. Figure 6 shows that the Noah LSM tended to become less accurate compared to the SCAN observations with depth while the POME generally showed the reverse.

The three data sets can be further compared through TC analysis. TC has the advantage that the SCAN observations are treated equally with the LSM and POME as just another estimate of the true SM state. The analysis is performed for three layers to be consistent with the LSM model configuration (Fig. 7). The surface results (0-10 cm) showed that in most instances the SCAN observations are closer to the true SM compared to the Noah and POME data; however, the latter two data sets also show high coefficient of determination ( $R^2$ ) values at several sites. The middle and bottom layer results appear to indicate that the Noah LSM is superior (with 5 and 9 instances of  $R^2 > 0.8$ , respectively), while the SCAN observations and the POME model track each other fairly well with six and five instances, respectively, of  $R^2 > 0.4$  for the POME and five and four such instances for SCAN observations. It should be noted here that although TC accounts for total error among the three data sets, the Noah results may be problematic in that, unlike the other two data sets, the deterministic SM equation (e.g., Richards Equation) governs the movement of moisture through the column and some of the random errors are eliminated. This would not affect the surface layer, which is governed by precipitation and surface evaporation. Thus, the errors in the LSM at the deeper layers may be dampened and thus affect the results.

#### 5 Error Characterization

15

The developed profile results are impacted by the boundary conditions applied to the POME as the integral serves to transition the profile between the upper and lower boundary conditions. The upper boundary is associated with the MW surface SM estimates while the lower boundary was assumed for this study and potentially could be parameterized or used as a calibration parameter. In addition, the mean SM estimated from ALEXI determines the total mass to be distributed. Earlier studies by Al-Hamdan and Cruise (2010) and Mishra et al. (2015) showed that the POME model is capable of producing profiles with significant accuracy with mean absolute errors in the range of 0.5-3.0% for known input conditions. However, in this study

inputs to the POME model are derived from remotely sensed measurements, in addition to a parameterized bottom boundary condition. Hence, profile errors may be characterized in terms of errors in input parameters.

Figures 8(a) and (b) shows the sensitivity of the profile in terms of bias and RMSD to variations in the mean and surface constraints. From Figure 8(a) it is clear that, even if the surface boundary condition is off by 50% (in effective SM), the overall profile RMSD and bias is less than 0.35 (in effective SM), and the maximum possible deviation in the surface boundary results in bias and RMSD of 0.62 and 0.67 (in effective SM), respectively. The sensitivity study of the mean moisture content (Fig. 8(b)) shows that the bias and RMSD of the profile (in terms of effective SM) are linearly related to the deviations in the assumed mean. Furthermore, Fig. 8 indicates that the profile is more sensitive to errors in the mean than it is to deviations in the surface boundary condition.

#### 5.0.1 Effect of Disaggregation of AMSR-E MW Data

## 5.1 Effect of Disaggregation of AMSR-E MW Data

Figure 8 shows that the POME profile is sensitive to the surface boundary conditions. In this study these conditions are provided by AMSR-E; therefore, it is instructive to examine the relative accuracy of the downscaled MW data. To that end, the AMSR-E surface SM before and after disaggregation is compared to both the Noah LSM and the *in-situ* SCAN data to quantify the effect of the SEE downscaling algorithm. The results from a temporal analysis between coarse and downscaled (fine) resolution MW surface SM with the Noah LSM surface is shown in Fig. 9 for the study domain. The figure shows that the generally negative bias of the original AMSR-E data (overall mean =  $-0.08 \text{ m}^3\text{m}^{-3}$ ) when compared to the Noah LSM was transformed by the disaggregation to a positive bias in the eastern half of the study area although the overall bias remained slightly negative. The positive bias in the eastern zone was largely in the 0.04 to 0.13 m<sup>3</sup>m<sup>-3</sup> range. It is also apparent that this same area exhibited a substantial increase in correlation between the downscaled MW and Noah data. Comparing Fig. 9 to the land cover image in Fig. 1, it can be see that the increase in correlation was largely in the agricultural bands in the southwestern Georgia leading into southeastern Alabama. However, a few areas, such as extreme southwestern and east-central parts of Alabama, showed degradation in correlation on downscaling. The land cover map shows that these areas are generally forested. Overall the temporal r showed a modest increase from 0.21 to 0.25 with downscaling for the study area indicating that downscaled AMSR-E is slightly more comparable to Noah LSM surface SM. Perusal of the figure shows that the poor results in Florida and along the eastern seaboard are primarily responsible for the low correlations. It also demonstrates the fundamental property that the downscaling process will be compromised in areas where the original MW data was of exceptionally poor quality to begin with.

It is difficult to determine the impact of the disaggregated MW surface SM estimates on the profiles compared to the LSM. First, the statistics shown in Fig. 9 are for the sensing depth of the raw AMSR-E data (0-2 .5-cm) while the relatively better statistics shown in Fig. 2 are for the top layer corresponding to the Noah LSM (0-10 cm). This disparity in depth is undoubtedly affecting the results. The introduction of the mean SM from ALEXI also affects the near surface layer in the POME profile since mass balance must be maintained throughout the soil column. In any case, comparison of Fig. 2 and 9 shows that the

profile statistics are considerably improved compared to the MW surface values and thus the noise in the MW data has a minimal effect when compared to the Noah LSM.

The results of the comparison with the SCAN sites are perhaps more instructive and are given in Table 3 below. The table shows that in terms of correlation, the disaggregated data were better related to the *in-situ* data than were the original coarse scale MW data (r = 0.53 vs r = 0.31). This result was particularly evident at the agricultural SCAN sites (r = 0.64 vs r = 0.42). These results were obtained at a slight cost in the bias (bias=0.07 vs bias=-0.02 m³m<sup>-3</sup>) and RMSD (RMSD=0.1 vs RMSD=0.12 m³m<sup>-3</sup>), although the difference was not as great in unbiased RMSD. In the case of Table 3, the SCAN depth is the same as the MW so comparisons are apt. In cases of relatively high bias in the MW data (e.g., sites 2009, 2114, **2053, 2078**) this error is introduced into the POME profile. Figure 8 shows that errors in the surface boundary of about 0.1 translate to bias and RMSD in the profile of about 0.05 (in effective SM). It appears from Table 3 that at the sites demonstrating the consistently higher bias and RMSD, the error in the surface boundary could be responsible for one third to one half of that total.

### 5.1.1 Effect of Mean SM Inputs

## **5.2** Effect of Mean SM Inputs

The mean SM content within soil column in this study obtained from TIR based ALEXI model served as one of the two remotely sensed input parameters for the POME model. Therefore the mean SM content retrieved from the ALEXI model is compared with the Noah LSM. The results of the temporal analysis between the two datasets are shown in Fig. 10. The overall bias between the two datasets is  $0.04 \text{ m}^3\text{m}^{-3}$ . The overall RMSD is  $0.08 \text{ m}^3\text{m}^{-3}$  with ubRMSD of  $0.04 \text{ m}^3\text{m}^{-3}$  indicating that the mean SM content of the two datasets is similar. In terms of correlation coefficient, the root zone correlation nearly doubled (r = 0.49) compared to the surface correlations (Fig. 9). Further, comparison of Fig. 10 with Fig. 1 reveals that, similar to the surface SM analysis, the mean SM content with the highest correlations (r > 0.5) are observed mostly in agriculture-dominated areas.

Figure 8(b) shows that the translation of the error in the mean SM content to errors in the POME profile is linear, so an error of 0.04 in the ALEXI mean compared to the LSM would translate into a similar error in the computed profile. Examination of column 2 (NP) in Table 2 above shows that this error represents the majority of the errors in the computed POME profiles compared to the LSM. Overall, the analysis revealed that the surface SM estimates accounted for, at most, for one third to one half of the error in the SM profiles and for most cases, the mean SM and the parameterized lower boundary accounted for the majority of the error. Recent advances such as the L-band sensor aboard the SMAP mission, offers the potential for even better correlated MW data. In addition, further analysis of the lower boundary condition parameterization could improve the profiles, particularly in the lower layers. For example, Mishra et al. (2013) used POME generated profiles to update SM within a crop model using the lower boundary condition from the model itself. If sufficient ground truth data are available, calibration could be accomplished, or the lower boundary could be set as a function of soil properties in the bottom layer of the profile.

