An Observing System Simulation Experiment for the Aquarius/SAC-D Soil Moisture Product

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***Abstract*—An Observing System Simulation Experiment (OSSE) for the Aquarius/SAC-D mission has been developed for assessing the accuracy of soil moisture retrievals from passive L-band remote sensing. The implementation of the OSSE is based on the following: a 1-km land surface model over the Red-Arkansas River Basin, a forward microwave emission model to simulate the radiometer observations, a realistic orbital and sensor model to resample the measurements mimicking Aquarius operation, and an inverse soil moisture retrieval model. The simulation implements a zero-order radiative transfer model. Retrieval is performed by direct inversion of the forward model. The Aquarius OSSE attempts to capture the influence of various error sources, such as land surface heterogeneity, instrument noise, and retrieval ancillary parameter uncertainty, all on the accuracy of Aquarius surface soil moisture retrievals. In order to assess the impact of these error sources on the estimated volumetric soil moisture, a quantitative error analysis is performed by comparison of footprint-scale synthetic soil moisture with "true" soil moisture fields obtained from the direct aggregation of the original 1-km soil moisture field input to the forward model. Results show that, in heavily vegetated areas, soil moisture retrievals have a positive bias that can be suppressed with an alternative aggregation strategy for ancillary parameter vegetation water content (VWC). Retrieval accuracy was also evaluated when adding errors to 1-km VWC (which are intended to account for errors in VWC derived from remote sensing data). For soil moisture retrieval root-mean-square error on the order of 0.05 m^3/m^3, the error in VWC should be less than 12%.**

***Index Terms*—Aquarius, Observing System Simulation Experiment (OSSE), soil moisture.**

I. Introduction

An Observing System Simulation Experiment (OSSE) is a simulation designed to mimic as closely as possible a given satellite mission to study one or several characteristics of its operation. In general, OSSEs are developed to study final product characteristics as a function of system characteristics. In the past, OSSEs have been implemented to study the impact of land surface heterogeneity [1] as well as instrument error and parameter uncertainty on several soil moisture products for the AMSR-E and Hydros missions [2]. In these studies, it was shown that OSSEs are a useful tool to analyze the error budget of a given sensor from a system theory point of view and to identify significant error sources, which can be reduced by relatively inexpensive means. Nevertheless, results obtained with OSSEs are dependent on the following: 1) the models implemented [i.e., microwave emission model (MEM), dielectric mixing model, and land surface model (LSM)]; 2) the simplifications performed; and 3) the error metrics selected to do the analysis.

Here, a similar analysis is performed using an OSSE specifically developed for the Aquarius/SAC-D mission. This mission is a collaboration between the National Aeronautics and Space Administration and the Space Agency of Argentina, i.e., Comisión Nacional de Actividades Espaciales. Its main scientific objective is to provide global measurements of sea surface salinity. To meet this objective, mission simulations have been conducted to study sea surface salinity retrieval [3]. In addition, measurements obtained from the L-band radiometer on board the satellite can be also used to generate global soil moisture maps [4], [5].

Aquarius soil moisture retrieval performance was examined in a previous OSSE [6] for both the Aquarius radiometer and scatterometer to estimate retrieved soil moisture errors and identify their sources. The objectives of [6] were as follows: 1) obtain and compare root-mean-square errors (RMSEs) and correlations of retrieved soil moisture from Aquarius' three beams; 2) describe soil moisture temporal variability; and 3) contrast retrieval performance between sparsely and densely vegetated areas. The primary focus of [6] was on quantifying the lumped impact of all major error sources on overall soil moisture retrieval accuracy.

This work attempts to extend earlier work in [6] by examining the relative impact of various error sources in isolation, thereby identifying particular aspects of the Aquarius soil moisture retrieval procedure that can be targeted for improvement. Error sources considered in this work include intrapixel heterogeneity, instrument noise, soil moisture composite strategy, vegetation water content (VWC) aggregation method, and ancillary parameter uncertainty. Despite the fact that both random errors and biases contribute to RMSE, this paper will mainly focus on quantifying random errors since retrieval bias is known to have less negative impact on the usefulness of soil moisture retrievals for data assimilation applications [7].

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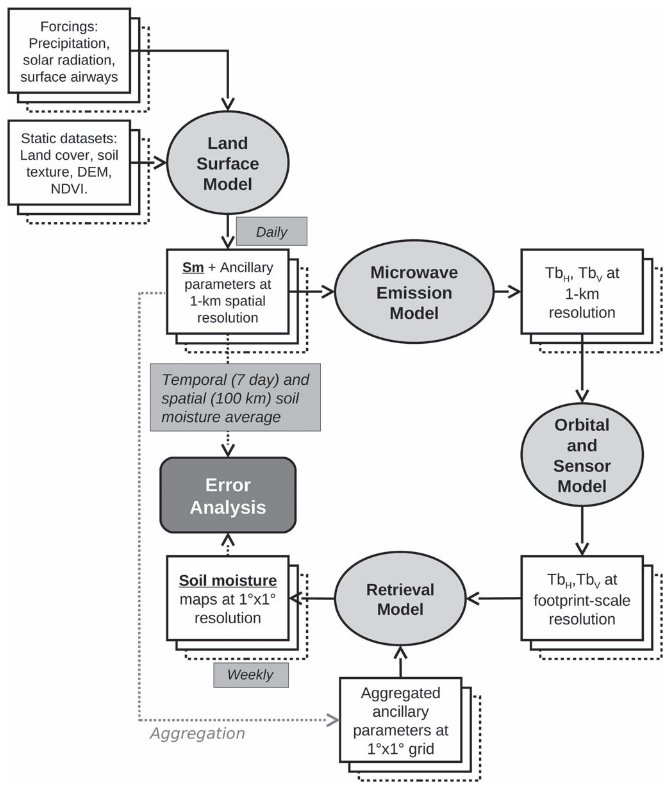

Fig. 1. OSSE block diagram.

To accomplish this objective, several different OSSEs were conducted and compared. Each OSSE implemented a different configuration (see Section III-A). Furthermore, a detailed analysis was conducted to quantify the impact of errors in ancillary parameter VWC value on soil moisture retrieval.

