Effect of Forward/Inverse Model Asymmetries Over Retrieved Soil Moisture Assessed With an OSSE for the Aquarius/SAC-D Mission

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***Abstract*—An Observing System Simulation Experiment (OSSE) for the Aquarius/SAC-D mission that includes different models for forward and retrieval processes is presented. This OSSE is implemented to study the errors related to the use of simple retrieval models in passive microwave applications. To this end, a theoretical forward model was introduced, which is suitable to reproduce some of the complexities related to canopy vegetation scattering. So far, this OSSE has been successfully exploited to study the artifacts in the retrieved soil moisture associated to: 1) uncertainties and aggregation of the ancillary parameters needed for the retrieval, and 2) instrumental noise effects. In this paper, we attempt to model the influence of this "model asymmetry" (different forward and inverse model) in the estimated soil moisture. These asymmetries are related to the fact that the emissivity of real surfaces is complex and strongly dependent on land cover type and condition. In particular, surface covered by average to dense vegetation presents complex scattering properties, related to canopy structure. Using this theoretical model, the difficulties related to retrieving soil moisture from passive data with a simple model are studied. The accuracy of the soil moisture estimation is analyzed in order to illustrate the impact of discrepancies between both models. In general, retrieved soil moisture performs worse over dense vegetated areas and under wet conditions. Furthermore, accuracy is highly dependent on land cover.**

***Index Terms*—Aquarius, OSSE, radiative transfer model, soil moisture, theoretical model.**

I. Introduction

An Observing System Simulation Experiment (OSSE) is a simulation designed to mimic as closely as possible a given Earth Observation satellite mission, in order to study one or several aspects of its operation. In general, OSSEs are developed to study the accuracy of final products given the terrain dynamics, the forward and inverse models and the orbital and instrumental characteristics.

OSSEs of passive microwave missions are usually designed to evaluate soil moisture errors as a function of antenna and electronics performance, since radiometer bias and stability has been a major concern in past missions. However, with the development of new generation radiometers, characterized by very low radiometric uncertainties ($< 1^{\circ}\mathrm{K}$), the contribution of system error to the overall soil moisture retrieval error is relatively low [1], [2].

Nevertheless, soil moisture retrievals obtained from passive microwave data are still relatively noisy. The uncertainties in the estimated soil moisture are related to several processes, but most studies [3]–[5] point out to the parameterization of the inverse model. First, in order to accurately estimate soil moisture, most retrieval models make extensive use of ancillary data about surface condition (e.g., vegetation water content, soil roughness, soil temperature, etc), which are usually available at higher resolutions than passive data. This gives rise to the problem of aggregating high resolution ancillary parameters to produce a low resolution (passive based) soil moisture product [6]. The effects of different aggregation strategies have been examined for other instruments and were recently studied for Aquarius soil moisture retrievals [7].

The second source of uncertainties in retrieved soil moisture is related to the formalism of the retrieval model itself. The most common retrieval model by far is based on a zero-order radiative transfer ω-τ formulation (RT-0) [8]. This model is usually selected, since it is able to relate surface brightness temperature to measurable surface parameters (soil moisture $[\mathrm{cm}^3/\mathrm{cm}^3]$ and vegetation water content (VWC) $[\mathrm{Kg/m}^2]$) in a simple way. Moreover, due to its simple formulation, a straightforward inversion is usually possible. However, this simplified model presents several drawbacks. The most important are that it neglects vegetation geometry and multiple scattering effects within vegetation canopies and at the vegetation soil interface. In particular, the relation between brightness temperature and bio-geophysical parameters (in particular VWC) is more complex than the one predicted by the RT-0 model [9]. As will be shown here, this has strong implications for the retrieval of soil moisture from L band data under heavy vegetation cover.

In a previous work [7], an OSSE for the Aquarius mission was implemented to model the influence of error sources such as heterogeneity effects, observations noise and ancillary parameters errors over the retrieved soil moisture. Different product design strategies were tested and it was shown that the soil moisture

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was highly sensitive to the aggregation method of the VWC parameter, as previously found in [10]. However, this analysis was implemented using the RT-0 model for both forward and retrieval model, so that no model asymmetries were considered in the analysis.