The relatively sparse (5-10 day recurrence interval) availability of the ALEXI TIR-based SM retrieval is the major weakness of the procedure and necessitated compositing of the data into three day running means. However, the issue is a function of

the semi-tropical humid climate of the Southeastern U.S. Drier regions of the world would not suffer as much from this issue. Thus it is possible that the proposed method could be employed to deduce vertical SM profiles in regions of the world where observed climate data are scarce or insufficient to drive ecological models. These profiles could be assimilated into the models to help correct for model bias due to the poor climate inputs.

#### 5 6 Conclusions

This study evaluated the feasibility of linking downscaled MW surface SM with TIR root zone estimates to develop entropy-based vertical SM profiles. The SM profiles (including surface values) were compared to *in-situ* data at the Southeastern U.S. as well as the Noah LSM within the NASA LIS. Initial results are encouraging. The SEE disaggregation method of Merlin et al. (2012), guided by high resolution TIR estimates from the ALEXI model, showed promise when compared to the *in-situ* and modeled estimates in a humid semi-tropical region of the U.S. The POME generated SM profiles generally compared favorably with the SCAN site profiles and the Noah LSM.

When the Noah LSM and the POME profiles were compared to the *in-situ* data in terms of bias, the POME-generated profiles were clearly superior in at four sites, the LSM was superior at four sites and the two methods were the same at the other sites. However it must be noted that there is a scale mismatch when comparing with *in-situ* observations, also biases may exist in SCAN observations as well as the models. The maximum correlation in the range of 0.4-0.65 was observed in agriculturally dominant areas. Further the highest correlations were found at the depth of 10-40 cm, coinciding with the maximum root density for crops and thus offering a better coupling between land and atmosphere. The ALEXI model was able to pick the wetting and drying trends in the root-zone consistently.

Compared to *in-situ* observations, the bias and RMSD of the Noah model often tended to degrade vertically with depth while the reverse was evident in most of the POME profiles. While acknowledging that the SCAN data contains biases and errors of their own, this characteristic of the remote sensing driven POME method seems to open the possibility that profiles from land surface models could be improved in terms of bias and RMSD through the assimilation of the remotely sensed profiles. This conclusion is bolstered by the results of previous studies (e.g., Al-Hamdan and Cruise (2010); Singh (2010); Mishra et al. (2015)) that have found that the when the input data are well defined, the POME profiles are highly accurate throughout the soil column. TC analysis revealed that the POME and observed SCAN site observations tracked well, while the LSM appeared to show less variability, possibly due to the use of the deterministic Richards Equation to model SM movement through the soil column.

Error analyses revealed that the majority of the error in the POME generated profiles was due to error in the mean SM deduced from the ALEXI retrievals and the parameterized lower boundary condition. The lower boundary was simply assumed to be 50% of available moisture capacity and this assumption proved to be incorrect in some cases where the lower layer in the soil column exhibited marked variability. The SEE downscaling procedure increased the correlation of the surface SM compared to both the LSM and the SCAN sites, especially in agricultural areas where correlations in the range of 0.5-0.8 were achieved. In the meantime, the overall bias was reduced by a factor of 4 and the RMSD was only slightly increased

(0.09 to 0.10 m<sup>3</sup>m<sup>-3</sup>). The error analysis suggested that at most the MW derived surface boundary accounted for at most one third to one half of the overall error in the POME profiles. Downscaling generally was less effective in locations where the AMSR-E demonstrated positive bias and appeared to lose effectiveness as the bias increased. MW surface observations can be contaminated when a high percentage of the pixel is dominated by water, as near large streams or lakes or in the near coastal region. Dense vegetation also tends to degrade the MW results.

## **Appendix A:** The Principle of Maximum Entropy (POME) Model

Three distinct SM profiles cases are possible: wet case- upper layer is wetter than the lower; dry case – upper layer is drier than the lower; and dynamic case: a mix of wet and dry case, typically has at least one prominent inflection point. The wet case arises right after an irrigation/precipitation event; dry case profiles result long time after precipitation/irrigation event. The dynamic case is caused some time after a precipitation/irrigation event when surface dries up but the middle layers still have elevated moisture contents from earlier precipitation/irrigation events. Figure A1 shows these three possible cases.

## **A1** Application of Entropy to SM Profile Development

25

The information in a system in state i according to classical Shannon entropy formulation is given as:

$$I_i = ln\left(\frac{1}{p_i}\right) \tag{A1}$$

Here  $p_i$  is the probability that the system is in state i, and ln is the natural logarithm. The mean information content of a variable or process is given by Shannon entropy formulation in continuous form:

$$H = -\int_{i=1}^{n} f(x)ln(f(x))dx$$
(A2)

Here, f(x) is continuous probability distribution function (pdf) and n is the number of values a variable can take. Higher values of entropy would mean the lesser prior information availability in other words higher entropy means the higher uncertainty. According to Mays et al. (2002), the informational entropy is a measure of the correspondence between the pdf of the dataset associated with a system and the pdf associated with the minimum information about the system. In case, the minimum a-priori information is available or the system is unpredictable, the probability distribution would be uniform and the entropy will be high (Pachepsky et al., 2006).

The principle of maximum entropy was developed by Jaynes (1957a, b) which proposes that if inferences has to be drawn from incomplete information then it should be drawn from a probability distribution that has the maximum entropy permitted by the a-priori information. Based on this concept, Al-Hamdan and Cruise (2010) developed an entropy-based algorithm to model SM profiles assuming uniform distribution throughout the soil column. The method was based on the approach developed to compute the vertical velocity distribution in open channels by Chiu (1987).

The application of POME to develop a one-dimensional SM profile requires two constraints; total probability:

$$\int_{\Theta_L}^{\Theta_0} f(\Theta) d\Theta = 1 \tag{A3}$$

and the mass balance constraint:

$$\int_{\Theta_L}^{\Theta_0} \Theta f(\Theta) d\Theta = \overline{\Theta} \tag{A4}$$

Here  $\Theta$  is the effective saturation and  $\overline{\Theta}$  is the mean moisture of the soil column; whereas  $\Theta_0$  and  $\Theta_L$  are the upper (surface) and lower (bottom) effective saturation. The effective SM is given as:  $(\theta - \theta_{wp})/(\theta_{fc} - \theta_{wp})$ . The second constraint serves to connect the first moment in probability space to the mean water content of the soil column in physical space. The Shannon entropy is given by Shannon (1948):

$$I = -\int_{0}^{\infty} f(x) ln(f(x)) dx$$
(A5)

Maximizing *I* in Eq. (A5) for the uniform pdf subject to the constraints, Chiu (1987) developed the 1-D profile of a variable decreasing monotonically from the surface down using the method of Lagrange multipliers. Al-Hamdan and Cruise (2010) applied the same technique to develop vertical SM profiles either increasing or decreasing with depth from the surface:

$$\Theta(z) = \frac{ln[exp(\lambda_2\Theta_0) \pm exp(1-\lambda_1)(\frac{z}{L})]}{\lambda_2}$$
(A6)

The Lagrange multipliers  $(\lambda's)$  can be determined from application of the constraints and boundary conditions (surface effective saturation,  $\Theta_0$ ) and mean effective saturation value of the soil column  $\overline{\Theta}$ , z is calculation depth, and L is total depth of the column. Equation (A6) is a monotonically increasing (+ sign) or decreasing (- sign) function, representing dry (increasing from the top boundary) and wet (increasing from the bottom boundary) case profiles (Fig. A1). The dynamic case can be handled by dividing the profiles into multiple monotonic profiles and running the wet/dry case models for each of those profiles separately while keeping the mass balance.

