Application of Triple Collocation in Ground-Based Validation of Soil Moisture Active/Passive (SMAP) Level 2 Data Products

Fan Chen, Wade T. Crow, *Member, IEEE*, Andreas Colliander, *Senior Member, IEEE*, Michael H. Cosh, *Member, IEEE*, Thomas J. Jackson, *Fellow, IEEE*, Rajat Bindlish, *Senior Member, IEEE*, Rolf H. Reichle, Steven K. Chan, *Senior Member, IEEE*, David D. Bosch, Patrick J. Starks, David C. Goodrich, and Mark S. Seyfried

***Abstract*—The validation of the soil moisture retrievals from the recently launched National Aeronautics and Space Administration (NASA) Soil Moisture Active/Passive (SMAP) satellite is important prior to their full public release. Uncertainty in attempts to characterize footprint-scale surface-layer soil moisture using point-scale ground observations has generally limited past validation of remotely sensed soil moisture products to densely instrumented sites covering an area approximating the satellite ground footprint. However, by leveraging independent soil moisture information obtained from land surface modeling and/or alternative remote sensing products, triple collocation (TC) techniques offer a strategy for characterizing upscaling errors in sparser ground measurements and removing the impact of such error on the evaluation of remotely sensed soil moisture products. Here, we propose and validate a TC-based strategy designed to utilize existing sparse soil moisture networks (typically with a single sampling point per satellite footprint) to obtain an unbiased correlation validation metric for satellite surface soil moisture retrieval products. Application of this TC strategy at five SMAP core validation sites suggests that unbiased estimates of correlation between the satellite product and the true footprint average can be obtained—even in cases where ground observations provide only one single reference point within the footprint. An example of preliminary validation results from the application of this TC strategy to the SMAP Level 2 Soil Moisture Passive (beta release version) product is presented.**

***Index Terms*—Remote sensing, soil moisture, Soil Moisture Active/Passive (SMAP), triple collocation (TC).**

I. Introduction

The Soil Moisture Active Passive (SMAP) satellite mission, launched in January 2015 by NASA, was designed to provide global mapping of soil moisture and landscape freeze/thaw state every 2–3 days on nested 3, 9, and 36-km Earth grids using L-band radar (1.26 GHz) and L-band radiometer (1.4 GHz) observations [1]. The SMAP mission requirement for soil moisture products in the top 5 cm of soil at 10-km and 40-km spatial resolutions is to meet a $0.04\,\mathrm{m}^3 \cdot \mathrm{m}^{-3}$ retrieval accuracy target [2]. On July 7, 2015 SMAPs on-board radar failed; however, the SMAP radiometer continues to function normally and produce a soil moisture product on a 36-km Equal Area Scalable Earth-2 (EASE2) grid.

As in previous satellite missions, assessment of SMAP soil moisture retrieval accuracy will be based mainly on comparisons with ground-based observations [3]–[5]. To this end, the SMAP mission subdivides the sources of such observations into two separate classes: 1) core validation sites which possess sufficient spatial sampling density (usually more than eight sampling points per SMAP footprint) to be aggregated into a representative estimate of footprint-scale soil moisture, and 2) sparse network sites that typically provide just one point-scale measurement in a satellite footprint.

Examples of core sites include dense soil moisture sampling networks installed within the United States Department of Agriculture (USDA)'s Agricultural Research Service (ARS) experimental watersheds [6], [7]. Examples of sparse validation networks include the USDA Soil Climate Analysis Network (SCAN) [8] and the National Oceanic and Atmospheric Administration (NOAA) U.S. Climate Reference Network (USCRN, or CRN) [9]. Both SCAN and CRN provide over 100 soil moisture sampling locations within the coterminous United States

Manuscript received January 13, 2016; revised April 13, 2016; accepted May 6, 2016. Date of publication June 15, 2016; date of current version January 23, 2017. This work was supported by the National Aeronautics and Space Administration, Soil Moisture Active/Passive mission via Wade Crow's membership on the SMAP Science Team

F. Chen and R. Bindlish are with Science System and Applications, Inc., Lanham, MD 20706 USA (e-mail: fan.chen@ars.usda.gov; rajat.bindlish@ars.usda.gov).

W. T. Crow, M. H. Cosh, and T. J. Jackson are with the Hydrology and Remote Sensing Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Beltsville, MD 20705 USA (e-mail: wade.crow@ars.usda.gov; Michael.Cosh@ars.usda.gov; tom.jackson@ars.usda.gov).

A. Colliander and S. K. Chan are with the NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109 USA (e-mail: andreas.colliander@jpl.nasa.gov; steven.k.chan@jpl.nasa.gov).

R. H. Reichle is with the Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, MD 20771 USA (e-mail: Rolf.Reichle@nasa.gov).

D. D. Bosch is with the Southeast Watershed Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Tifton, GA 31793 USA (e-mail: david.bosch@ars.usda.gov).

P. J. Starks is with the Grazinglands Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, El Reno, OK 73036 USA (e-mail: patrick.starks@ars.usda.gov).

D. C. Goodrich is with the Southwest Watershed Research Center, Agricultural Research Service, U.S. Department of Agriculture, Tucson, AZ 85719 USA (e-mail: dave.goodrich@ars.usda.gov).