The OSSE described here includes four elements: 1) an LSM to generate 1-km resolution geophysical data fields; 2) a MEM to simulate soil surface brightness temperature, i.e., Tb, from soil properties at 1-km resolution; 3) a system and orbital model (SOM) to simulate Aquarius measurements at 100-km resolution (which includes instrument and acquisition strategy artifacts); and 4) a retrieval model (RM) to estimate soil moisture from Aquarius measurements at 100-km resolution and aggregated ancillary data. Fig. 1 illustrates the relationship between these components and the data flow.

Generally speaking, there are four types of error sources captured by the OSSE.

1) *Heterogeneity effects*: sampling and nonlinearity effects associated with land surface heterogeneity and performing the retrieval at a coarser spatial resolution than the forward model. These errors include the effect of nonlinearities in the MEM and the RM and the gridding effects associated with the gain function.
2) *Observation noise effects*: errors that arise when adding synthetic noise to the footprint-scale Tb. These errors correspond to system measurement errors.
3) *Retrieval parameter error effects*: errors that arise when adding synthetic noise to the footprint-averaged retrieval parameters. These errors are related to uncertainties in the ancillary parameters needed in the RM.
4) *Forward/retrieval model incompatibilities*: errors that arise when the RM is structurally inadequate [8].

Of course, actual retrievals are degraded by all four error sources. An advantage of OSSEs is that they present an opportunity to decompose total retrieval errors into the separate contribution of each of these effects. Here, we focus on OSSEs that isolate the impact of 1) land surface heterogeneity effects, 2) observation noise effects, and 3) retrieval parameter error effects. OSSEs are conducted for all cases, and a case-by-case description of how errors evolve is presented.

II. Methodology

A. LSM

High-resolution geophysical variables used as "true" nature run fields were generated for the simulation using an LSM at 1-km spatial resolution within the 250 000-km^2 Red-Arkansas River Basin (South-Central U.S.) between April 2 and July 31, 1994. The static data set used for the nature run includes a land cover and soil texture database, a digital elevation model, and a Normalized Difference Vegetation Index (NDVI) database, all at 1-km resolution. The LSM used for the simulations was the TOPMODEL-Based Land Surface-Atmosphere Transfer Scheme hydrological model [9]. The three LSM predictions were as follows: 0- to 5-cm integrated surface soil moisture in volumetric ($\mathrm{m}^3/\mathrm{m}^3$) units, surface "skin" temperature, and 5-cm soil temperature. Outputs were generated at 6 P.M. local time in the Central U.S., corresponding to the Aquarius ascending overpass time. Therefore, only ascending results were simulated and analyzed.

It is worth noting that, although the simulation is not run at global scale, land conditions in the Southern Great Plains are typical for areas of the world in which soil moisture is a limiting factor for key land surface processes.

B. MEM

Radiometer observations were simulated in the Aquarius frequency band (1.413 GHz), polarization (h and v), and incidence angles (28.7°, 37.8°, and 45.6° for inner, middle, and outer beams, respectively) at 1-km spatial resolution. Radiometer brightness temperature was computed based on a zero-order radiative transfer model that includes vegetation and soil components as [10]

$$Tb_p = Ts(1-r_p)\exp\left(-\frac{\tau}{\cos\theta}\right) + Tc(1-\omega) \times \left(1-\exp\left(-\frac{\tau}{\cos\theta}\right)\right)\left(1+r_p\exp\left(-\frac{\tau}{\cos\theta}\right)\right) \quad (1)$$

where p refers to polarization, Ts to 5-cm soil temperature, Tc to surface skin temperature (both derived from the LSM), r_p to soil reflectivity, θ to incidence angle, τ to nadir vegetation opacity, and ω to vegetation single scattering albedo. Vegetation opacity is assumed to be unpolarized and is defined as $\tau = b\,\mathrm{VWC}$, where b is a land-cover-dependent coefficient, and VWC is vegetation water content (in kilograms per square meter).

The surface roughness effect on the modeled brightness temperature was approximated as $r_p = r_{sp} \exp(-h)$, where h is related to the root-mean-square surface height, and r_{sp} refers to the reflectivity of the equivalent smooth soil surface. Values for these land-cover-dependent ancillary parameters were obtained from [1]. Finally, a dielectric constant was obtained from soil moisture and soil type using the semiempirical dielectric mixing model proposed by [11]. High-resolution inland water pixels were not considered in the analysis.

According to the Aquarius simulated Level-2 data set available at ftp://saltmarsh.jpl.nasa.gov/, the atmospheric contributions to the top-of-atmosphere brightness temperature at L-band over the Red-Arkansas River Basin can vary from 1.5 to 3.5 K. However, no atmospheric effects were considered in this study. Moreover, the objective of this paper was not to consider all possible sources of error in the retrieved soil moisture, which are many and may be very complex to simulate. On the contrary, we focused on a subset of error sources, which are mainly related to the retrieval process and are known to strongly influence overall soil moisture retrieval accuracy [12]. Therefore, our focus was on land surface processes having the largest impact on observed Tb.

C. SOM

The SOM is based on a MATLAB routine that implements the simplified general perturbation (SGP4) orbit propagator. Aquarius orbital parameters considered in the SOM were the following: 98.0126° inclination, 0.0012 eccentricity, 18:00 mean local mean time of ascending node, 7028.871-km mean semimajor axis, 90° mean argument of perigee, and 657-km satellite height.

The synthetic 1-km Tb obtained from (1) are weighted by a sinc^2 function applied as a theoretical approximation of the Aquarius antenna patterns. The theoretical approximation matches the actual −3-dB footprints for each of the three Aquarius radiometers. The ground projected axes of the footprints are as follows: 74 km along track × 94 km across track for the inner beam, 84 × 120 km for the middle beam, and 96 × 156 km for the outer beam, yielding a swath width of 390 km [13]. For each of the three beams, 1-km resolution gain patterns were projected on the ground as in [14]. Patterns were rotated and located to move along with the satellite. Geolocation of observations was associated with the latitude and longitude of the center of each footprint. The varying incidence angle within each of the Aquarius footprints was also computed. Spatially independent Gaussian noise with a standard deviation of 1 K in brightness temperature was added to the measurements to account for the effect of radiometer instrument noise. The chosen measurement error is large, considering the 0.38-K error expected per observation described in [15]. Observations were then averaged to a time interval of 1.44 s (i.e., 12 Tb samples) to match the temporal resolution of Aquarius Level-2 products [16] and the Aquarius measurement procedure [13].