#### 20 Appendix B: Soil Water Characteristics

The soil water characteristics used in this study to map effective to volumeteric SM and *vice-versa* is obtained from the values reported by Rawls et al. (1982) in their study. Table A1 summarizes the properties used for each soil types.

Acknowledgements. The authors would like to express their sincere gratitude to the anonymous reviewers for their constructive comments towards the improvement of this manuscript. This study is supported by NASA Headquarters under the NASA Earth and Space Science Fellowship (NESSF) Program - Grant NNX15AN58H. The authors are also thankful of agencies such as NASA, NRCS for making soil moisture data publicly available.

#### References

5

10

30

- Aghakouchak, A., Farahmand, A., Melton, F. S., Teixeira, J., Anderson, M. C., Wardlow, B. D., and Hain, C. R.: Remote sensing of drought: Progress, challenges and opportunities, Reviews of Geophysics, 53, 452–480, https://doi.org/10.1002/2014RG000456, 2015.
- Al-Hamdan, O. Z. and Cruise, J. F.: Soil Moisture Profile Development from Surface Observations by Principle of Maximum Entropy, Journal of Hydrologic Engineering, 15, 327–337, https://doi.org/10.1061/(ASCE)HE.1943-5584.0000196, 2010.
- Alfieri, J. G., Anderson, M. C., Kustas, W. P., and Cammalleri, C.: Effect of the revisit interval and temporal upscaling methods on the accuracy of remotely sensed evapotranspiration estimates, Hydrol. Earth Syst. Sci, 21, 83–98, https://doi.org/10.5194/hess-21-83-2017, 2017.
- Anderson, M. C., Norman, J. M., Diak, G. R., and Kustas, W. P.: A Two-Source Time-Integrated Model for Estimating Surface Fluxes Using Thermal Infrared Remote Sensing, Remote Sensing of Environment, 60, 195–216, https://doi.org/10.1016/S0034-4257(96)00215-5, 1997.
- Anderson, M. C., Norman, J. M., Mecikalski, J. R., Otkin, J. A., and Kustas, W. P.: A climatological study of evapotranspiration and moisture stress across the continental United States based on thermal remote sensing: 2. Surface moisture climatology, Journal of Geophysical Research D: Atmospheres, 112, https://doi.org/10.1029/2006JD007507, 2007.
- Anderson, M. C., Hain, C., Wardlow, B., Pimstein, A., Mecikalski, J. R., and Kustas, W. P.: Evaluation of drought indices based on Thermal remote sensing of evapotranspiration over the continental United States, Journal of Climate, 24, 2025–2044, https://doi.org/10.1175/2010JCLI3812.1, 2011a.
  - Anderson, M. C., Kustas, W. P., Norman, J. M., Hain, C. R., Mecikalski, J. R., Schultz, L., Gonzlez-Dugo, M. P., Cammalleri, C., D'Urso, G., Pimstein, A., and Gao, F.: Mapping daily evapotranspiration at field to continental scales using geostationary and polar orbiting satellite imagery, Hydrology and Earth System Sciences, 15, 223–239, https://doi.org/10.5194/hess-15-223-2011, 2011b.
- Anderson, M. C., Allen, R. G., Morse, A., and Kustas, W. P.: Use of Landsat thermal imagery in monitoring evapotranspiration and managing water resources, Remote Sensing of Environment, 122, 50–65, https://doi.org/10.1016/j.rse.2011.08.025, 2012.
  - Anderson, M. C., Hain, C., Otkin, J., Zhan, X., Mo, K., Svoboda, M., Wardlow, B., and Pimstein, A.: An Intercomparison of Drought Indicators Based on Thermal Remote Sensing and NLDAS-2 Simulations with U.S. Drought Monitor Classifications, Journal of Hydrometeorology, 14, 1035–1056, https://doi.org/10.1175/JHM-D-12-0140.1, 2013.
- 25 Arya, L. M. and Richter, J. C.: Estimating Profile Water Storage From Surface Zone Soil Moisture Measurements Under Bare Field Conditions, Water Resources Research, 19, 403–412, 1983.
  - Bastiaanssen, W., Menenti, M., Feddes, R., and Holtslag, A.: A remote sensing surface energy balance algorithm for land (SEBAL). 1. Formulation, Journal of Hydrology, 212-213, 198–212, https://doi.org/10.1016/S0022-1694(98)00253-4, 1998.
  - Brocca, L., Hasenauer, S., Lacava, T., Melone, F., Moramarco, T., Wagner, W., Dorigo, W., Matgen, P., Martínez-Fernández, J., Llorens, P., Latron, J., Martin, C., and Bittelli, M.: Soil moisture estimation through ASCAT and AMSR-E sensors: An intercomparison and validation study across Europe, Remote Sensing of Environment, 115, 3390–3408, https://doi.org/10.1016/j.rse.2011.08.003, 2011.
  - Budyko, M.: Heat banace of the Earth's surface, Soviet Geogrphy, 2, 3–13, 1961.
  - Chen, N., He, Y., and Zhang, X.: NIR-Red Spectra-Based Disaggregation of SMAP Soil Moisture to 250 m Resolution Based on SMAPEx-4/5 in Southeastern Australia, Remote Sensing, 9, 51, https://doi.org/10.3390/rs9010051, 2017.
- 35 Chiu, C. L.: Entropy and Probability Concepts in Hydraulics, Journal of Hydraulic Engineering, 113, 583–599, https://doi.org/10.1061/(ASCE)0733-9429(1987)113:5(583), 1987.

- Cho, E., Choi, M., and Wagner, W.: An assessment of remotely sensed surface and root zone soil moisture through active and passive sensors in northeast Asia, Remote Sensing of Environment, 160, 166–179, https://doi.org/10.1016/j.rse.2015.01.013, 2015.
- Cosgrove, B. A.: Real-time and retrospective forcing in the North American Land Data Assimilation System (NLDAS) project, Journal of Geophysical Research, 108, 8842, https://doi.org/10.1029/2002JD003118, 2003.
- 5 Crow, W. T., Lei, F., Hain, C., Anderson, M. C., Scott, R. L., Billesbach, D., and Arkebauer, T.: Robust estimates of soil moisture and latent heat flux coupling strength obtained from triple collocation, Geophysical Research Letters, 42, 8415–8423, https://doi.org/10.1002/2015GL065929, 2015.
  - Djamai, N., Magagi, R., Goita, K., Merlin, O., Kerr, Y., and Walker, A.: Disaggregation of SMOS soil moisture over the Canadian Prairies, Remote Sensing of Environment, 170, 255–268, https://doi.org/10.1016/j.rse.2015.09.013, 2015.
- Draper, C., Mahfouf, J. F., Calvet, J. C., Martin, E., and Wagner, W.: Assimilation of ASCAT near-surface soil moisture into the SIM hydrological model over France, Hydrology and Earth System Sciences, 15, 3829–3841, https://doi.org/10.5194/hess-15-3829-2011, 2011.
  - Ellenburg, W. L., McNider, R. T., Cruise, J. F., and Christy, J. R.: Towards an understanding of the twentieth-century cooling trend in the Southeastern United States: Biogeophysical impacts of land-use change, Earth Interactions, 20, https://doi.org/10.1175/EI-D-15-0038.1, 2016.
- Entekhabi, D., Njoku, E. G., O'Neill, P. E., Kellogg, K. H., Crow, W. T., Edelstein, W. N., Entin, J. K., Goodman, S. D., Jackson, T. J., Johnson, J., Kimball, J., Piepmeier, J. R., Koster, R. D., Martin, N., McDonald, K. C., Moghaddam, M., Moran, S., Reichle, R., Shi, J. C., Spencer, M. W., Thurman, S. W., Tsang, L., and Van Zyl, J.: The soil moisture active passive (SMAP) mission, Proceedings of the IEEE, 98, 704–716, https://doi.org/10.1109/JPROC.2010.2043918, 2010a.
  - Entekhabi, D., Reichle, R. H., Koster, R. D., and Crow, W. T.: Performance Metrics for Soil Moisture Retrievals and Application Requirements, Journal of Hydrometeorology, 11, 832–840, https://doi.org/10.1175/2010JHM1223.1, 2010b.