Hence, the objective of this work is to extend the results previously obtained in order to include error effects associated with the use of a simplified retrieval model (RT-0). To this end, a theoretical forward model is introduced, which can estimate terrain brightness temperature as a function of terrain dielectric and geometric parameters, using an approach based on a detailed description of vegetation geometry and high order radiative transfer approach. Most critically, this model captures several processes that are neglected in the RT-0 model used in the retrieval portion of the OSSE. This forward/retrieval model asymmetry is likely to be present in any real soil moisture retrieval, since the emissivity of vegetated surfaces is complex and cannot be fully modeled at the typical scales of passive microwaves.

II. Methodology

The implementation of the OSSE is based on: (1) a land surface model at 1-km spatial resolution within the 250,000-km^2 Red-Arkansas River Basin (south-central US) for 3 months during the summer of 1994, (2) a forward theoretical microwave emission model based on the electromagnetic modeling of vegetation elements (branches and trunk as cylinders, leaves as disks, etc) and high order radiative transfer theory [11] to simulate brightness temperature, (3) an orbital and sensor model to simulate the radiometer observations, and (4) a retrieval model based on the RT-0 model. Coarse resolution VWC needed for the retrieval was obtained aggregating high resolution values through two different strategies: linear averaging (AVE) and an aggregation method (AGG) proposed by Zhan *et al.* [10]. Gridded soil moisture was composed by three sampling methods: nearest neighbor (NN), weighing function (WF) and local polynomial fitting (LP) with 100-km bandwidth [7]. In order to test the performance of the retrieval scheme using different forward and inverse models, the OSSE was run assuming neither instrumental error nor uncertainties in the auxiliary parameters.

A. Microwave Emission Model: Theoretical Model

The theoretical model describes a vegetated terrain as subdivided into three main regions: crown, trunks, and soil. The crown is filled with scatterers representing leaves, needles and branches. Several approximations were used to model the electromagnetic properties of different crown elements [11]. The Integral equation model has been adopted in this paper to model soil scattering. More details about model characteristics and implementation are given in [11].

Since this model takes as input a large set of vegetation characteristics, allometric equations for every landcover were implemented. In this way, vegetation geometry can be related to key variables (diameter at breast height (dbh), LAI, crop height, etc). These allometric equations were obtained from bibliography [9] and databases, to model as best as possible the land covers characteristics of the Red Arkansas Basin.

It is important to note that this theoretical model was validated with field campaigns on different observations conditions (incidence angle, frequencies, polarizations) and over different landcovers, from bare soils and crops [12], to forests [11], [13].

The main advantage of this model is that it is able to capture the complexities of vegetation emissivity as a function of a comprehensive set of both geometrical and dielectrical properties of the canopy. These types of models are currently not used in retrieval algorithms, since the number of variables required for a univocal estimation of soil moisture using this model is large. Nevertheless, this model is well suited to our purpose: to study the problems arising from the use of a simple retrieval scheme with synthetic data describing complex emission and scattering effects.

From the operational point of view, due to the theoretical model's computational complexity, look up tables were generated for 5 different land covers: broadleaf forest (FB), needleleaf forest (FN), tall grass (TG), short grass (SG), and shrubs (SH). Brightness temperature Tb of two pure land covers was averaged together to obtain the Tb for mixed land covers such as needleleaf forest mixed with tall grass (FN+TG) or short grass mixed with tall grass (MG).

B. Retrieval Model: RT-0

The retrieval is based on an RT-0 model, which is derived from the zero-order radiative transfer theory by summing the terms of the emitted radiation of different surface components [8]. Vegetation is characterized by three parameters, vegetation single scattering albedo ω, vegetation attenuation coefficient b and vegetation water content VWC. Soil is characterized by its dielectric constant ε and an overall roughness parameter h. As stated, this model has the main advantage of being both physically-based and simple, allowing for a straightforward retrieval. Its main drawbacks are related to the disregard of the effects of canopy geometry.