D. RM

The OSSE implements the single channel retrieval algorithm (SCA) [17] to estimate soil moisture from simulated brightness temperature. This is accomplished by directly inverting the implemented forward model. It is worth noting that the SCA is not quite a perfect inversion of the forward model since it assumes $Tc = Ts$ in (1). Soil moisture was retrieved from the reflectivity coefficient via the Fresnel equations and the Dobson soil dielectric mixing model used in the MEM. Auxiliary data for estimating soil moisture are the ancillary parameters (Ts, Tc, θ, τ, ω, b, sand, and clay) at footprint scale. These values are derived by linearly averaging 1-km emission parameters used as inputs to the MEM.

In previous studies [18], it was shown that VWC is the most critical quantity in soil moisture retrieval errors. To evaluate the effect of subfootprint-scale land surface heterogeneity, two methods of aggregating VWC were evaluated. Linear averaging (AVE) of 1-km VWC and an alternative aggregation (AGG) scheme for VWC, derived from theoretical considerations (see [12]), is

$$\text{VWC}_{\text{agg}} = \left[\ln \left(\sum_{i=1}^{n} A^{\text{VWC}_\text{i}} \right) - \ln(n) \right] / \ln(A) \qquad (2)$$

where $A = \exp(-2b/\cos\theta)$, with θ being the Aquarius incidence angle and b the vegetation parameter that relates vegetation opacity to VWC. Uncertainties in ancillary parameters were accounted for by adding synthetic noise to some footprint-resolution parameters. These perturbations were generated using Gaussian noise with zero mean and standard deviations of 1 K for Ts and Tc; 1% relative error for sand, clay, and VWC; and 0.005 for b and h (in centimeters).

E. Compositing

To mimic Aquarius Level-3 processing, retrieved soil moisture at footprint center locations for the three beams were mapped onto a fixed weekly soil moisture product with 1° spatial resolution. Composite pixels may arise from observations of different beams, and the resulting image will be the standard Aquarius soil moisture product. To generate the composite, three sampling methods were implemented: 1) nearest neighbor (NN); 2) weighting function (WF); and 3) local quadratic polynomial (LP) fitting with a bandwidth of 100 km [19]. In WF interpolation, soil moisture retrievals for individual footprints, i.e., X_i, were weighted according to their distance, i.e., d, from the grid center using

$$Y = \frac{\sum_{i=1}^{n} X_i/d_i}{\sum_{i=1}^{n} 1/d_i} \qquad (3)$$

where Y refers to the image pixel value. Image pixel values derived using NN and WF interpolation were obtained by binning the Level-2 soil moisture product onto a 1° grid (see Fig. 2), i.e., only footprints whose center falls within a particular 1° box were used to determine Y for that box. This methodology, combined with considering only ascending passes, led to spatial gaps in simulated Level-3 soil moisture products.

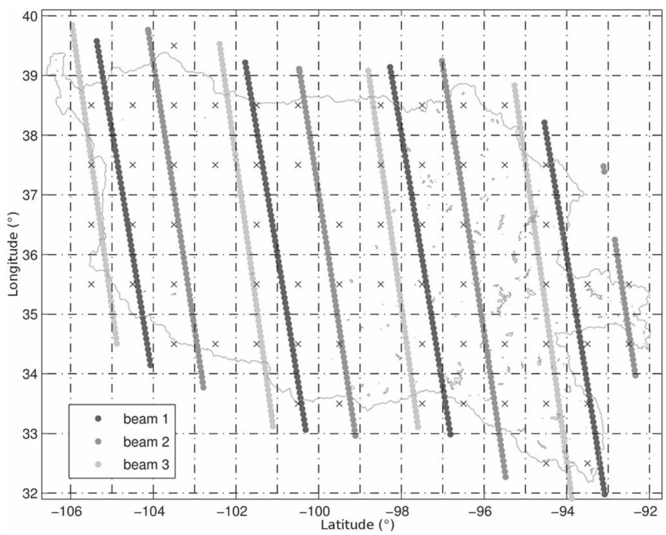

Fig. 2. The 1° grid of the weekly composited soil moisture product derived from the three Aquarius beams. The centers of composite grids are marked with "×," and Aquarius footprint centers (of the three beams) are marked with "•."

III. Results

Soil moisture runs from April 2 to July 31, 1994, were used in this analysis. Since Aquarius has a seven-day repeat pass orbit, 17 weekly product images were obtained. Each seven-day retrieved soil moisture image was obtained by compositing observations from seven consecutive days.

A. Total Error Analysis

The OSSE's soil moisture was retrieved with the SCA for the following cases: two polarization channels, three Aquarius beams, two VWC aggregation strategies, and three soil moisture compositing strategies. For each of the cases, three separate OSSE's were conducted: 1) a no-noise case (nn); 2) the Tb with Gaussian noise case (i) (observation noise effects described in Section II-C); and 3) the Tb and ancillary parameters with Gaussian noise case (i + p) (observation noise and retrieval parameter error effects described in Section II-D). To assess the impact of these different error sources and to quantify their influence on the final product (weekly soil moisture), two separate error metrics were taken into consideration. For every output, correlation, i.e., ρ, and RMSE between synthetic soil moisture (sm_0) and weekly averaged "true" soil moisture degraded at coarse resolution through lineal averaging (sm_g) were computed as

$$\sigma_{\mathrm{sm}_0} = \sqrt{\sum_{i=1}^{n} \left(\mathrm{sm}_{0i} - E[\mathrm{sm}_0]\right)^2}$$

$$\sigma_{\mathrm{sm}_g} = \sqrt{\sum_{i=1}^{n} \left(\mathrm{sm}_{gi} - E[\mathrm{sm}_g]\right)^2}$$

$$\rho = \frac{\sum_{i=1}^{n} \left(\mathrm{sm}_{0i} - E[\mathrm{sm}_0]\right)\left(\mathrm{sm}_{gi} - E[\mathrm{sm}_g]\right)}{\sigma_{\mathrm{sm}_0}\sigma_{\mathrm{sm}_g}} \tag{4}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\mathrm{sm}_{0i} - \mathrm{sm}_{gi})^2}. \tag{5}$$

Error metrics for each case are displayed in Table I. In all the tested cases, soil moisture retrievals obtained from the vertical polarization channel exhibit slightly better accuracy than retrievals from the horizontal channel. This result may seem controversial since it does not agree with either field experiments [20] or theoretical results [21], which predict a higher sensitivity to soil moisture in the horizontal channel. However, it can be explained by the fact that no bias was introduced in the radiometric measurements; hence, there is no larger bias in vertical polarization than in horizontal polarization. Actual retrievals will be impacted by the varying bias between polarizations (and between the different beams). Nevertheless, it is difficult to estimate how the actual bias over land will vary with beam and polarization.