20

25

- Fang, B. and Lakshmi, V.: AMSR-E Soil Moisture Disaggregation Using MODIS and NLDAS Data, in: Remote Sensing of the Terrestrial Water Cycle, edited by Lakshmi, V., Alsdorf, D., Anderson, M., Biancamaria, S., Cosh, M., Entin, J., Huffman, G., Kustas, W., Oevelen, P., Painter, T., Parajka, J., Rodell, M., and Rudiger, C., pp. 277–304, John Wiley & Sons, Inc, Hoboken, NJ, 2014.
- Gruber, A., Su, C., Zwieback, S., Crow, W., Dorigo, W., and Wagner, W.: Recent advances in (soil moisture) triple collocation analysis, International Journal of Applied Earth Observation and Geoinformation, 45, 200–211, 2016.
- Gruhier, C., de Rosnay, P., Kerr, Y., Mougin, E., Ceschia, E., Calvet, J.-C., and Richaume, P.: Evaluation of AMSR-E soil moisture product based on ground measurements over temperate and semi-arid regions, Geophysical Research Letters, 35, L10405, https://doi.org/10.1029/2008GL033330, 2008.
- Hain, C. R., Mecikalski, J. R., and Anderson, M. C.: Retrieval of an Available Water-Based Soil Moisture Proxy from Thermal Infrared
  Remote Sensing. Part I: Methodology and Validation, https://doi.org/10.1175/2008JHM1024.1, 2009.
  - Hain, C. R., Crow, W. T., Mecikalski, J. R., Anderson, M. C., and Holmes, T.: An intercomparison of available soil moisture estimates from thermal infrared and passive microwave remote sensing and land surface modeling, Journal of Geophysical Research Atmospheres, 116, 1–18, https://doi.org/10.1029/2011JD015633, 2011.
  - Hamon, W.: Computation of Direct Runoff Amounts From Storm Rainfall, Int. Assoc. Sci. Hydrol., Pub. 63, 52–62, 1963.
- Jackson, T. J., Cosh, M. H., Bindlish, R., Starks, P. J., Bosch, D. D., Seyfried, M., Goodrich, D. C., Moran, M. S., Du, J., Goodrich, D. C., and Moran, M. S.: Validation of Advanced Microwave Scanning Radiometer Soil Moisture Products, IEEE Transactions on Geoscience and Remote Sensing, 48, https://doi.org/10.1109/TGRS.2010.2051035, 2010.

- Jaynes, E. T.: Information Theory and Statistical Mechanics, Physical Review, 106, 620–630, https://doi.org/10.1103/PhysRev.106.620, 1957a.
- Jaynes, E. T.: Information Theory and Statistical Mechanics II, Physical Review, 108, 171-190, 1957b.
- Kerr, Y. H., Waldteufel, P., Wigneron, J.-P., Delwart, S., Cabot, F., Boutin, J., Escorihuela, M.-J., Font, J., Reul, N., Gruhier, C., Juglea, S. E.,
- 5 Drinkwater, M. R., Hahne, A., Martin-Neira, M., and Mecklenburg, S.: The SMOS Mission: New Tool for Monitoring Key Elements of the Global Water Cycle, Proceedings of the IEEE, 98, 666–687, https://doi.org/10.1109/JPROC.2010.2043032, 2010.
  - Komatsu, T. S.: Towards a robust phenomenological expression of evaporation efficiency for unsaturated soil surfaces, Journal of Applied Meteorology, 42, 1330–1334, 2003.
- Kondratyev, K. Y., Melentyev, V. V., Rabinovich, Y. I., and Shulgina, E. M.: Passive Microwave Remote Sensing Of Soil Moisture, in:
   Proceedings of 11th International Symposium on Remote Sensing Environment, University of Michigan, Ann Arbor, April 25-29, 1977.,
   1977.
  - Kostov, K. G. and Jackson, T. J.: Estimating profile soil moisture from surface-layer measurements: a review, in: Optical Engineering and Photonics in Aerospace Sensing, edited by Nasr, H. N., pp. 125–136, International Society for Optics and Photonics, https://doi.org/10.1117/12.154681, 1993.
- 15 Kumar, S., Peters-Lidard, C., Tian, Y., Houser, P., Geiger, J., Olden, S., Lighty, L., Eastman, J., Doty, B., Dirmeyer, P. A., Adams, J., Mitchell, K. E., Wood, E. F., and Sheffield, J.: Land information system: An interoperable framework for high resolution land surface modeling, Environmental Modelling and Software, 21, 1402–1415, https://doi.org/10.1016/j.envsoft.2005.07.004, 2006.
  - Kustas, W., Diak, G. R., and Norman, J.: Time Difference Methods for Monitoring Regional Scale Heat Fluxes with Remote Sensing, in: Land Surface Hydrology, Meteorology, and Climate: Observations and Modeling, edited by Lakshmi, V., Albertson, J., and Schaake, J., Water Science and Application, American Geophysical Union, Washington, D. C., https://doi.org/10.1029/WS003, 2001.
  - Lee, T. J. and Pielke, R. A.: Estimating the soil surface specific humidity, Journal of Applied Meteorology, 31, 480–484, 1992.

20

35

- Leng, P., Li, Z.-L., Duan, S.-B., Gao, M.-F., and Huo, H.-Y.: A practical approach for deriving all-weather soil moisture content using combined satellite and meteorological data, ISPRS Journal of Photogrammetry and Remote Sensing, 131, 40–51, https://doi.org/10.1016/j.isprsiprs.2017.07.013, 2017a.
- 25 Leng, P., Li, Z.-L., Duan, S.-B., Tang, R., and Gao, M.-F.: A Method for Deriving All-Sky Evapotranspiration From the Synergistic Use of Remotely Sensed Images and Meteorological Data, Journal of Geophysical Research: Atmospheres, pp. 1–15, https://doi.org/10.1002/2017JD027880, 2017b.
  - Lin, Y. and Mitchell, K. E.: The NCEP Stage II/IV hoissny precipitation analyses: development and applications, 9th Conf. on Hydrology, American Meteorological Society, San Diego, CA, 9-13 January 2005, Paper 1.2, pp. 2–5, 2005.
- Lu, J., Sun, G., McNulty, S. G., and Amatya, D. M.: A Comparison of Six Potential Evapotranspiration Methods For Regional Use in The Southeastern United States, Journal of the American Water Resources Association, 41, 621–633, https://doi.org/10.1111/j.1752-1688.2005.tb03759.x, 2005.
  - Malbéteau, Y., Merlin, O., Molero, B., Rüdiger, C., and Bacon, S.: DisPATCh as a tool to evaluate coarse-scale remotely sensed soil moisture using localized in situ measurements: Application to SMOS and AMSR-E data in Southeastern Australia, International Journal of Applied Earth Observation and Geoinformation, 45, 221–234, https://doi.org/10.1016/j.jag.2015.10.002, 2016.
  - Manabe, S.: Climate and ocean circulation. I. The atmospheric circulation and the hydrology of the Earth's surface, Monthly weather review, 97, 739–774, 1969.