III. Results

A. Impact of Model Asymmetries: OSSE Overall Outputs

In a previous work [7] the OSSE was implemented considering no model asymmetries in order to study the sensitivity of soil moisture retrieval to VWC aggregation strategies and compositing. Overall, retrieval accuracy was acceptable. However errors arising from adopting the RT-0 model as both forward and inverse were not considered. Therefore, our first goal is to study how the aggregation errors compare to model asymmetry errors. To this end, the OSSE was run for all the design strategies proposed in [7] but considering different forward and retrieval models.

As an example, Fig. 1 shows, for one OSSE's configuration run, a comparison between true ground soil moisture and retrievals obtained using both the same (a) and different (b) forward and retrieval models. In view of these results and the previous error analysis performed in [7], it is clear that model discrepancies are, by far, the most significant source of error in the estimated soil moisture. Whereas in [7] improving the VWC aggregation strategy could lead to a 1% decrease in the estimation

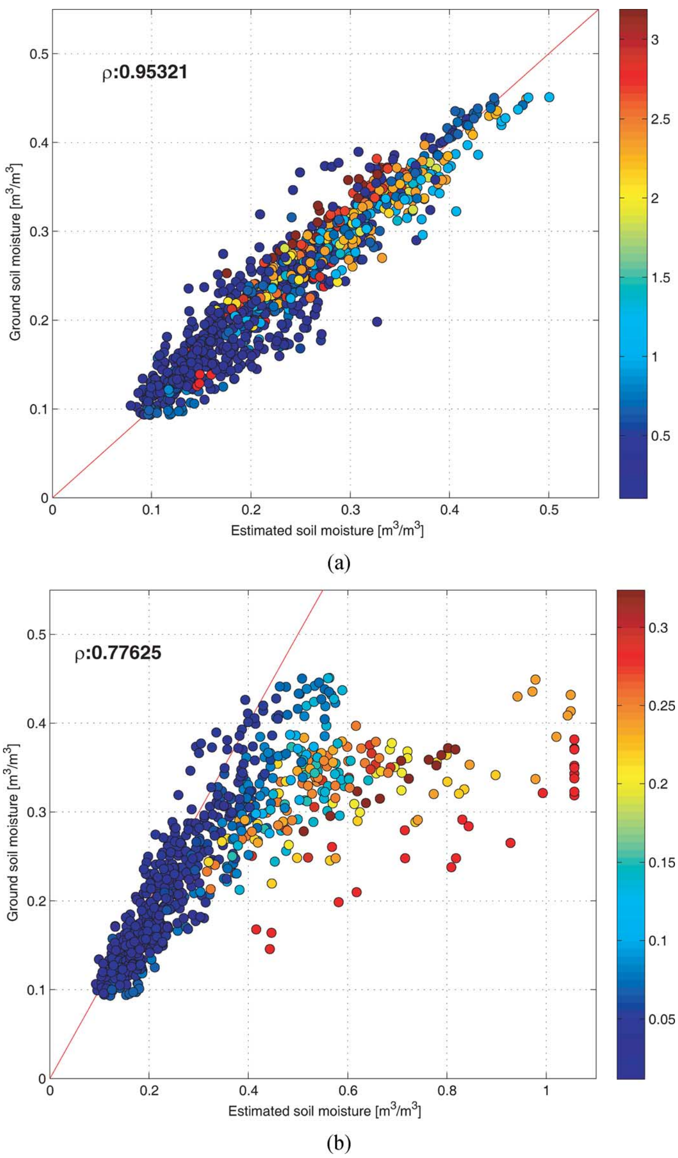


Fig. 1. Retrieved soil moisture vs. ground soil moisture for H polarization implementing Zhan aggregation of VWC and nearest neighbor composite considering: RT-0 as both the forward and inverse model (a) and the presence of asymmetric forward and inverse models (b). The color axes correspond to VWC [kg/m2] values.