With regard to VWC aggregation, applying the alternative aggregation method proposed in [12] results in improved soil moisture retrieval accuracy for all cases. In addition, errors associated with the compositing strategy were evaluated. The estimation performance slightly improves in comparison with both NN and LP when using the WF compositing approach. Furthermore, WF interpolation has less sensitivity to instrumental noise and parameter uncertainty than either NN or LP has.

The total error as a function of which Aquarius beam was used was also evaluated. Differences in retrieval performance between beams are expected since the three Aquarius beams have different incidence angles and footprint dimensions. Since error analysis is performed after compositing, beam performance differentiation cannot be directly assessed. Nevertheless, simulated Level-2 soil moisture results demonstrate that retrievals based on middle beam observations have the best accuracy and the outer beam the worst. As an example, in the case where neither instrumental noise nor ancillary parameter uncertainties are added and AGG VWC aggregation is applied, the inner beam has $\rho_h = 0.969$, $\mathrm{RMSE}_h = 0.023$, $\rho_v = 0.976$, and $\mathrm{RMSE}_v = 0.020$; the middle beam has $\rho_h = 0.984$, $\mathrm{RMSE}_h = 0.017$, $\rho_v = 0.986$, and $\mathrm{RMSE}_v = 0.016$; and the outer beam has $\rho_h = 0.959$, $\mathrm{RMSE}_h = 0.027$, $\rho_v = 0.960$, and $\mathrm{RMSE}_v = 0.027$. Nevertheless, since the soil moisture composite is constructed using all three beams, these effects are not relevant to the Level-3 product.

B. VWC Parameter

1) VWC Aggregation: Resolution degradation of VWC was obtained through two different aggregation approaches, namely, AVE and AGG [see (2)], to degrade high-resolution VWC to final product spatial resolution. An error analysis was performed to derive the accuracy of synthetic soil moisture retrieved with each of the schemes [see Fig. 3(a) and (b)]. Results suggest that AVE of VWC overestimates soil moisture for heavily vegetated surfaces. The AGG strategy gives rise to lower VWC, in turn leading to lower retrieved soil moisture and a reduction in retrieval bias. Therefore, the AGG method results in improved soil moisture estimation accuracy.

TABLE I
ERROR METRICS ASSOCIATED WITH VARIOUS VWC AGGREGATION AND SOIL MOISTURE COMPOSITING STRATEGIES

		NN				**WF**				**LP**			
		Tb_h		Tb_v		Tb_h		Tb_v		Tb_h		Tb_v	
		ρ	RMSE	ρ	RMSE	ρ	RMSE	ρ	RMSE	ρ	RMSE	ρ	RMSE
AV	nn	0.941	0.034	0.952	0.030	0.947	0.031	0.955	0.029	0.935	0.034	0.951	0.030
	i	0.940	0.034	0.952	0.030	0.947	0.031	0.955	0.029	0.935	0.035	0.948	0.031
	i+p	0.937	0.036	0.950	0.031	0.946	0.032	0.955	0.029	0.933	0.035	0.943	0.032
AGG	nn	0.953	0.028	0.957	0.027	0.957	0.027	0.959	0.026	0.948	0.029	0.952	0.028
	i	0.953	0.028	0.957	0.027	0.957	0.027	0.959	0.026	0.939	0.032	0.950	0.029
	i+p	0.951	0.028	0.956	0.027	0.956	0.027	0.959	0.026	0.931	0.033	0.941	0.031

RMSE: Root Mean Square Error (m^3/m^3)