M. S. Seyfried is with the Northwest Watershed Research Center, Agricultural Research Service, U.S. Department of Agriculture, Boise, ID 83712 USA (e-mail: mark.seyfried@ars.usda.gov).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/JSTARS.2016.2569998

(CONUS). The presence of error in reference soil moisture values obtained from ground measurements complicates efforts to validate satellite-based retrievals. Even sites equipped with a dense observing network can suffer from spatial representativeness error due to suboptimal spatial coverage and/or spatial aggregation functions, etc. This challenge is especially acute when utilizing sparse ground sites and attempting to represent true footprint-scale soil moisture using only a single point-scale observation. Left uncorrected, such upscaling errors will spuriously inflate retrieval error estimates obtained via comparison against sparse ground-based observations [10].

In response to this challenge, triple collocation (TC) [11] techniques have been proposed to estimate true satellite product root-mean-squared-error (RMSE) from ground-based point observations via correction of the spatial representativeness error in the *in situ* data [12]. Likewise, the recent development of so-called extended triple collocation (ETC) techniques [13], [14] also demonstrates the possibility of obtaining unbiased estimates of correlation coefficients between satellite retrievals and the true (but unknown) footprint value. Such correlation-based approaches overcome ambiguities commonly noted in the application of TC to estimate RMSE [15]. In addition to providing validation information for satellite retrievals, TC and ETC can also be potentially used to assess the spatial representativeness of the *in situ* observations relative to the true average conditions within the satellite footprint.

This paper seeks to expand upon [12] by establishing a stronger theoretical basis for the application of TC to obtain soil moisture validation metrics corrected for the impact of spatial representativeness errors on sparse ground-based observations. In this way, we hope to ensure the credible application of TC as a statistical tool for validating SMAP soil moisture products utilizing observations obtained from sparse networks. A secondary goal is evaluating the accuracy of benchmark footprint-average soil moisture time series obtained from selected SMAP core validation sites as well as the spatial representativeness of the point-scale sparse network sites to be used in SMAP validation.

This paper is organized as follows. Section II describes the TC and ETC approaches and clarifies untested assumptions underlying earlier TC-based upscaling work presented in [12]. It also describes the potential range of anomaly preprocessing methods required by a TC analysis. Section III describes the various *in situ*, remote sensing, and model-derived surface soil moisture data products used in our analysis. Section IV presents a verification of the proposed TC strategy at a subset of SMAP core validation sites, and Section V evaluates the potential application of TC at SMAP sparse network sites. Guided by TC verification results in Sections IV and V, Section VI describes a specific strategy for utilizing sparse network measurements for SMAP soil moisture validation and presents a preliminary assessment of the SMAP Level 2 Soil Moisture (Passive, L2SMP) beta release product.

II. METHODOLOGY

A. Classic TC

TC was originally designed to obtain the calibration constants against a chosen reference dataset [11]. It is based on the availability of three collocated, independent measurement systems (X_i, X_j, and X_k) which describe the same geophysical variable, each of which is related to the unknown true quantity in the linear form

$$X_i = \beta_i + \alpha_i T + \varepsilon_i \tag{1}$$

where T is the unknown truth; β_i and α_i are the additive and multiplicative bias terms, and ε_i is the mean-zero random error. Similarly, the calibration constants α_j, β_j, α_k, β_k and error terms ε_j, ε_k are defined for X_j and X_k.

In addition to the assumed linear model between measurement systems and the true soil moisture signal in (1), the following underlying assumptions are required for the collocation technique [14]–[16]: 1) zero error cross-correlation, 2) zero correlation between errors and the true signal, and 3) stationary of signal and error statistics. In reality, the three soil moisture products often represent different soil depths and/or spatial scales and present varying dynamic ranges and climatologies as impacted by physical processes of different spatio-temporal scales and instrumental characteristics [17], [18]. In addition, temporal variations in α and β can result in nonlinearities between the products and/or nonzero error cross-correlation (for further discussion, refer to [14] and [19]).

To minimize this possibility, soil moisture products are often first transformed into anomaly time-series relative to some baseline mean prior to the application of TC. Any soil moisture product can be decomposed into its mean ($\bar{X}_i$) and anomaly (X_i') components where

$$X_i = \bar{X}_i + X_i' \tag{2}$$

(similar for X_j, X_k, and T). Here $\bar{X}_i$ is not limited to a single value of arithmetic mean—instead it can also be defined as either a climatology for each day-of-year or a time-series of moving-window average (see Section II-D). Combining (1) and (2), the anomaly of X_i can be expressed as

$$X_i' = \alpha_i\, T' + \varepsilon_i, \tag{3}$$

where T' is the anomaly of the (unknown) truth, and similar expressions apply for ${X_j}'$ and ${X_k}'$.

Following [11] and taking X_i as the reference dataset, the relative magnitude of calibration constants for X_j and X_k (versus X_i) can be derived from the covariances of anomalies

$$\begin{cases} \alpha_j = \alpha_i \dfrac{\langle X_j' X_k' \rangle}{\langle X_i' X_k' \rangle} = \alpha_i c_j \\ \alpha_k = \alpha_i \dfrac{\langle X_j' X_k' \rangle}{\langle X_i' X_j' \rangle} = \alpha_i c_k \end{cases} \tag{4}$$

where the brackets indicate time averaging and

$$c_j = \frac{\langle X_j' X_k' \rangle}{\langle X_i' X_k' \rangle}, \quad c_k = \frac{\langle X_j' X_k' \rangle}{\langle X_i' X_j' \rangle}.$$

It is now possible to estimate the variances of ε_i, ε_j, ε_k by eliminating T', α_i, α_j, α_k from (3). First, the two nonreference datasets are scaled to the reference dataset using the scaling constants in (4)

$$\begin{cases} X_i^* = X_i' = \alpha_i\, T' + \varepsilon_i^* \\ X_j^* = \dfrac{1}{c_j} X_j' = \alpha_i\, T' + \varepsilon_j^* \\ X_k^* = \dfrac{1}{c_k} X_k' = \alpha_i\, T' + \varepsilon_k^*. \end{cases} \tag{5}$$