- Mays, D. C., Faybishenko, B. A., and Finsterle, S.: Information entropy to measure temporal and spatial complexity of unsaturated flow in heterogeneous media, Water Resources Research, 38, 49–1–49–11, https://doi.org/10.1029/2001WR001185, 2002.
- McCabe, M. F., Gao, H., and Wood, E. F.: Evaluation of AMSR-E-Derived Soil Moisture Retrievals Using Ground-Based and PSR Airborne Data during SMEX02, Journal of Hydrometeorology, 6, 864–877, https://doi.org/10.1175/JHM463.1, 2005.
- McColl, K. A., Vogelzang, J., Konings, A. G., Entekhabi, D., Piles, M., and Stoffelen, A.: Extended triple collocation: Estimating errors and correlation coefficients with respect to an unknown target, Geophysical Research Letters, 41, 6229–6236, https://doi.org/10.1002/2014GL061322, 2014.
  - McNider, R. T., Christy, J. R., Moss, D., Doty, K., Handyside, C., Limaye, A., Garcia y Garcia, A., and Hoogenboom, G.: A Real-Time Gridded Crop Model for Assessing Spatial Drought Stress on Crops in the Southeastern United States, Journal of Applied Meteorology and Climatology, 50, 1459–1475, https://doi.org/10.1175/2011JAMC2476.1, 2011.

10

20

25

35

- McNider, R. T., Handyside, C., Doty, K., Ellenburg, W., Cruise, J., Christy, J., Moss, D., Sharda, V., Hoogenboom, G., and Caldwell, P.: An integrated crop and hydrologic modeling system to estimate hydrologic impacts of crop irrigation demands, Environmental Modelling & Software, 72, 341–355, https://doi.org/10.1016/J.ENVSOFT.2014.10.009, 2015.
- Merlin, O., Al Bitar, A., Walker, J. P., and Kerr, Y.: An improved algorithm for disaggregating microwave-derived soil moisture based on red, near-infrared and thermal-infrared data, Remote Sensing of Environment, 114, 2305–2316, https://doi.org/10.1016/j.rse.2010.05.007, 2010.
  - Merlin, O., Rudiger, C., Al Bitar, A., Richaume, P., Walker, J. P., and Kerr, Y. H.: Disaggregation of SMOS Soil Moisture in Southeastern Australia, IEEE Transactions on Geoscience and Remote Sensing, 50, 1556–1571, https://doi.org/10.1109/TGRS.2011.2175000, 2012.
  - Merlin, O., Escorihuela, M. J., Mayoral, M. A., Hagolle, O., Al Bitar, A., and Kerr, Y.: Self-calibrated evaporation-based disaggregation of SMOS soil moisture: An evaluation study at 3km and 100m resolution in Catalunya, Spain, Remote Sensing of Environment, 130, 25–38, https://doi.org/10.1016/j.rse.2012.11.008, 2013.
  - Merlin, O., Malbeteau, Y., Notfi, Y., Bacon, S., Er-Raki, S., Khabba, S., and Jarlan, L.: Performance metrics for soil moisture downscaling methods: Application to DISPATCH data in central Morocco, Remote Sensing, 7, 3783–3807, https://doi.org/10.3390/rs70403783, 2015.
  - Miller, D. A. and White, R. A.: A Conterminous United States Multilayer Soil Characteristics Dataset for Regional Climate and Hydrology Modeling, Earth Interactions, 2, 1–26, https://doi.org/10.1175/1087-3562(1998)002<0001:ACUSMS>2.3.CO;2, 1998.
  - Mishra, V., Cruise, J. F., Mecikalski, J. R., Hain, C. R., and Anderson, M. C.: A remote-sensing driven tool for estimating crop stress and yields, Remote Sensing, https://doi.org/10.3390/rs5073331, 2013.
  - Mishra, V., Ellenburg, W., Al-Hamdan, O., Bruce, J., and Cruise, J.: Modeling Soil Moisture Profiles in Irrigated Fields by the Principle of Maximum Entropy, Entropy, 17, 4454–4484, https://doi.org/10.3390/e17064454, 2015.
- 30 Mishra, V., Ellenburg, W. L., Griffin, R. E., Mecikalski, J. R., Cruise, J. F., Hain, C. R., and Anderson, M. C.: An initial assessment of a SMAP soil moisture disaggregation scheme using TIR surface evaporation data over the continental United States, Int J Appl Earth Obs Geoinformation, 68, 92–104, https://doi.org/10.1016/j.jag.2018.02.005, 2018.
  - Molero, B., Merlin, O., Malbéteau, Y., Al Bitar, A., Cabot, F., Stefan, V., Kerr, Y., Bacon, S., Cosh, M. H., Bindlish, R., and Jackson, T. J.: SMOS disaggregated soil moisture product at 1km resolution: Processor overview and first validation results, Remote Sensing of Environment, 180, 361–376, https://doi.org/10.1016/j.rse.2016.02.045, 2016.
  - Njoku, E.: AMSR-E/Aqua Daily L3 Surface Soil Moisture, Interpretive Parameters, & QC EASE-Grids. Version 2., https://doi.org/10.5067/AMSR-E/AE\_LAND3.002., 2004.

- Njoku, E., Ashcroft, P., Chan, T., and Li Li: Global survey and statistics of radio-frequency interference in AMSR-E land observations, IEEE Transactions on Geoscience and Remote Sensing, 43, 938–947, https://doi.org/10.1109/TGRS.2004.837507, 2005.
- Njoku, E. G., Jackson, T. J., Lakshmi, V., Chan, T. K., and Nghiem, S. V.: Soil moisture retrieval from AMSR-E, IEEE Transactions on Geoscience and Remote Sensing, 41, 215–228, https://doi.org/10.1109/TGRS.2002.808243, 2003.
- Noilhan, J. and Planton, S.: A simple parameterization of land surface processes for meteorological models, Monthly weather review, 117, 536–549, 1989.
  - Norman, J. M., Divakarla, M., and Goel, N. S.: Algorithms for extracting information from remote thermal-IR observations of the Earth's surface., Remote Sensing of Environment, 51, 157–168, 1995.
- Norman, J. M., Anderson, M. C., Kustas, W. P., French, a. N., Mecikalski, J., Torn, R., Diak, G. R., Schmugge, T. J., and Tanner, B. C. W.: Remote sensing of surface energy fluxes at 10 1 -m pixel resolutions, Water Resources Research, 39, https://doi.org/10.1029/2002WR001775, 2003.
  - Pachepsky, Y., Guber, A., Jacques, D., Simunek, J., Van Genuchten, M. T., Nicholson, T., and Cady, R.: Information content and complexity of simulated soil water fluxes, Geoderma, 134, 253–266, https://doi.org/10.1016/j.geoderma.2006.03.003, 2006.
- Paloscia, S., Macelloni, G., Santi, E., and Koike, T.: A multifrequency algorithm for the retrieval of soil moisture on a large scale using microwave data from SMMR and SSM/I satellites, IEEE Transactions on Geoscience and Remote Sensing, 39, 1655–1661, https://doi.org/10.1109/36.942543, 2001.
  - Pan, F., Pachepsky, Y. A., Guber, A. K., and Hill, R. L.: Information and complexity measures applied to observed and simulated soil moisture time series, Hydrological Sciences Journal, 56, 1027–1039, https://doi.org/10.1080/02626667.2011.595374, 2011.
  - Penna, D., Brocca, L., Borga, M., and Dalla Fontana, G.: Soil moisture temporal stability at different depths on two alpine hillslopes during wet and dry periods, Journal of Hydrology, 477, 55–71, https://doi.org/10.1016/j.jhydrol.2012.10.052, 2013.
  - Priestley, C. and Taylor, R.: On the assessment of surface heat flux and evaporation using large-scale parameters, Monthly weather review, pp. 81–92, 1972.
  - Rawls, W., Brakensiek, D., and Saxton, K.: Estimation of Soil Water Properties, Transactions of the ASCE, 25, 1316–1320, 1982.