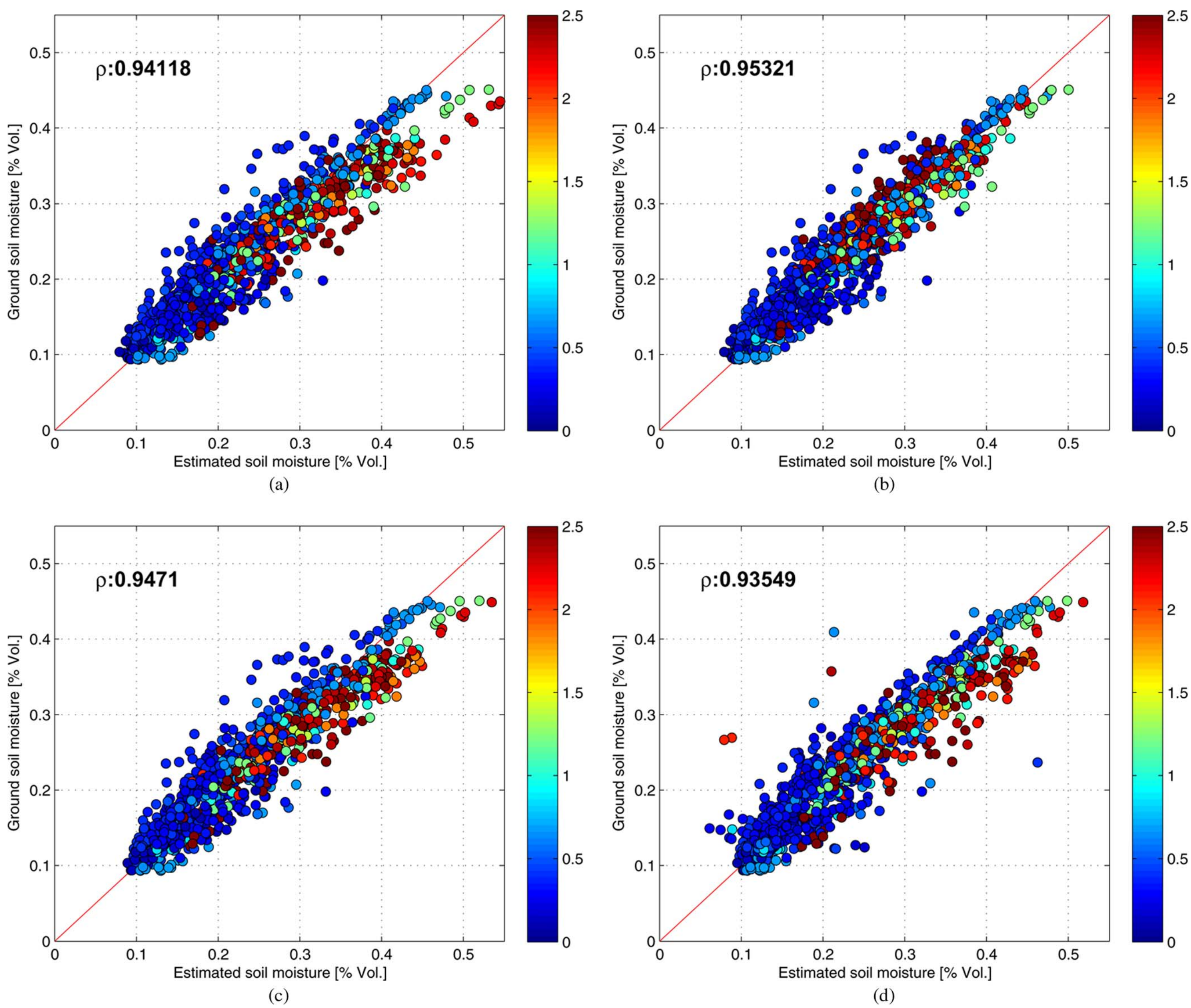

Fig. 3. Ground soil moisture versus estimated soil moisture from horizontal polarization channel for different VWC aggregation methods and soil moisture composites. (a) AVE and NN. (b) AGG and NN. (c) AVE and WF. (d) AVE and LP. The color corresponds to VWC (in kilograms per square meter) levels, as shown in the color bars.

To understand the errors that arise from the two different approaches, comparison between AVE-based and AGG-based VWCs with the corresponding effective (EFF) VWC values was performed following the methodology in [12] over the 17-week simulation period. EFF values are defined as the VWC that minimizes RMSE in soil moisture retrievals for a given condition. Results are illustrated in Fig. 4, where the values of the b parameters needed for the AGG approach were obtained through linear averaging of b at 1-km resolution. As shown, the AGG-based VWC shows better agreement with EFF than the

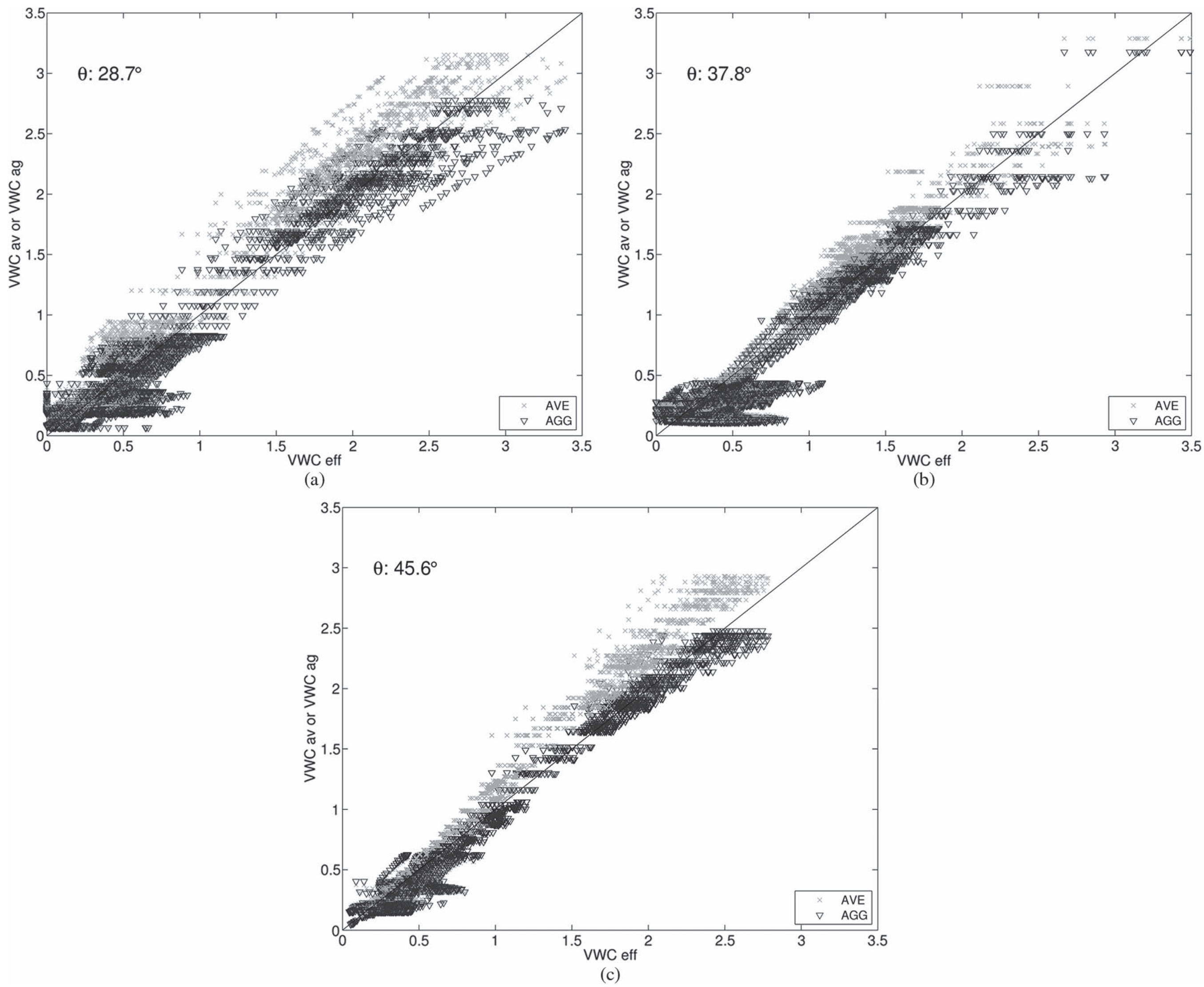

Fig. 4. Comparison between averaged (AVE) and aggregated (AGG) VWC values and corresponding effective (EFF) VWC values at three incidence angles corresponding to the Aquarius (a) inner, (b) middle, and (c) outer footprints.