Next the error variances of the scaled datasets, expressed in the reference space of X_i, are estimated as

$$\begin{cases} \sigma^2_{\varepsilon_i^*} = \langle \left(X_i^* - X_j^*\right)\left(X_i^* - X_k^*\right)\rangle \\ \sigma^2_{\varepsilon_j^*} = \langle \left(X_j^* - X_i^*\right)\left(X_j^* - X_k^*\right)\rangle \\ \sigma^2_{\varepsilon_k^*} = \langle \left(X_k^* - X_i^*\right)\left(X_k^* - X_j^*\right)\rangle . \end{cases} \tag{6}$$

The absolute random error variances of X_i, X_j, and X_k anomalies can then be expressed as $\sigma^2_{\varepsilon_i} = \sigma^2_{\varepsilon_i^*}$, $\sigma^2_{\varepsilon_j} = c_j^2 \sigma^2_{\varepsilon_j^*}$, and $\sigma^2_{\varepsilon_k} = c_k^2 \sigma^2_{\varepsilon_k^*}$.

Note that these error variances are anomaly based, which—in the case of soil moisture—is sensitive to the ability of the products to capture individual wet/dry events or episodes (depending on the exact definition of "mean" and "anomaly"—see Section II-D) rather than the absolute biases of the raw time series.

B. *Correcting Soil Moisture RMSE Acquired Using Point-Scale Observations*

In order to evaluate remotely sensed soil moisture retrievals resolved at satellite footprint scales (X_{RS}) with ground-based soil moisture observations acquired at a point scale (X_{pt}), Miralles *et al.* [12] proposed applying TC to correct for the upscaling error of X_{pt} contained in the mean-squared-difference (MSD) between X_{RS} and X_{pt}, and therefore obtain the MSD between X_{RS} and the true footprint-scale state (T). Taking the square-root of this corrected MSD potentially recovers the true RMSE of the satellite product.

The difference between the anomalies of X_{RS} and X_{pt} can be expressed as

$$X'_{\mathrm{RS}} - X'_{\mathrm{pt}} = \left(X'_{\mathrm{RS}} - T'\right) + \left(T' - X'_{\mathrm{pt}}\right) \tag{7}$$

where the single quotation mark indicates an anomaly time series. Assuming $\varepsilon_{\mathrm{RS}}\varepsilon_{\mathrm{pt}} = 0$, (7) can be rewritten in terms of MSD

$$MSD(X'_{\mathrm{RS}}, X'_{\mathrm{pt}}) = MSD\left(X'_{\mathrm{RS}}, T'\right) + MSD\left(X'_{\mathrm{pt}}, T'\right). \tag{8}$$

By inserting (3) into (8), $MSD(X'_{\mathrm{RS}}, X'_{\mathrm{pt}})$ can then be expanded as follows:

$$MSD\ \left(X'_{\mathrm{RS}}, X'_{\mathrm{pt}}\right) = \sigma^2_{\varepsilon_{\mathrm{pt}}} + \sigma^2_{\varepsilon_{\mathrm{RS}}} + \left(\alpha_{\mathrm{pt}} - \alpha_{\mathrm{RS}}\right)^2 \sigma_T^2 \tag{9}$$

where $\sigma^2_{\varepsilon_{\mathrm{pt}}}$ and $\sigma^2_{\varepsilon_{RS}}$ are the random error variances in point ground observations and remote sensing retrievals relative to the footprint-scale truth, and σ_T^2 is the temporal variance of this unknown truth, respectively.

$MSD(X'_{\mathrm{RS}}, X'_{\mathrm{pt}})$ in (9) represents the quantity that can be directly sampled via the comparison of satellite retrievals and point-scale observations. In contrast, the MSD between the remote sensing retrievals and true footprint-scale soil moisture (i.e., the ultimate target metric of SMAP validation activities) can be written as follows:

$$MSD\ \left(X'_{\mathrm{RS}}, T'\right) = \sigma^2_{\varepsilon_{\mathrm{RS}}} + \left(1 - \alpha_{\mathrm{RS}}\right)^2 \sigma_T^2. \tag{10}$$

The challenge is thus transforming the *available* quantity in (9) to conform to the *validation goal* represented by (10).

The basis of [12] is that $\sigma^2_{\varepsilon_{\mathrm{pt}}}$ can be estimated via (6) by utilizing soil moisture time series estimates derived from: 1) a land surface model (LSM), 2) a remote sensing product, and 3) a single point-scale ground observation site. This estimation of $\sigma^2_{\varepsilon_{\mathrm{pt}}}$ can be subtracted from (9) in order to replicate the random error component of (10). However, TC only provides information regarding the *relative* ratio between α for various measurement systems—see (4) above—and therefore no means for estimating absolute values of α. As a result, TC cannot directly estimate the relative difference between the $(1 - \alpha_{\mathrm{RS}})^2 \sigma_T^2$ term in (10) and the $(\alpha_{\mathrm{pt}} - \alpha_{\mathrm{RS}})^2 \sigma_T^2$ term in (9).

The approach in [12] side-steps this issue by using a sparse, point-scale observation as the reference dataset and implicitly assuming $\alpha_{\mathrm{pt}} = 1$. However, this (untested) assumption must be verified before any TC-based MSD (and RMSE) correction can be applied with confidence during SMAP validation activities. See Section V-A for a more detailed discussion.