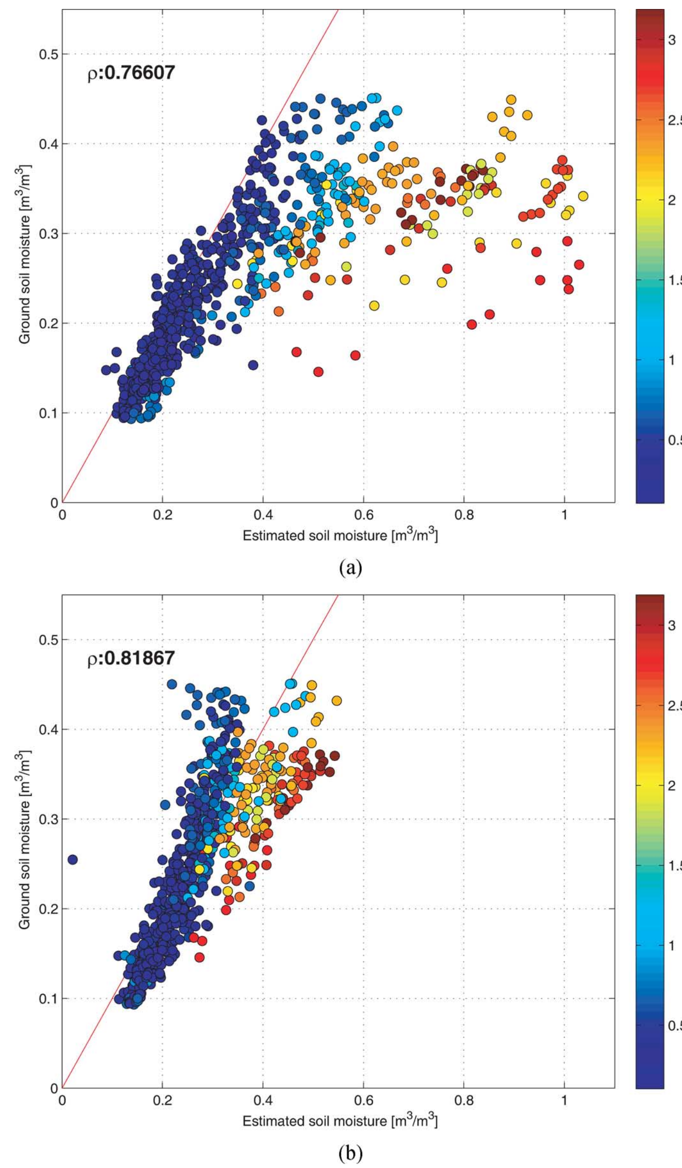


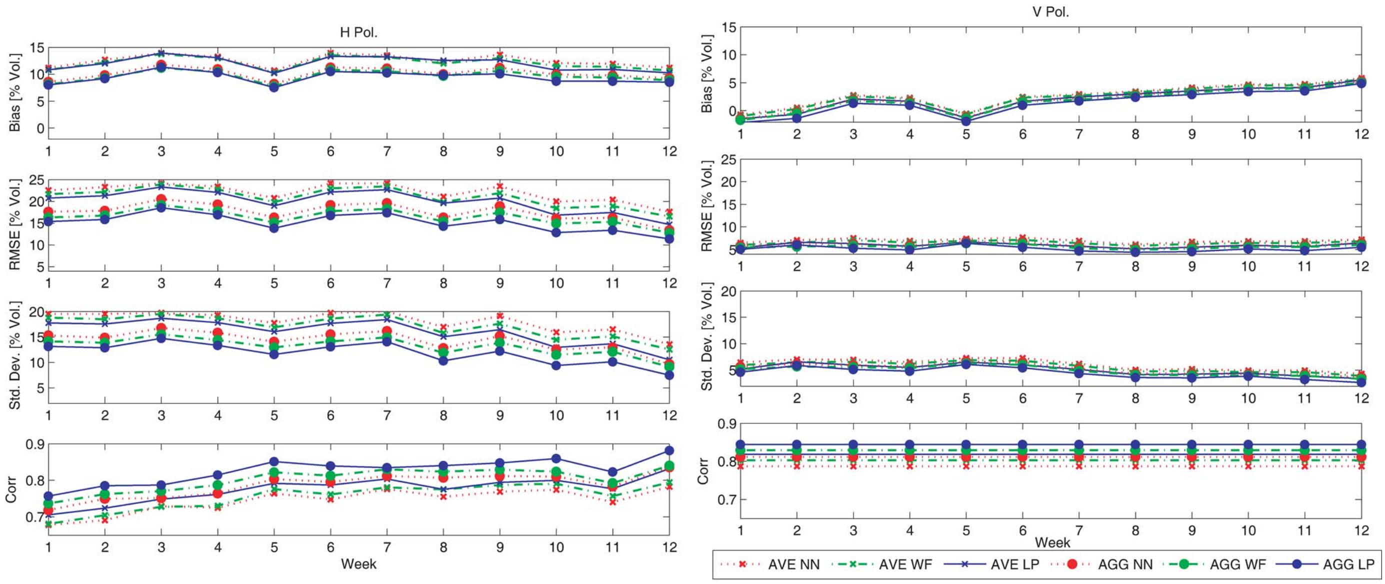
Fig. 2. Retrieved soil moisture vs. ground soil moisture for H (a) and V (b) polarization implementing linear averaging aggregation of VWC and local polynomial fitting composite considering model asymmetries. The color axes correspond to VWC $[\mathrm{kg/m^2}]$ values.