AVE-based one does. In particular, for high VWC values, the agreement between EFF and AGG is significantly better than that between EFF and AVE. For low VWC values, although the difference is not so remarkable, a slight improvement is achieved by implementing the AGG method instead of the AVE method. These results agree with the outputs of the OSSE where AVE-derived VWC shows a positive bias, which increases as vegetation becomes denser and produces a positive bias in estimated soil moisture. On the contrary, soil moisture retrieved using the AGG approach shows better agreement with nature run soil moisture. The impact of changing the aggregation method is small for sparsely vegetated areas and increases as vegetation becomes denser.

An important feature shown in Fig. 4 is a horizontal striped pattern. This artifact is produced because, for a given pixel, VWC and b parameters remain constant over the simulation period, but the effective VWC changes with time. Effective VWC changes imply that the VWC value that will lead to the minimum error in soil moisture estimation also changes with time. This change should be related to the variables that change with time in the OSSE, i.e., soil moisture, soil temperature, and canopy temperature. Therefore, the change in effective VWC is presumably related to the aggregation method of these parameters. Although these errors are small compared with VWC ones, the aggregation strategy of these parameters should be taken into account in any actual retrieval scheme.

2) Errors in VWC: Since ancillary VWC estimates are known to be a major source of soil moisture retrieval error [18], it is useful to determine the maximum tolerable error in this parameter to keep soil moisture error below a given threshold. To this end, synthetic error was added to the 1-km^2 ancillary parameter VWC before aggregation. To simulate both a systematic bias and variance in VWC, errors were added as Gaussian noise $\mathcal{N}(0, \sigma^2)$, with a higher standard deviation for areas with denser vegetation and a bias to account for nonlinearity between VWC and its satellite-derived proxy, NDVI, and Normalized Difference Water Index (NDWI). Noisy VWC of 1° resolution is then used in soil moisture retrieval, and the synthetic product performance is assessed. Results are summarized in Table II.

TABLE II
ERROR METRICS ASSOCIATED WITH BIASES AND RANDOM ERRORS IN VWC

VWC Agg.		No Error	5% bias +10% σ	5% bias +15% σ	5% bias +25% σ	8% bias +15% σ	8% bias +25% σ	12% bias +15% σ	25% bias +25% σ
AVE	ρ_h	0.941	0.933	0.933	0.933	0.929	0.929	0.918	0.878
	$RMSE_h$	0.034	0.040	0.040	0.040	0.044	0.043	0.052	0.083
	ρ_v	0.952	0.950	0.950	0.950	0.949	0.949	0.946	0.937
	$RMSE_v$	0.030	0.033	0.033	0.033	0.034	0.034	0.037	0.048
AGG	ρ_h	0.953	0.925	0.925	0.924	0.924	0.923	0.920	0.911
	$RMSE_h$	0.028	0.035	0.036	0.036	0.036	0.037	0.039	0.048
	ρ_v	0.957	0.927	0.926	0.926	0.926	0.926	0.924	0.921
	$RMSE_v$	0.027	0.036	0.036	0.036	0.036	0.037	0.038	0.042

RMSE: Root Mean Square Error (m^3/m^3)

As expected, linear averages of VWC obtained using the AVE approach demonstrate strong sensitivity to bias in high-resolution VWC. On the other hand, the performance of the AGG method remains generally constant when bias is added to VWC. Furthermore, for high-bias cases (more than 25%), applying the AGG method yields better accuracy soil moisture retrievals than the AVE approach does. Both aggregation methods exhibit low sensitivity to Gaussian noise on 1-km resolution VWC. This result is expected since random error (i.e., nonbias based) added is spatially independent in neighboring 1-km pixels. As a result, it can be effectively eliminated by spatial averaging. In summary, although accuracy gets worse when VWC error increases (both bias and variance), the RM proves to be quite robust even when using low-quality VWC estimates. However, low VWC bias is advantageous to meet the Aquarius soil moisture retrieval error target of 0.05 m^3/m^3. As an example, for the case in which the horizontal polarization Tbs are used as inputs to the SCA and the AVE approach is implemented, VWC bias should be lower than 12% so that RMSE will remain below 0.05 m^3/m^3 (see Table II). The VWC bias threshold is allowed to be higher if the AGG method and/or the vertical polarization are used instead.

C. Compositing

Results for the three different compositing strategies introduced in Section II-E (i.e., NN, WF, and LP) are shown in Fig. 3. Since only ascending passes were considered in the simulation, composited soil moisture does not precisely represent the Level-3 data (in fact, the NN and WF compositing methods led to some "holes" in the soil moisture imagery). Nevertheless, several conclusions can still be extracted from the analysis. Interpolations NN and WF display the most similar results. However, the NN compositing approach is more sensitive to noise in radiometer Tb observations. Moreover, with this configuration, LP fitting displays the worst accuracy. Nevertheless, further analysis should be carried out to derive the optimal bandwidth for the LP composite. A similar analysis can be performed for the WF composite. Linear averaging can be tweaked with a coefficient to adjust the distance weighting to slightly improve the retrieved soil moisture. However, this analysis is outside of the scope of this paper, and results obtained here suggest that the improvement that can be achieved by optimizing the compositing approach is smaller than that possible by using an alternative VWC aggregation approach.

IV. DISCUSSION AND CONCLUSION

Using an OSSE for Aquarius, this paper has evaluated the accuracy of retrieving soil moisture from radiometer observations and the potential impact of specific error sources on Level-2 and Level-3 soil moisture retrieval products. By extending past work primarily intended to estimate the lumped impacted of all major error sources [6], our emphasis here is on evaluating the relative impact of various error sources in isolation and thereby identifying high-priority errors for the improvement of Aquarius soil moisture retrieval accuracy.