20

25

- Sahoo, A. K., Houser, P. R., Ferguson, C., Wood, E. F., Dirmeyer, P. A., and Kafatos, M.: Evaluation of AMSR-E soil moisture results using the in-situ data over the Little River Experimental Watershed, Georgia, Remote Sensing of Environment, 112, 3142–3152, https://doi.org/10.1016/j.rse.2008.03.007, 2008.
- Santanello, J. and Friedl, M.: Diurnal variation in soil heat flux and net radiation., Journal of Applied Meteorology, 42, 851–862, 2003.
- Schaefer, G. L., Cosh, M. H., and Jackson, T. J.: The USDA Natural Resources Conservation Service Soil Climate Analysis Network (SCAN), Journal of Atmospheric and Oceanic Technology, 24, 2073–2077, https://doi.org/10.1175/2007JTECHA930.1, 2007.
- Schmugge, T., Jackson, T., Kustas, W., and Wang, J.: Passive microwave remote sensing of soil moisture: results from HAPEX, FIFE and MONSOON 90, ISPRS Journal of Photogrammetry and Remote Sensing, 47, 127–143, https://doi.org/10.1016/0924-2716(92)90029-9, 1992.
  - Scipal, K., Holmes, T., de Jeu, R., Naeimi, V., and Wagner, W.: A possible solution for the problem of estimating the error structure of global soil moisture data sets, Geophysical Research Letters, 35, L24 403, https://doi.org/10.1029/2008GL035599, 2008.
- Scott, C. A., Bastiaanssen, W. G. M., and Ahmad, M.-u.-D.: Mapping Root Zone Soil Moisture Using Remotely Sensed Optical Imagery, Journal of Irrigation and Drainage Engineering, 129, 326–335, https://doi.org/10.1061/(ASCE)0733-9437(2003)129:5(326), 2003.
  - Shannon, C. E.: A Mathematical Theory of Communication, Bell System Technical Journal, 27, 379–423, https://doi.org/10.1002/j.1538-7305.1948.tb01338.x, 1948.

Singh, V. P.: Hydrologic Systems: Watershed Modeling 2, Prentice Hall, Engelwood Cliffs, NJ, 1988.

5

20

25

- Singh, V. P.: Entropy theory for movement of moisture in soils, Water Resources Research, 46, https://doi.org/10.1029/2009WR008288, 2010.
- Song, J., Wesely, M. L., Coulter, R. L., and Brandes, E. A.: Estimating Watershed Evapotranspiration with PASS. Part I: Inferring Root-Zone Moisture Conditions Using Satellite Data, 2000.
- Srivastava, S., Yograjan, N., Jayaraman, V., Rao, P., and Chandrasekhar, M.: On the relationship between ERS-1 SAR/backscatter and surface/sub-surface soil moisture variations in vertisols, Acta Astronautica, 40, 693–699, https://doi.org/10.1016/S0094-5765(97)00125-2, 1997.
- Starks, P. J., Heathman, G. C., Ahuja, L. R., and Ma, L.: Use of limited soil property data and modeling to estimate root zone soil water content, Journal of Hydrology, 272, 131–147, https://doi.org/10.1016/S0022-1694(02)00260-3, 2003.
  - Stoffelen, A.: Toward the true near-surface wind speed: Error modeling and calibration using triple collocation, JOURNAL OF GEOPHYS-ICAL RESEARCH, 103, 7755–7766, https://doi.org/10.1029/97JC03180, 1998.
  - Su, C.-H., Ryu, D., Crow, W. T., and Western, A. W.: Beyond triple collocation: Applications to soil moisture monitoring, Journal of Geophysical Research: Atmospheres, 119, 6419–6439, https://doi.org/10.1002/2013JD021043, 2014.
- 15 Su, Z.: The Surface Energy Balance System (SEBS) for estimation of turbulent heat fluxes, Hydrology and Earth System Sciences Discussions, 6, 85–100, 2002.
  - Wagner, W., Blöschl, G., Pampaloni, P., Calvet, J.-C., Bizzarri, B., Wigneron, J.-P., and Kerr, Y.: Operational readiness of microwave remote sensing of soil moisture for hydrologic applications, Hydrology Research, 38, 2007.
  - Wetzel, P. J. and Chang, J.-T.: Concerning the Relationship between Evapotranspiration and Soil Moisture, Journal of Climate and Applied Meteorology, 26, 18–27, https://doi.org/10.1175/1520-0450(1987)026<0018:CTRBEA>2.0.CO;2, 1987.
  - Wu, J., Zhang, R., and Gui, S.: Modeling soil water movement with water uptake by roots, Plant and Soil, 215, 7–17, https://doi.org/10.1023/A:1004702807951, 1999.
  - Xia, Y., Mitchell, K., Ek, M., Sheffield, J., Cosgrove, B., Wood, E., Luo, L., Alonge, C., Wei, H., Meng, J., Livneh, B., Lettenmaier, D., Koren, V., Duan, Q., Mo, K., Fan, Y., and Mocko, D.: Continental-scale water and energy flux analysis and validation for the North American Land Data Assimilation System project phase 2 (NLDAS-2): 1. Intercomparison and application of model products, Journal of Geophysical Research: Atmospheres, 117, n/a–n/a, https://doi.org/10.1029/2011JD016048, 2012.
  - Yilmaz, M. T., Crow, W. T., Yilmaz, M. T., and Crow, W. T.: Evaluation of Assumptions in Soil Moisture Triple Collocation Analysis, Journal of Hydrometeorology, 15, 1293–1302, https://doi.org/10.1175/JHM-D-13-0158.1, 2014.
- Overview of study area showing location of all active SCAN sites. The dark blue circles indicate sites with most consistent data availability and are being used for comparison and validation in this study. The right figure shows a land cover map (MODIS-2008) for the study area.

## **Tables**

Map of bias, RMSD, ubRMSD and correlation coefficient between Noah and POME SM profiles over multiple years (2006-2010) at different layer depths: top panel: 0-10 cm; middle panel: 10-40 cm and bottom panel: 40-100 cm.

Comparison of Noah and POME SM profiles at multiple layer depths by Land Cover across Southeast United States

5 Statistics at SCAN sites showing bias, Correlation, RMSD and ubRMSD between SCAN observations and POME SM profiles at multiple layer depths.

Time series of soil moisture condition at 10 NRCS SCAN sites from the POME model (Blue); Noah LSM (green) and *in-situ* observations (red) at three layer depths (2006-2010)

POME and Noah SM profiles statistics at all SCAN sites compared against *in-situ* observations averaged across layer depths

Triple collocation analyses of SM profiles from Noah (green), POME (blue) and *in-situ* observations (red) at scan site locations at the depths of 0-10; 10-40 and 40-100 cm

POME model sensitivity to (a) boundary condition; (b) sensitivity to profile mean input towards profile Bias and RMSD in terms of effective SM.

Map of Southeast United States demonstrating temporal statics in bias, RMSD, ubRMSD and correlation between coarse (top panel) and fine (bottom panel) resolution AMSR-E (MW) and Noah LSM surface SM (2006-2010)

Map of temporal statistics between root zone ALEXI and Noah SM (2006-2010).

**Table 1.** SCAN site 5 km dominant land cover (MODIS 2008) and soil characteristics (SCAN) at surface and depth of 100 cm [S-Sand; L-Loam; C-Clay and Si-Silt]. Soil information was not available for sites 2037 and 2038.