error (RMSE), including model asymmetries lowers the accuracy more than 4 times with respect to the no model asymmetries case (Fig. 1).

In the case where the theoretical model is implemented as forward model, retrieved soil moisture obtained from vertically (V) polarized observations outperform retrievals obtained from horizontally (H) polarized data (see Fig. 2). This result is expected since variations between RT-0 and the theoretical model are larger at H-polarization than at V-polarization (see Section III.B).

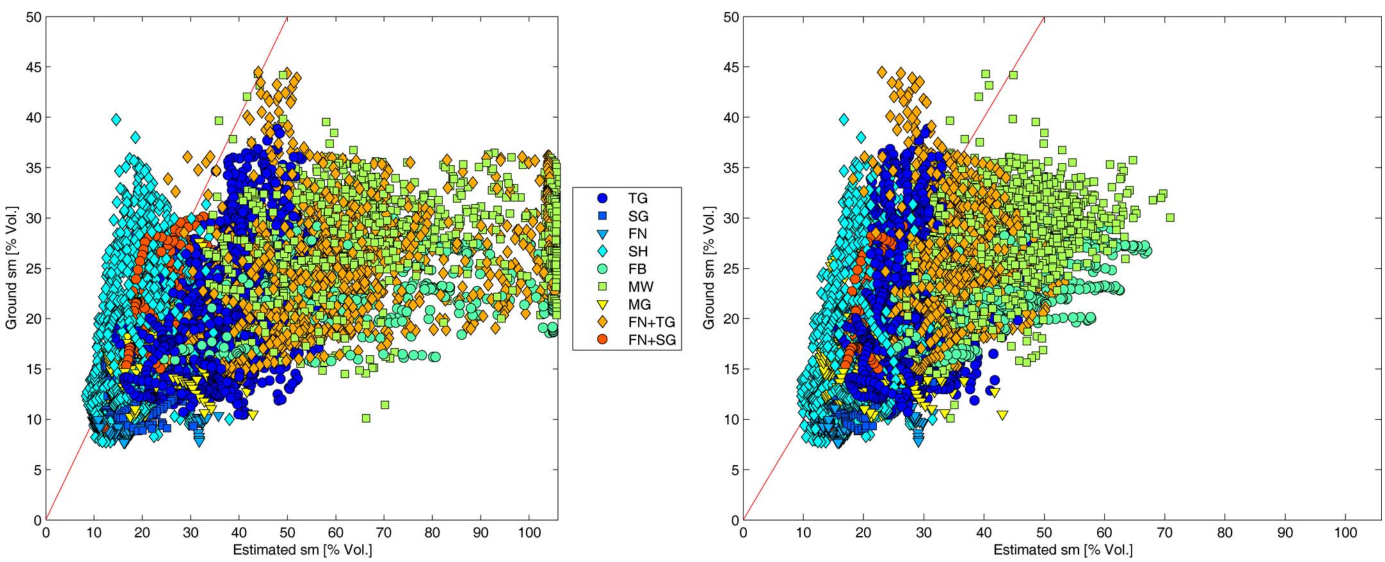
A comparison between coarse resolution ground soil moisture and retrieved soil moisture from horizontal polarization observations is shown in Fig. 2(a). Marker colors correspond to different VWC values. Error in estimated soil moisture increases mainly with increasing VWC. Wherever coarse resolution VWC is higher than 2 kg/m2, soil moisture values are overestimated in at least 0.1 cm3/cm3. The error increases as the soil moisture condition increases and is land cover dependent (see Fig. 4). On the other hand, V polarization presents no overall bias since soil moisture for low VWC areas is underestimated and over dense vegetation areas is overestimated. However, the retrieval accuracy is much higher for the V case.