It is worth noting that the main objective of this study was not to replicate Aquarius' Tb observations perfectly but rather to use the OSSE as a tool to estimate sensitivities, study aggregation strategies, and describe error propagation, assuming that the forward model produces "realistic" outputs. Therefore, to perform representative analysis, it is important that the data set contains a representative range of surface states and Tbs. As a matter of fact, OSSEs are not expected to correspond exactly to the real world. In particular, the variability of Tbs of a real scenario can be only partially explained by a simulated database. As stated in [22], a fair degree of realism is usually assumed to be sufficient to develop and test retrieval methods in OSSE. Evaluation of product performance depends on the error metrics used, and the conclusions derived are highly dependent on the models implemented (i.e., MEM, SCA, Dobson, etc.).

After evaluating error metrics (correlation and RMSE), it has been shown that the single channel algorithm for retrieving soil moisture from brightness temperature observations exhibits good sensitivity to optical depth and VWC aggregation technique [18]. Moreover, the results exhibited a bias toward highly vegetated areas for synthetic soil moisture values retrieved from passive microwave observations when linear averaging was used to aggregate VWC. The impact of aggregation of VWC was greater for denser vegetation.

OSSE simulations were also used to evaluate and compare three compositing methods to obtain Level-3 product imagery. Results suggest that choosing an optimal soil moisture composite has a smaller impact on retrieval accuracy than the corresponding improvement that can be achieved by implementing proper ancillary parameter aggregation methods.

Finally, both parameter uncertainty and instrumental errors were considered. Despite the small errors in auxiliary parameters considered, the retrieval was found to be more sensitive to ancillary parameter errors than to footprint-scale noise added to observations. Moreover, using OSSE outputs, both systematic and random errors in VWC data were studied for two different aggregation techniques (AVE and AGG approaches [12]). For large values of VWC, overestimation of soil moisture is observed when averaging is used to degrade the spatial resolution of VWC. Regarding vegetation effects, overestimation of soil moisture is related to overestimation of VWC. Indeed, for a given value of measured Tb_H, the RM will assign a higher soil moisture value to more heavily vegetated areas. Therefore, the overestimation in soil moisture observed when averaging is used should be related to overall overestimation of VWC for areas with large VWC values (> 2 kg/m^2).

From previous studies [18] and the results of this paper, we establish that, to first order, VWC is the parameter that controls estimated soil moisture error. Therefore, its absolute error and aggregation strategy should be comprehensively studied. In this paper, two types of VWC error were modeled: zero-mean Gaussian noise and systematic bias (see Table II). As expected, an increase in VWC errors degrades soil moisture estimation. A linear aggregation scheme is sensitive to biases in VWC. As already noted, errors associated with the AGG approach remain generally constant when VWC bias is introduced. In general, although accuracy decreases when VWC error increases, retrievals are robust even in the presence of large errors in VWC. Nevertheless, based on these simulations, maximum values of VWC errors (bias and standard deviation) can be defined before Aquarius soil moisture error will rise above its threshold value of 0.05 $\mathrm{m}^3/\mathrm{m}^3$. As a conservative estimate, for the data set and configuration used in this OSSE, 12% was found to be the maximum relative bias in VWC that can be tolerated without exceeding the threshold retrieval error of 0.05 $\mathrm{m}^3/\mathrm{m}^3$. However, this maximum can vary depending on the SCA polarization channel and the VWC aggregation method used.

It is interesting to contrast these values with those available in the literature. VWC data used for passive microwave soil moisture retrieval are generally estimated using a combination of remote sensing proxies: NDVI [5], NDWI [23], and microwave polarization indices [24]. All of these methods are land cover dependent, i.e., the equations that relate the proxy value to VWC depend on assumptions about land cover. In addition, few VWC estimation strategies are well validated or provide uncertainty estimates. As an example, [25] provides an RMSE estimate of ~0.6 kg/m^2 for the retrieval of VWC from NDWI (for corn and soybean), and this RMSE estimate is ~10% of the observed range of VWC for these crops. Based on our analysis, this level of error seems generally acceptable for VWC inputs into an Aquarius soil moisture retrieval algorithm. Nevertheless, results in [25] also demonstrate strong field-to-field discrepancies using the proposed VWC-NDVI model and indicate even nonlinear relationships between NDVI and VWC, which could lead to bias in VWC [26]. Unfortunately, this kind of exhaustive analysis is not available for all land covers, and therefore, it is difficult to assess whether current VWC estimation strategies are robust enough to be used as global inputs to an Aquarius soil moisture retrieval scheme.

REFERENCES

[1] W. T. Crow, M. Drusch, and E. F. Wood, “An observation system simulation experiment for the impact of land surface heterogeneity on AMSR-E soil moisture retrieval,” *IEEE Trans. Geosci. Remote Sens.*, vol. 39, no. 8, pp. 1622–1631, Aug. 2001.

[2] W. T. Crow, S. T. K. Chan, D. Entekhabi, P. R. Houser, A. Y. Hsu, T. J. Jackson, E. G. Njoku, P. E. O’Neill, J. Shi, and X. Zhan, “An Observing System Simulation Experiment for Hydros radiometer-only soil moisture products,” *IEEE Trans. Geosci. Remote Sens.*, vol. 43, no. 6, pp. 1289–1303, Jun. 2005.

[3] D. M. Le Vine, E. P. Dinnat, S. Abraham, P. de Matthaeis, and F. J. Wentz, “The Aquarius simulator and cold-sky calibration,” *IEEE Trans. Geosci. Remote Sens.*, vol. 49, no. 9, pp. 3198–3210, Sep. 2011.

[4] E. G. Njoku and D. Entekhabi, “Passive microwave remote sensing of soil moisture,” *J. Hydrol.*, vol. 184, no. 1/2, pp. 101–129, Oct. 1996.

[5] T. J. Jackson, D. M. Le Vine, A. Y. Hsu, A. Oldak, P. J. Starks, C. T. Swift, J. D. Isham, and M. Haken, “Soil moisture mapping at regional scales using microwave radiometry: The Southern Great Plains hydrology experiment,” *IEEE Trans. Geosci. Remote Sens.*, vol. 37, no. 5, pp. 2136–2151, Sep. 1999.