SCAN	Lat/Lon	Land cover	Soil Type (SCAN)		
Site			Surface	100cm	
2009	30.3/-84.4	Savannas/Mix Forest	S	S	
2013	33.8/-83.4	Crop/Savannas	SL	C	
2027	31.5/-83.5	Cropland	S	SL	
2037	34.3/-79.7	Crop/Shurbland	-	-	
2038	32.6/-81.2	Crop / Savannas	-	-	
2053	34.9/-86.5	Cropland	SiCL	SiC	
2078	34.9/-86.6	Cropland	SiCL	C	
2113	34.2/-86.8	Crop/Savannas	L	SCL	
2114	32.6/-88.2	Savannas	SCL	CL	
2115	32.4/-85.7	Savannas	LS	SC	

**Table 2.** Results of temporal comparisons in absolute bias( $m^3m^{-3}$ ), RMSD ( $m^3m^{-3}$ ), ubRMSD ( $m^3m^{-3}$ ) and correlation at 10 sites between the developed profile and Noah SM profiles against SCAN observations at 0-10; 10-40 and 40-100cm depths [NP - Noah vs POME; SP - SCAN vs POME; and NS - Noah vs SCAN]

C!4	Bias			RMSD			ubRMSD			Correlation			
Site	NP	SP	NS	NP	SP	NS	NP	SP	NS	NP	SP	NS	
2009	0.02	0.13	0.11	0.05	0.14	0.12	0.04	0.04	0.03	0.12	0.23	0.56	
2014	0.00	-0.10	-0.10	0.06	0.13	0.11	0.06	0.07	0.03	0.54	0.50	0.85	
2015	0.01	0.15	0.14	0.07	0.16	0.14	0.07	0.06	0.00	0.50	0.54	0.72	
2027	0.09	0.19	0.10	0.10	0.20	0.11	0.06	0.07	0.05	0.64	0.49	0.70	
2053	0.05	0.03	-0.02	0.07	0.06	0.04	0.05	0.06	0.03	0.77	0.75	0.85	0-10 cm
2078	0.05	0.03	-0.02	0.09	0.09	0.05	0.07	0.08	0.05	0.73	0.69	0.72	cm
2113	0.00	0.02	0.03	0.06	0.08	0.06	0.06	0.08	0.05	0.41	0.51	0.86	
2037	0.06	0.08	0.02	0.09	0.10	0.04	0.07	0.06	0.03	0.40	0.63	0.72	
2038	0.02	0.02	0.16	0.06	0.06	0.04	0.05	0.05	0.04	0.34	0.37	0.62	
2013	0.04	0.07	0.23	0.07	0.09	0.04	0.05	0.05	0.03	0.59	0.67	0.88	
2009	0.06	0.18	0.12	0.08	0.19	0.13	0.05	0.03	0.05	0.21	0.17	0.37	
2014	0.02	-0.14	-0.16	0.05	0.14	0.17	0.04	0.04	0.06	0.69	0.60	0.78	
2015	0.00	0.04	0.04	0.04	0.06	0.05	0.04	0.04	0.03	0.52	0.51	0.80	
2027	0.06	0.14	0.08	0.07	0.14	0.09	0.04	0.05	0.04	0.70	0.56	0.63	
2053	0.00	0.03	0.03	0.05	0.07	0.06	0.05	0.06	0.05	0.67	0.51	0.74	10-40 cm
2078	0.01	-0.06	-0.06	0.05	0.07	0.09	0.05	0.05	0.06	0.69	0.56	0.56	0 cm
2113	0.04	0.03	-0.01	0.08	0.06	0.03	0.06	0.05	0.03	0.37	0.37	0.91	_
2037	0.07	0.10	0.02	0.08	0.10	0.03	0.03	0.03	0.02	0.57	0.55	0.78	
2038	0.08	-0.01	-0.09	0.09	0.04	0.10	0.05	0.04	0.04	0.44	0.39	0.55	
2013	0.07	0.05	-0.02	0.10	0.08	0.04	0.07	0.06	0.03	0.29	0.27	0.88	
2009	0.09	0.20	0.11	0.10	0.20	0.12	0.05	0.03	0.05	0.22	0.16	0.33	
2014	0.04	-0.17	-0.21	0.08	0.17	0.22	0.07	0.02	0.07	0.65	0.59	0.68	
2015	0.00	-0.02	-0.02	0.04	0.08	0.06	0.04	0.07	0.05	0.48	0.45	0.81	
2027	0.08	0.05	-0.02	0.10	0.06	0.06	0.06	0.03	0.06	0.38	0.40	0.58	4
2053	0.01	-0.04	-0.04	0.08	0.06	0.06	0.08	0.05	0.05	0.49	0.51	0.85	40-100
2078	0.03	-0.08	-0.11	0.08	0.09	0.13	0.08	0.04	0.06	0.54	0.54	0.74	0 cm
2113	0.07	-0.03	-0.10	0.11	0.06	0.11	0.08	0.05	0.05	0.32	0.27	0.85	=
2037	0.09	0.04	-0.04	0.10	0.05	0.06	0.04	0.03	0.03	0.52	0.45	0.68	
2038	0.13	-0.10	-0.22	0.14	0.10	0.23	0.06	0.03	0.06	0.42	0.40	0.35	
2013	0.12	0.08	-0.04	0.15	0.12	0.09	0.09	0.09	0.07	0.16	0.10	0.65	

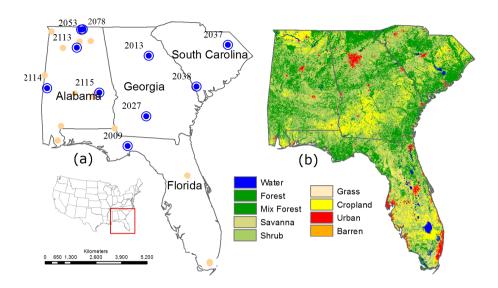
**Table 3.** Statistical comparison before and after disaggregation of coarse resolution MW SM against SCAN observations  $[r - correlation coefficient; bias, RMSD and ubRMSD in <math>m^3m^{-3}$ ; N – number of days data points was available; maximum possible N = 1825];\*non-significant correlation using two-tailed t-test at 99% CI

	Mean SM				SCAN/MW(25km)				SCAN/MW(5k)			
Site	SCAN	MW (25k)	MW (5k)	N	Bias	RMSD	ubRMSD	r	Bias	RMSD	ubRMSD	r
2009	0.06	0.18	0.19	841	0.12	0.12	0.02	-0.12*	0.13	0.14	0.04	0.17
2014	0.26	0.15	0.19	1055	-0.11	0.14	0.09	0.30	-0.07	0.12	0.09	0.47
2015	0.08	0.15	0.25	1103	0.08	0.09	0.04	0.42	0.17	0.19	0.08	0.60
	•	Mean			0.03	0.12	0.05	0.22	0.08	0.15	0.07	0.42
2027	0.08	0.13	0.29	1241	0.05	0.06	0.03	0.48	0.21	0.22	0.08	0.50
2053	0.24	0.14	0.32	1160	-0.10	0.13	0.08	0.43	0.08	0.10	0.06	0.74
2078	0.25	0.14	0.31	1080	-0.12	0.13	0.05	0.34	0.06	0.10	0.08	0.68
		Mean			-0.06	0.10	0.05	0.42	0.12	0.14	0.07	0.64
2113	0.20	0.14	0.18	1014	-0.06	0.12	0.10	0.44	-0.02	0.10	0.09	0.47
2037	0.16	0.14	0.21	1157	-0.02	0.06	0.05	0.11	0.06	0.10	0.09	0.62
2038	0.14	0.16	0.16	1067	0.02	0.05	0.04	0.45	0.02	0.06	0.06	0.31
2013	0.21	0.15	0.23	1218	-0.06	0.09	0.06	0.21	0.02	0.05	0.05	0.55
Mean				-0.03	0.08	0.06	0.26	0.02	0.08	0.07	0.53	
	Overall Mean				-0.02	0.10	0.06	0.31	0.07	0.12	0.07	0.53

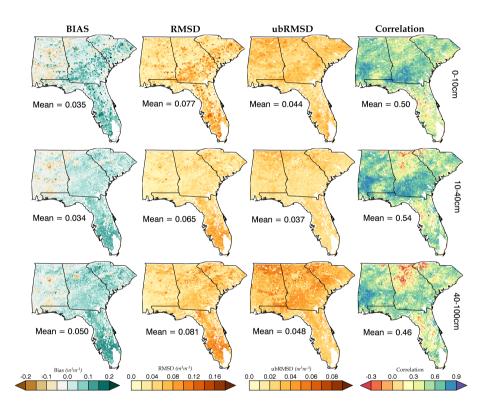
**Table A1.** The soil water characteristic values used in this study based on the earlier study by Rawls et al. (1982)

Soil Type	Residual (m³m⁻³)	Wilting Point (m³m⁻³)	Field Capacity (m <sup>3</sup> m <sup>-3</sup> )	Porosity (m³m-³)
Sand	0.020	0.033	0.091	0.437
Loamy Sand	0.035	0.055	0.125	0.437
Sandy Loam	0.041	0.095	0.207	0.453
Silt Loam	0.015	0.133	0.330	0.501
Silt	0.020	0.110	0.370	0.481
Loam	0.027	0.117	0.270	0.463
Sandy Clay Loam	0.070	0.148	0.255	0.398
Silty Clay Loam	0.040	0.208	0.366	0.471
Clay Loam	0.075	0.197	0.318	0.464
Sandy Clay	0.109	0.239	0.339	0.430
Silty Clay	0.056	0.250	0.387	0.479
Clay	0.090	0.272	0.396	0.475

## **Figures**



**Figure 1.** (a)Overview of study area showing location of all active SCAN sites. The dark blue circles indicate sites with most consistent data availability and are being used for comparison and validation in this study.(b) The figure shows a land cover map (MODIS-2008) for the study area.