Moreover, unlike results obtained considering no model asymmetries, when model asymmetries are present, VWC aggregation strategy (AGG) cannot lower the positive bias of soil moisture (although it slightly enhances the accuracy of the retrieval). In particular, for the H polarization, the sensitivity to the aggregation scheme is higher than for the V case. Similarly, but in less significant way, the different composite methods implemented vary the results on the retrieval with the local polynomial fitting interpolation the one exhibiting the best performance.



(a) (b)

Fig. 3. Time series of bias, RMSE, standard deviation and correlation of retrieved and coarse resolution ground soil moisture for H (a) and V (b) polarization, for different VWC aggregation methods (AVE, average and AGG, alternative aggregation method) and for three different compositing strategies (NN, nearest neighbor, WF, weighing function and LP, local polynomial).



(a) (b)

Fig. 4. Retrieved soil moisture vs. ground soil moisture for H (a) and V (b) polarization implementing linear averaging aggregation of VWC and before compositing. Saturated retrieved soil moisture values correspond to constrains on the minimization of the RT-0 model.

In Fig. 3 the error metrics for all the configuration runs are summarized. For each simulation configuration, the OSSE is run for a 12-week period in order to capture different soil moisture conditions.

1) Land Cover Analysis: To study the impact of forward/retrieval model asymmetries over retrieved soil moisture for different land covers, soil moisture pixels were classified before compositing according to their majority land cover type. Results are shown in Fig. 4.

In particular, for FB, woodlands (MW, mixed needleleaf and broadleaf forest) and FN+TG land cover areas, retrieved soil moisture values higher than 0.5 cm3/cm3 are to be found. Better retrieval performance is achieved in areas covered with SH and SG. However, in these areas coarse resolution VWC is less than 0.5 kg/m2.

To a lesser extent, the error in the estimation increases when soil moisture increases. For high ground soil moisture values, all land covers tend to overestimate soil moisture, except for the areas covered with shrubs where values are generally underestimated. Overall, the estimation worsens significantly as soil moisture increases, especially in areas where VWC is high.

Although there is a general overestimation of soil moisture, this behavior is more remarkable in H than in V channel. Nonetheless, the difference between H and V is more noticeable for some land cover types (e.g., FB, MW, TG and FN+TG). These results are expected, since for these particular

TABLE I
SCATTERING MODELS INPUT PARAMETERS

	Input parameters	Value
RT-0 model	Vegetation single scattering albedo ω	0.1
	Vegetation attenuation coefficient b	0.12
	Soil roughness parameter h	0.1
Theoretical model	Vegetation main species (related to a set of allometric equations)	Aspen
	Range distribution for trunks dimensions (min, max)	5 – 70 cm
	Wood water content (Trunks, branches, leaves)	0.5, 0.6 cm^3/cm^3
	Soil roughness parameter h	0.1

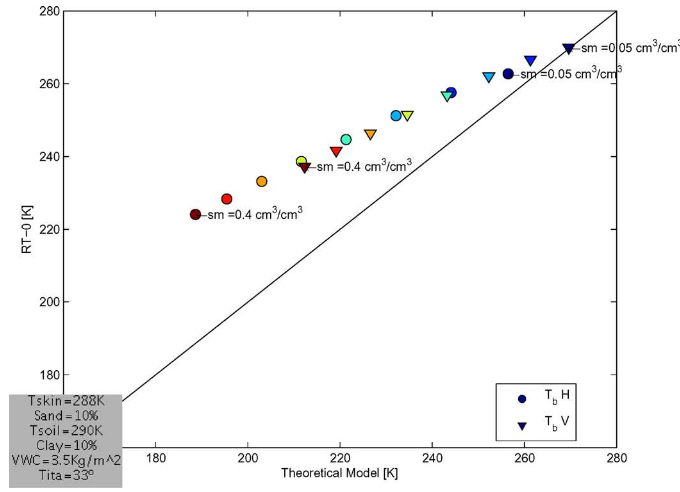
land covers, the behaviors of the theoretical model and RT-0 are more similar for the V channel than for the H channel. To illustrate the previous, a detailed comparison of the two models for the broadleaf forest is described in Section III.B.