C. *Extended Triple Collocation*

As noted above, uncertainty regarding the absolute values of α in (1) leads to ambiguity in the application of TC to correct MSD-based evaluation metrics. However, this ambiguity can be avoided via the use of TC to estimate correlation-based evaluations metrics. In particular, McColl *et al.* [13] introduced the ETC approach by which the correlation between any of the three independent products and the unknown truth can be resolved. When both $\varepsilon_i, T = 0$ and $\varepsilon_i, \varepsilon_j = 0$ are satisfied, the covariance between two datasets (X_i, X_j) can be written as

$$\sigma_{\mathrm{ij}} = \begin{cases} \alpha_i \alpha_j \sigma_T^2, & \text{for i} \neq \text{j} \\ \alpha_i^2 \sigma_T^2 + \sigma^2_{\varepsilon_i}, & \text{for i} = \text{j} \end{cases} \tag{11}$$

where α is defined as in (1), and σ_T^2 is the variance of true state T. Then, the error variance can be estimated as

$$\sigma^2_{\varepsilon_i} = \sigma_i^2 - \frac{\sigma_{\mathrm{ij}}\sigma_{\mathrm{ik}}}{\sigma_{\mathrm{jk}}} \tag{12}$$

where σ_i^2 is the variance of X_i. Note that (12) is equivalent to (6) for the reference dataset when calculated with anomalies. Therefore, the simple form of (12) can be used to obtain the same TC error variance from (4) to (6) without the need to designate a reference dataset and compute calibration constants. The relationship between the ordinary least-squares slope α_i and the correlation between X_i and the true state (ρ_{T,X_i}) can be expressed as

$$\alpha_i = \rho_{T,X_i} \frac{\sigma_i}{\sigma_t}. \tag{13}$$

Combining (11–13), ρ_{T,X_i} can be obtained via

$$\rho_{T,X_i} = \pm \sqrt{\frac{\sigma_{\mathrm{ij}}\sigma_{\mathrm{ik}}}{\sigma_i^2 \sigma_{\mathrm{jk}}}}. \tag{14}$$

In practice, the sign ambiguity in (14) is resolved by assuring positive correlation between the measurement systems and the true state using the pretest procedure described below.

Prior to the calculation of ρ_{T,X_i}, a pre-test must be conducted to confirm: 1) positive correlation exists between any two of the three anomaly time series and 2) calculated error variances (e.g., $\sigma^2_{\varepsilon_i}$) are real, positive numbers. Datasets that fail this test are deemed unqualified and masked from the ETC analysis. Note that the ρ_{T,X_i} metric in (14) is essentially complementary to the fractional RMSE metric proposed in [15] in the way that the squared sum of both metrics equals unity. However, the correlation metric is preferred here because it has been widely used in validation studies (see e.g., [6], [7] and [20]) and is (arguably) more straightforward to interpret.

If applied to a triplet of ground-based, model-based, and satellite-based soil moisture retrievals, (14) can be used to adjust correlations sampled from sparse point sites for the impact of spatial representativeness errors. Furthermore, unlike the earlier MSD-based analysis in [12], such a correlation-based analysis does not require any assumption regarding α.

D. Definition of Anomalies

Soil moisture inputs for TC analysis are typically time-series anomalies that represent deviation from some predefined "mean" condition. However, the exact definition of this condition can affect the accuracy and interpretation of TC results. Commonly used definitions in the TC literature fall in three categories: 1) a long-term arithmetic average, 2) a long-term seasonal climatology, and 3) a moving window average. The details of anomaly calculation approaches based on these three definitions are discussed below.

1) Anomaly Against Arithmetic Mean: The straight-forward removal of a single, long-term arithmetic mean from the entire time series is the simplest method for the calculation of anomalies. However, this method fails to resolve nonstationarity due to (potentially varying) seasonality in multiple soil moisture products. As a result, past work has cautioned against its application in soil moisture TC studies [12], [15].

2) Anomaly Against Long-Term Seasonality: This approach is popular in TC soil moisture studies due to the fact that different measurement systems often present different soil moisture seasonalities [17], [18]. For example, long-term seasonality is calculated by averaging soil moisture estimates within 31-day windows centered on each day-of-year (DOY) across multiple years of a single dataset. Once obtained, this seasonal climatology can be subtracted from the original time series to obtain a time series of interannual and seasonal anomalies relative to a fixed climatology. Ideally, this approach requires at least 3 years of continuous historical data. For retrieval time-series containing large temporal gaps (e.g., due to long periods of frozen conditions), calculated seasonality for certain DOYs can contain large uncertainty.

3) Anomaly Against a Moving Window: Another possible approach is applying a high-pass filter by removing an average value sampled within a moving window. As such, the resulting anomalies reflect high-frequency variations relative to the mean condition of the chosen window length. The moving window length is often set to a monthly time scale (see e.g., [21]). Relative to the two climatologically based approaches described above, this technique has less stringent requirements regarding the historical length of data sets. However, when a period of anomalously dry or wet conditions persists at time scales exceeding the window length, this signal will be effectively filtered. Therefore, this approach runs the risk of neglecting potentially important temporal anomaly signals in a soil moisture time series.

The numeric values (and exact definitions) of α, β, and ε—as well as the interpretation of subsequent RMSE and correlation results—will vary depending on which mean/anomaly definition is adopted in a TC analysis. The sensitivity of soil moisture TC results to such definition will be discussed further in Section IV-A.