[6] Y. Luo, X. Feng, P. Houser, V. Anantharaj, X. Fan, G. De Lannoy, X. Zhan, and L. Dabbiru, “Potential soil moisture products from the Aquarius radiometer and scatterometer using an Observing System Simulation Experiment,” *Geosci. Instrum., Methods Data Syst. Discuss.*, vol. 2, no. 2, pp. 457–476, 2012.

[7] W. T. Crow, R. D. Koster, R. H. Reichle, and H. O. Sharif, “Relevance of time-varying and time-invariant retrieval error sources on the utility of spaceborne soil moisture products,” *Geophys. Res. Lett.*, vol. 32, no. 24, p. L24405, 2005.

[8] A. G. Konings, D. Entekhabi, S. T. K. Chan, and E. G. Njoku, “Effect of radiative transfer uncertainty on L-band radiometric soil moisture retrieval,” *IEEE Trans. Geosci. Remote Sens.*, vol. 49, no. 7, pp. 2686–2698, Jul. 2011.

[9] C. D. Peters-Lidard, M. S. Zion, and E. F. Wood, “A soil vegetation–atmosphere transfer scheme for modeling spatially variable water and energy balance processes,” *J. Geophys. Res.*, vol. 102, no. D4, pp. 4303–4324, Feb. 1997.

[10] T. J. Jackson and T. J. Schmugge, “Vegetation effects on the microwave emission of soil,” *Remote Sens. Environ.*, vol. 36, no. 3, pp. 203–212, Jun. 1991.

[11] M. C. Dobson, F. T. Ulaby, M. T. Hallikainen, and M. A. El-Rayes, “Microwave dielectric behavior of wet soil—Part II: Dielectric mixing models,” *IEEE Trans. Geosci. Remote Sens.*, vol. GE-23, no. 1, pp. 35–46, Jan. 1985.

[12] X. Zhan, W. T. Crow, T. J. Jackson, and P. E. O’Neill, “Improving spaceborne radiometer soil moisture retrievals with alternative aggregation rules for ancillary parameters in highly heterogeneous vegetated areas,” *IEEE Geosci. Remote Sens. Lett.*, vol. 5, no. 2, pp. 261–265, Apr. 2008.

[13] D. M. Le Vine, G. S. E. Lagerloef, S. Yueh, F. Pellerano, E. Dinnat, and F. Wentz, “Aquarius mission technical overview,” in *Proc. IGARSS*, Jul. 2006, pp. 1678–1680.

[14] A. S. Limaye, W. L. Crosson, and C. A. Laymon, “Estimating accuracy in optimal deconvolution of synthetic AMSR-E observations,” *Remote Sens. Environ.*, vol. 100, no. 1, pp. 133–142, Jan. 2006.

[15] Y. Chao, “L2a Aquarius science requirements,” Jet Propulsion Lab., Pasadena, CA, USA, Tech. Rep., Jul. 2008.

[16] G. Foti and C. Finch, “Aquarius user guide,” Jet Propulsion Lab., Pasadena, CA, USA, Tech. Rep., 2011.

[17] T. J. Jackson, “Measuring surface soil moisture using passive microwave remote sensing,” *Hydrol. Process.*, vol. 7, no. 2, pp. 139–152, 1993.

[18] C. A. Bruscantini, F. M. Grings, P. Perna, H. Karszenbaum, W. T. Crow, and J. C. A. Jacobo, “An Observing System Simulation Experiment (OSSE) for the Aquarius/SAC-D soil moisture product,” in *Proc. 12th Spec. Meet. MicroRad*, Mar. 2012, pp. 1–4.

[19] J. M. Lilly and G. S. E. Lagerloef, Aquarius level 3 processing algorithm theoretical basis document, Part II. Implementation, Feb. 2009.

[20] J.-C. Calvet, J.-P. Wigneron, J. Walker, F. Karbou, A. Chanzy, and C. Albergel, "Sensitivity of passive microwave observations to soil moisture and vegetation water content: L-band to W-band," *IEEE Trans. Geosci. Remote Sens.*, vol. 49, no. 4, pp. 1190–1199, Apr. 2011.

[21] F. T. Ulaby, R. K. Moore, and A. K. Fung, *Microwave Remote Sensing: Active and Passive. From Theory to Applications*. Norwood, MA, USA: Artech House, 1986.

[22] T. Pellarin, J.-P. Wigneron, J.-C. Calvet, M. Berger, H. Douville, P. Ferrazzoli, Y. H. Kerr, E. Lopez-Baeza, J. Pulliainen, L. P. Simmonds, and P. Waldteufel, "Two-year global simulation of L-band brightness temperatures over land," *IEEE Trans. Geosci. Remote Sens.*, vol. 41, no. 9, pp. 2135–2139, Sep. 2003.

[23] D. Chen, T. J. Jackson, F. Li, M. H. Cosh, C. Walthall, and M. Anderson, "Estimation of vegetation water content for corn and soybeans with a Normalized Difference Water Index (NDWI) using Landsat Thematic Mapper data," in *Proc. IEEE IGARSS*, 2003, vol. 4, pp. 2853–2856.

[24] T. Jing, S. Jiancheng, T. J. Jackson, D. Jinyang, R. Bindlish, and Z. Lixin, "Monitoring vegetation water content using microwave vegetation indices," in *Proc. IEEE IGARSS*, 2008, vol. 1, pp. I-197–I-200.

[25] D. Chen, J. Huang, and T. J. Jackson, "Vegetation water content estimation for corn and soybeans using spectral indices derived from MODIS near- and short-wave infrared bands," *Remote Sens. Environ.*, vol. 98, no. 2/3, pp. 225–236, Oct. 2005.

[26] T. J. Jackson, D. Chen, M. Cosh, F. Li, M. Anderson, C. Walthall, P. Doriaswamy, and E. Ray Hunt, "Vegetation water content mapping using Landsat data derived Normalized Difference Water Index for corn and soybeans," *Remote Sens. Environ.*, vol. 92, no. 4, pp. 475–482, Sep. 2004.

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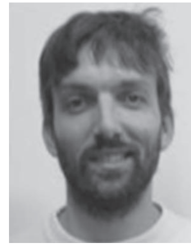

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