**Figure 2.** Map of bias, RMSD, ubRMSD and correlation coefficient between Noah and POME SM profiles over multiple years (2006-2010) at different layer depths: top panel: 0-10 cm; middle panel: 10-40 cm and bottom panel: 40-100 cm.

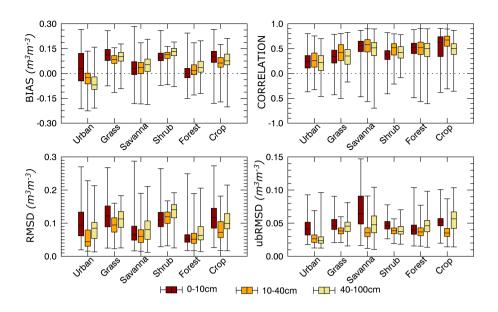
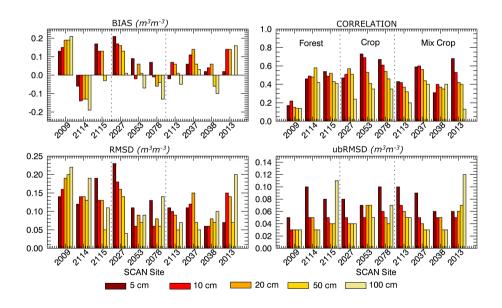
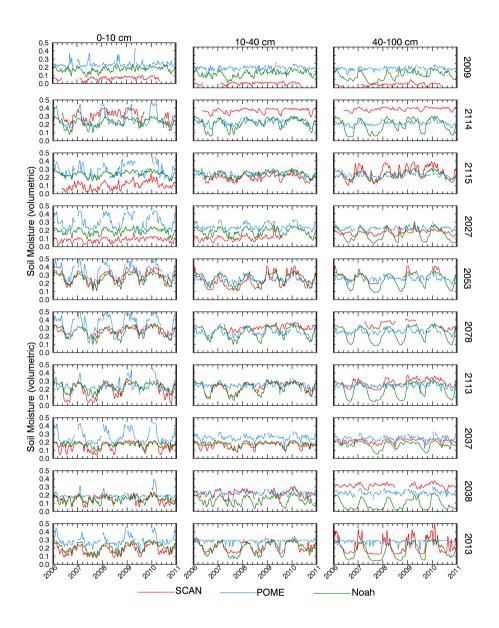


Figure 3. Comparison of Noah and POME SM profiles at multiple layer depths by Land Cover across Southeast United States



**Figure 4.** Statistics at SCAN sites showing bias, Correlation, RMSD and ubRMSD between SCAN observations and POME SM profiles at multiple layer depths.



**Figure 5.** Time series of soil moisture condition (every 8-day interval) at 10 NRCS SCAN sites from the POME model (Blue); Noah LSM (green) and *in-situ* observations (red) at three layer depths (2006-2010)

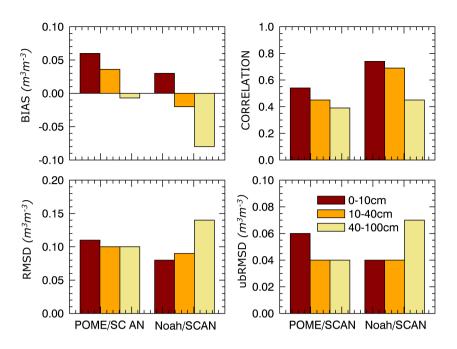
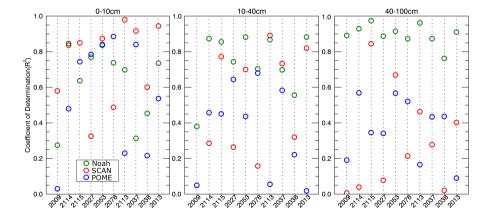
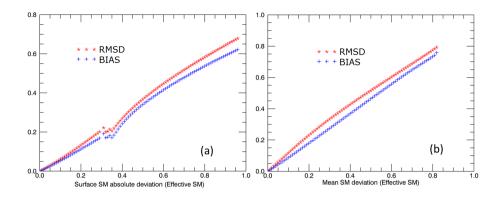


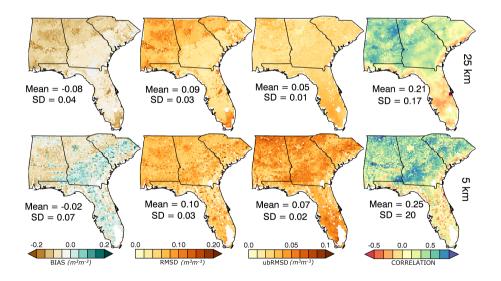
Figure 6. POME and Noah SM profiles statistics at all SCAN sites compared against in-situ observations averaged across layer depths



**Figure 7.** Triple collocation analyses of SM profiles from Noah (green), POME (blue) and *in-situ* observations (red) at scan site locations at the depths of 0-10; 10-40 and 40-100 cm



**Figure 8.** POME model sensitivity to (a) boundary condition; (b) sensitivity to profile mean input towards profile Bias and RMSD in terms of effective SM.



**Figure 9.** Map of Southeast United States demonstrating temporal statics in bias, RMSD, ubRMSD and correlation between coarse (top panel) and fine (bottom panel) resolution AMSR-E (MW) and Noah LSM surface SM (2006-2010)

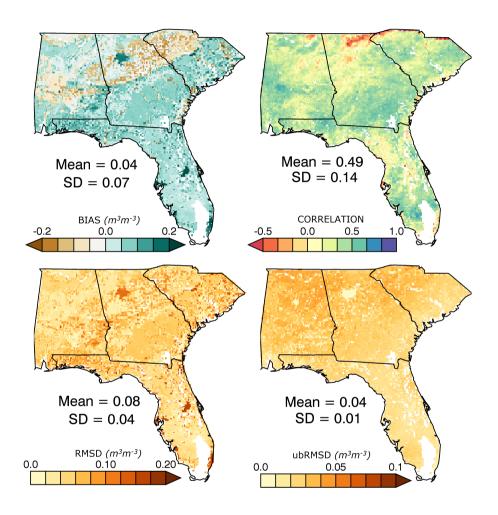


Figure 10. Map of temporal statistics between root zone ALEXI and Noah SM (2006-2010).

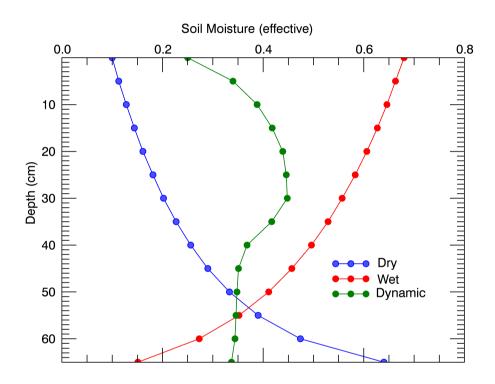


Figure A1. Plot displaying the three possible cases of the soil moisture profile