III. Data

A variety of data sources are exploited to provide the required remote sensing, land surface modeling, and ground-observing datasets for our TC analysis. Due to the relatively short data length of the SMAP data product, the analysis will first utilize existing longer term satellite datasets to evaluate TC as a viable soil moisture validation tool.

A. Soil Moisture Ocean Salinity (SMOS) Level 2 Soil Moisture

The SMOS satellite was launched in 2009 by the European Space Agency [22] and measures L-band microwave emission (1.400–1.427 GHz) with equatorial ascending/descending overpasses at 6 AM/PM local solar time and a 3-day revisit period at the equator. The SMOS Level 2 soil moisture user data product [23] used in this study includes retrievals from both ascending and descending overpasses acquired from version 5.01 (Jan. 12, 2010–Apr. 22, 2012) and 5.51 (Apr. 23, 2012–Dec. 31., 2014) of the SMOS soil moisture retrieval algorithm on an equal-area ISEA 4H9 15-km grid [24].

B. Advanced Scatterometers (ASCAT) Soil Moisture Product

The ASCAT onboard the Meteorological Operational (Met Op-A, MetOp-B) satellites [25] measure C-band (5.255 GHz) radar backscatter since 2006, with approximately 25-km spatial resolution and equatorial ascending/descending overpasses at 9:30 PM/AM local solar time and a revisit frequency of 1–2 days. ASCAT is sensitive to the soil moisture in the top 0–3 cm of soil layer. The soil moisture retrieval product utilized here is based on the change-detection algorithm developed by the Vienna University of Technology (Version 2.2 of the Water Retrieval Package 5) [26], [27]. Both ascending and descending retrievals for the period Jan. 1, 2010–Jun. 29, 2014 are used.

C. SMAP Level 2 Passive Soil Moisture

The standard SMAP L2SMP product is generated on a fixed EASE2 grid with a nominal 36-km grid size that is close to the resolution of the radiometer [28]. In order to minimize the spatial mismatch and the associated geolocation error between

TABLE I
SUMMARY OF THE SMAP CORE VALIDATION SITES/USDA-ARS EXPERIMENTAL WATERSHED SOIL MOISTURE NETWORKS

Watershed	Size (km^2)	Number of sensors	Climate	Annual rainfall (mm)	Topography	Land use
Little Washita, OK	610	20	Subhumid	750	Rolling	Range/wheat
Fort Cobb, OK	813	15	Subhumid	750	Rolling	Crop/range
Walnut Gulch, AZ	148	29	Semiarid	320	Rolling	Range
Little River, GA	334	28	Humid	1200	Flat	Row crop/forest
Reynolds Creek, ID	238	20	Semiarid	300	Mountainous	Range

the standard grid product and ground-based estimates (especially with the effective spatial support of the core validation sites, see Section III-E), a "validation grid" L2SMP product is also generated with a 36-km spatial resolution and a 3-km grid spacing [29]. For each core validation site, a particular validation grid cell is chosen which maximizes the correspondence with the spatial distribution of *in situ* measurement locations. In this way, the validation grid allows for greater flexibility in choosing the spatially appropriate grid-cells for the fixed ground validation sites.

Preliminary assessment is performed on the SMAP L2SMP beta release validation grid product (Mar. 31–Nov. 18, 2015, Composite Release Identifier, or CRID, T11880) baseline single channel algorithm (applied to vertical polarization brightness temperature). At present, only retrievals from the 6 AM descending passes are a standard product and applied in this analysis.

D. *LSM Soil Moisture Product*

The LSM data used here are the top-layer (0–5 cm) soil moisture output from the SMAP Nature Run, version 3 (NRv3). The NRv3 data were generated with an early version of the SMAP Level 4 Surface and Root Zone Soil Moisture (L4_SM) algorithm by the NASA Goddard Space Flight Center Global Modeling and Assimilation Office [30], which was applied in model-only configuration using a single ensemble member, without perturbations and without assimilation of SMAP observations. Surface meteorological forcing data come from the NASA GEOS-5 Forward Processing for Instrument Teams (FP-IT; GEOS-5.9.1, 0.5° resolution) product for the period 2001–2013 and from the GOES-5 Forward Processing (FP; GEOS-5.11–GEOS-5.13, 0.25° resolution) product thereafter (https://gmao.gsfc.nasa.gov/products). Precipitation forcing is corrected with the NOAA Climate Prediction Center "Unified" ½ degree, global gauge-based product [31]. Land model parameters are based on [32] and [33]. Modeled soil moisture is output every 3 h on the global cylindrical 9-km EASE2 grid from Jan 1, 2001 to present.

E. *SMAP Core Validation Sites (CVS): USDA-ARS Research Watersheds*

Soil moisture monitoring networks in five long-term experimental watersheds operated by USDA-ARS have been designated core soil moisture validation sites for the SMAP