B. Model Comparison as Forward Models: Case Study

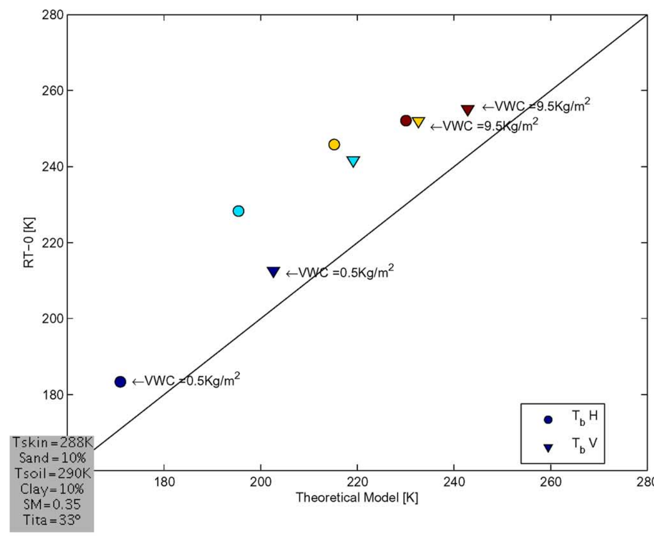
One of the most critical (and difficult) land covers to retrieve soil moisture from is a broadleaf forest. Therefore, for illustration proposes, it was selected as a test-case to perform a detailed study of its emissivity properties using the RT-0 and the theoretical model. The analysis is based on simulations for a general sparse broadleaf forest. Input model parameters are given in Table I. The purpose of this comparison is to evaluate the intrinsic behavior and sensitivity of Tb predicted by both models in terms of ground soil moisture and VWC. This procedure sets the base on what to expect for OSSE's simulation over land covers of similar characteristics.

The comparison between the simulated brightness temperatures for RT-0 and the theoretical model is presented in Fig. 5. It illustrates the comparison of brightness temperature predicted by the RT-0 and the theoretical model for different soil moisture values (a) and VWC values (b), having the remaining parameters fixed at expectable values, as shown in the chart.

For low VWC, both models present similar trends in almost all its dynamic range for both Tbv and Tbh. When VWC increases, both models Tb's sensitivity to variations of soil moisture decreases, as expected from theory. But RT-0 model presents a smaller range than the theoretical model. This is strongly related to differences in the approach used to estimate vegetation opacity and scattering within different models (see [11] and [8]), in particular the value of b selected for broadleaf forests (see Table I). The behavior as a function of VWC for different soil moisture values is also interesting. At low soil moisture, Tbs are large and dynamic ranges are small, as predicted by the theory. But when soil moisture increases, RT-0 presents a complex increasing trend of Tb as a function of VWC; models disagree for intermediate values of VWC, but produce similar results in the extremes. These results depend critically on values of ω and b and the set of allometric equations selected. Different model parameters and different sets of allometric equations will lead to different results.



(a)



(b)

Fig. 5. Brightness temperature for H and V polarization predicted by the theoretical model vs. the RT-0, varying soil moisture (a) or VWC (b) with all remaining parameters held fixed. Darker marker colors correspond to lower values of soil moisture (a)/VWC (b).

However, these discrepancies have strong implications for the retrieval using the RT-0 model. When VWC is small, RT-0 approximations are adequate to model surface emissivity and the retrieval uncertainties related to the inverse model are low. But when VWC increases, there is a systematic bias for higher values of soil moisture, which will produce an increase in estimated soil moisture. This effect will be strongly dependent on VWC value, but the dependence is complex.