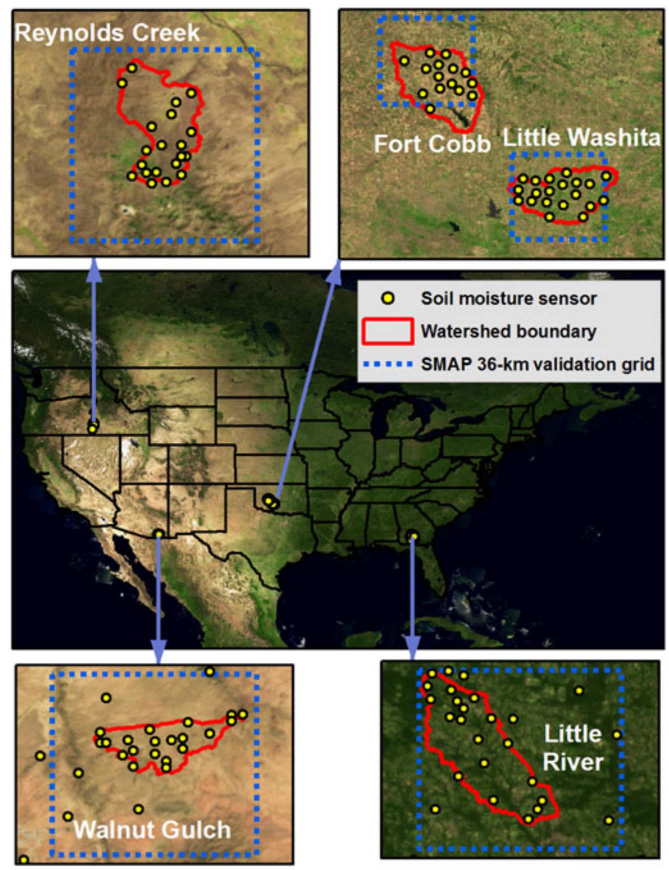

Fig. 1. Map of SMAP core validation sites located at five USDA-ARS experimental watersheds (solid red lines), their network sampling locations (yellow dots), and corresponding 36-km validation grid cells (dotted blue boxes).

mission: Walnut Gulch (WG), Little Washita (LW), Fort Cobb (FC), Little River (LR), and Reynolds Creek (RC) (see Table I) [2]. In each watershed, a representative sampling network of Stevens Hydra Probes has been used to produce reliable estimates of spatially averaged surface soil moisture at a 36-km SMAP grid product scale (referred to as "watershed average soil moisture" or WASM) using spatially weighted scaling functions that have been validated using gravimetric measurements acquired during intense field campaigns [33]–[35]. These sites have played important roles in the validation of existing remotely sensed surface soil moisture products [6], [7]. Locations of soil moisture sensors within these core sites and the corresponding validation grid boxes are shown in Fig. 1.

F. Sparse Networks

TC will primarily be applied to sparse ground-based observations of surface soil moisture acquired from the SCAN and CRN networks within the contiguous United States.

1) Soil Climate Analysis Network: The SCAN, established in 1999, is a cooperative continental-scale soil moisture and climate information system led by the USDA's Natural Resources Conservation Service [8]. Designed to focus on agricultural areas and represent the predominant climate regime, the network currently comprises over 200 stations nationwide. Each station collects hourly soil moisture data at 5, 10, 20, 50, and 100-cm (where possible) depths using a Hydra Probe dielectric constant measuring sensor.

2) Climate Reference Network: The U.S. CRN operated by NOAA was established in 2004 to provide science-quality, long-term air temperature, and precipitation measurements at over 100 locations. In 2011, the installation of triplicate soil moisture probes (Hydra Probe II) at five standard depths (5, 10, 20, 50, and 100 cm) was completed at each CONUS station. These sensors currently provide measurements at subhourly (15-min for most depths) intervals [9] that are averaged to generate an hourly soil moisture product.

G. Data Processing

To obtain the SMAP, SMOS, ASCAT, and NRv3 data for each sparse site, corresponding validation grid-cells are chosen from the global 3-km grid spacing cells based on two criteria: 1) they must contain perfectly nested 4×4 9-km EASE2 grid-cells; and 2) minimized distance between center of the grid-cell and the sparse ground site. The SMOS, ASCAT, and NRv3 data are then regridded at the selected validation grid pixels (for both core and sparse validation sites) by spatial averaging of nearest-neighbor pixels from their native grids. The model and *in situ* datasets are then matched separately to any of the remote sensing time-series with a minimal temporal offset, allowing no more than 2 h apart for a given retrieval for the 5-year analysis period (2010–2014).

IV. Application of TC at Core Validation Sites

Although our primary focus is the application of TC to observations obtained from sparse ground-based data networks, it is useful to start with the initial goal of utilizing TC to verify core site WASM values used as benchmark data for validating SMAP retrievals. Once verified in this way, WASM values can then be used as a source of verification for later analysis focused on the application of TC to sparse networks (see Section V). In addition, the core sites provide a well-controlled environment to examine the impact of various soil moisture mean/anomaly definitions described in Section II-D.

A. Assessment of WASM at Core Validation Sites

Using TC based on a triplet of: 1) WASM *in situ* measurements, 2) remotely sensed surface soil moisture retrievals, and 3) model-based surface soil moisture estimates, the variance of random errors contained in WASM anomalies can be obtained from (6). Fig. 2 plots estimated RMSE (i.e., the squared root of the error variance) obtained for WASM in this way. Note that this analysis is based on the use of WASM values as the scaling reference and the implicit assumption that WASM is perfectly calibrated (i.e., $\alpha_{\mathrm{WASM}} = 1$). This assumption is generally supported by past work comparing WASM values to independent gravimetric sampling performed during intensive field campaigns [34]–[36].

TC results are organized to reflect variations in the type of anomaly calculated (see Section II-D) and the particular datasets used to construct the soil moisture triplet. For the moving-window anomaly method, an empirical window length of 30 days is used. In addition, the following three triplets are applied: WASM-ASCAT-LSM, WASM-SMOS-LSM, and WASM-SMOS-ASCAT to calculate WASM RMSE via (6). As noted above, WASM is utilized as the TC scaling reference in all three cases. Plotted RMSE values in Fig. 2 should reflect the inherent accuracy of the WASM anomalies and therefore be independent of the particular combination of remote sensing (RS) and/or LSM products used to complete the soil moisture triplet. This is generally the case for Fig. 2(a) where anomalies are defined via the removal of a 30-day moving average. However, such consistency breaks down slightly for the case where anomalies are calculated via the removal of long-term seasonality [see Fig. 2(b)] and, for the most part, falls apart completely for the case of anomaly versus a single long-term mean [see Fig. 2(c)].