These previous results agree with the results achieved from the OSSE runs, and a similar analysis can be performed on the rest of the land covers following the same methodology.

IV. CONCLUSIONS

As well stated in [5], simulation test environments need different parameterizations in the forward and retrieval models in order to assess the potential effect of different source of errors on the retrieved soil moisture accuracy. In a previous work [7] carried out with the Aquarius OSSE, the retrieval algorithm was not considered as a source of uncertainty since the RT-0 model was implemented as both forward and retrieval models. Nevertheless, the impact of several error sources (e.g., ancillary parameter aggregation scheme, soil moisture composite and instrumental noise) was assessed. To extend the analysis, the Aquarius OSSE used in [7] was adjusted in this paper to include the errors due to uncertainties in the retrieval algorithm. To this end, different models for forward and retrieval processes were presented. A theoretical model was introduced as a forward model, which is suitable to simulate some of the geometrical effects related to different vegetation types. The objective was to study the uncertainties related to the use of simple retrieval models in passive microwave applications, such as the RT-0 model.

As in [7], the simulation was carried out using a 12-week OSSE run within the Red-Arkansas River basins located in the South-Central United States. The retrieved soil moisture were compared with coarse resolution synthetic soil moisture "truth" fields (used as input into the OSSE experiment), in order to estimate retrieval errors for different land cover types as a function of soil moisture.

Results presented in this paper are strongly dependent on the chosen simulation configuration. Even though they can help guiding efforts to improve soil moisture retrieval, they may not completely agree with actual observations. One of the main reasons is that the forward model implemented is not the "truth", but a model with its own uncertainties, as the retrieval model is. Furthermore, the land surface model used in the simulation to obtain the inputs needed for the OSSE is also a model characterized with uncertainties. Thus, though biophysical layers attempt to represent real variables, they are not actual ground measurements. It is practically impossible to have enough real data at high spatial resolution to perform a similar analysis.

Nevertheless, the analysis of models' simulation presented the opportunity to test in which cases RT-0 is able to successfully model complex surface emissivities. Comparing the results obtained in this analysis and previous results [7], model discrepancies were pinpointed to be the most significant source of retrieval error. Therefore, efforts to increase the accuracy on the retrieval should be orientated towards improving/refining the retrieval model, by optimally selecting the ancillary vegetation parameters or including more emissivity terms in the formalism.

As expected, in the cases where RT-0 and theoretical model mismatches are important, effects in the retrieval were significant. Moreover, retrieval errors were found to be strongly dependent on land cover type within the Aquarius footprint. This result was expected since both the RT-0 and the theoretical model use different parameterizations. Whereas the RT-0 mainly considers vegetation as an opacity layer, the theoretical model accounts for complex vegetation geometry. As a consequence, retrieval errors are also dependent on VWC. In the cases where VWC is low, as well as heavily vegetated areas, both models behave in a similar way. However, at average biomass model mismatches are important. Therefore, lower accuracy on the retrieval was obtained on areas with relatively high VWC. However, since the dependence between Tb's and VWC is complex for both models, in general it is not easy to predict the magnitude and sign of the overall retrieval errors.

The retrieval errors related to the observed effect can be reduced in several ways. First, the values of vegetation single scattering albedo and vegetation opacity can be carefully selected for a given land cover in order to minimize model discrepancies. Optimal values of the vegetation parameter for every polarization (i.e., bH and bV) can be fitted for every land cover, matching as best as possible both models outputs thus minimizing the error in the retrieved soil moisture. Second, there are several different approaches available (dual channel algorithm, minimizations) which allow for the simultaneous estimation of certain ancillary parameters (e.g., ω or vegetation opacity) along with surface soil moisture. Such approaches may be able to recover effective parameters which minimize errors in soil moisture retrievals obtained from simplified models

Finally, it is important to note that although the specific conclusions obtained depends on the characteristics of the theoretical model used, any complex model will present trends which disagree with RT-0 predictions. Therefore, any robust retrieval scheme based on simplified models should be able to successfully deal with the effects of the models asymmetries.

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