Anomaly time-series relative to a fixed long-term mean can result in violation of TC assumptions and consequently, invalid TC output (suggested by missing results for RC, WG, and LR in Fig. 2(c). When data products present different seasonality, removing a single (fixed) long-term mean does not eliminate their mutual systematic differences. Such systematic differences are then leaked into the ostensibly random error term ε in (3) which may result in the violation of assumptions underlying TC. This result, consistent with earlier advice presented in [12] and [15], suggests that low-frequency variability should be removed from soil moisture time series prior to the application of TC.

In Section II-D, two methods are described for removing such low-frequency variability, i.e., the subtraction of: 1) a fixed seasonal cycle or 2) a 30-day moving window average. Comparison of Fig. 2(a) and (b) suggests that the 30-day moving average approach leads to a more robust TC analysis. This may be due to the presence of longer scale variability in the seasonal anomaly time-series and the tendency of such variability to increase sampling errors (relative to the moving window case where such variability is explicitly filtered). Therefore, the use of soil moisture anomalies obtained via the subtraction of a 30-day moving window average is recommended and all TC results presented below are based on anomalies calculated in this way. However, it should be stressed that such high-pass filtering will make TC blind to the presence of low-frequency errors in soil moisture estimates.

Assuming that WASM is calibrated to the true domain average (i.e., $\alpha_{\mathrm{WASM}} = 1$), the values plotted in Fig. 2 can be taken to represent the absolute RMSE of WASM anomalies (given the various ways in which these anomalies are defined). It is worth noting that WASM RMSE values plotted in Fig. 2(a) (based on

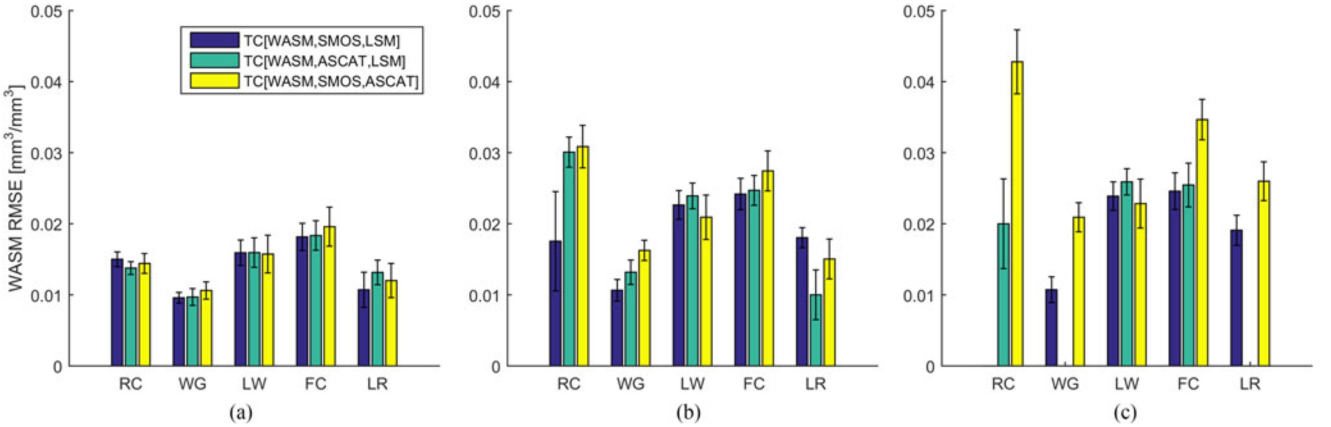

Fig. 2. Using different combinations of passive (SMOS), active (ASCAT) satellite retrievals and LSM data at the five SMAP core validation sites in Fig. 1, TC-based RMSE estimates of WASM anomalies calculated relative to: (a) a 30-day moving average; (b) a long-term seasonal climatology, and (c) a single long-term mean. Error bars show 95% confidence intervals obtained from a 1000-member bootstrapping analysis.

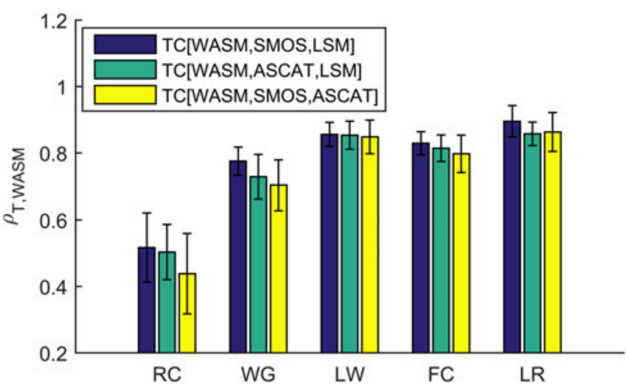

Fig. 3. Comparison of the TC-derived correlation between anomalies of WASM and footprint truth based on different combinations of passive (SMOS), active (ASCAT) satellite retrievals and modeling data acquired at the five SMAP core validation sites shown in Fig. 1. Error bars show 95% confidence intervals obtained from a 1000-member bootstrapping analysis.

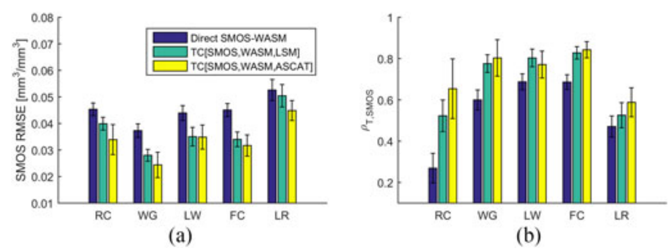

Fig. 4. (a) SMOS retrieval error (RMSE) estimated via both TC (based on two sets of triplets) and direct comparison with WASM; (b) same as (a) but for the correlation coefficient. Anomalies are used in both TC and direct correlation calculations. Error bars show 95% confidence intervals obtained from a 1000-member bootstrapping analysis.

the removal of a 30-day moving average window) agree well with earlier assessments of WASM by comparison with dense gravimetric sampling results obtained during short-term field experiments [34]–[36].

Using the TC-based approach shown in (14), $\rho_{T,\mathrm{WASM}}$ is estimated using the same data triplets as in Fig. 2 with anomalies calculated relative to a 30-day moving average (see Fig. 3). The natural variation in the dynamic range and variability in surface soil moisture across different geophysical locations or regions are likely to complicate the cross-comparison of estimated RMSE values [37] (e.g., note the—due to overall relatively low soil moisture at the site—very low RMSE value obtained at WG site [see Fig. 2(a)] versus the corresponding relatively low correlation in Fig. 3). In contrast, the correlation metric is also sensitive to the calibration constant (α_i) and true variability (σ_T^2) in addition to error variance ($\sigma_{\varepsilon_i}^2$)—see (13)—and therefore provides information about the unbiased signal-to-noise ratio that can be fairly compared across space [13]. The WASM obtained at five ARS watersheds present overall strong correlation with the truth (all above 0.70 except RC) and are relatively insensitive to the choice of SMOS, ASCAT, or NRv3 data to complete the TC triplet.

The relatively low $\rho_{T,\mathrm{WASM}}$ value found at the RC site (see Fig. 3) likely reflects the increased difficulty of establishing a representative network for a domain consisting of complex terrain and uneven rainfall distribution. Therefore, a TC-derived $\rho_{T,\mathrm{WASM}}$ metric can be a complementary option to the absolute accuracy metrics in core site network assessment and potentially be used to guide the adjustment of scaling functions used to acquire WASM based on distributed observations within a soil moisture network.

B. Validation of Satellite Retrievals Over Core Sites

The validation of satellite soil moisture retrievals at core validation sites can also be supplemented with TC analysis (see Fig. 4). TC has the advantage of not having to assume that WASM is free from random errors—thus providing a truly unbiased assessment of the satellite product being evaluated. This is particularly useful for newer or complex core sites like RC where there is considerable uncertainty in WASM due to challenges such as complex topography or high land surface variability.

SMOS RMSE (based on 30-day anomalies, same for WASM) derived by direct comparison with WASM is shown to be consistently larger than the RMSE relative to truth derived from

TC using either a SMOS-WASM-LSM or a SMOS-WASM-ASCAT soil moisture triplet [see Fig. 4(a)]. Likewise, results in Fig. 4(b) show direct SMOS-WASM correlation has a negative bias relative to $\rho_{T,\mathrm{SMOS}}$ obtained via the application of TC to the same triplets.

However, cross-correlated error between data products is known to cause a negative bias in TC-estimated random error variance [15], [38]. As seen in Fig. 4, generally lower error (and higher correlation) estimates are acquired using a SMOS-WASM-ASCAT triplet versus a SMOS-WASM-LSM triplet. This suggests that the error correlation between passive (SMOS) and active (ASCAT) satellite soil moisture products is non-negligible (also see [38]). Left uncorrected, such error correlation will result in an overly optimistic TC assessment of SMOS retrieval accuracy. Therefore, caution is recommended when applying TC to a triplet that includes both active and passive remote sensing products. Instead, applying TC to a triplet consisting of satellite-, ground-, and LSM-based products (e.g., SMOS-WASM-LSM) appears to be a more robust choice.

V. Application of TC at Sparse Network Sites

In contrast to WASM values obtained via averaging of multiple ground-based observations sites, the reliability of validation metrics for satellite retrievals calculated via comparisons against a single point-scale, ground observation time series is highly questionable. Here, we will examine the application of TC tools to enhance the validation of satellite-based surface soil moisture products from sparse ground networks. In this set of results, WASM-based validation metrics obtained from core validation sites will be used solely as a source of verification information for TC-based estimates derived from individual sensors within each core site. In this way, the core sites can be subsampled to simulate the spatial sampling characteristics of a sparse network. Once verified, TC can then be applied with confidence to actual sparse soil moisture networks.

A. Distribution of α_{pt}

An important initial issue is defining which type of validation metric will serve as the target of the TC analysis. TC can potentially be applied to estimate both RMSE and correlation-type validation information. However, as discussed in Section II-B, the total RMSE of satellite retrievals (versus footprint-scale truth) cannot be directly estimated unless the sparse *in situ* time series is perfectly calibrated (i.e., $\alpha = 1$).

Utilizing WASM time-series from the core sites, the distribution of α_{pt} for individual sensors within each core site can be obtained by applying the ordinary least squares method to solve the equation $X_{pt} = \alpha_{pt} \cdot X_{\mathrm{WASM}} + \beta$. These distributions are plotted in Fig. 5. The range of linear scaling factors between individual soil moisture measurement sites and WASM suggests that α_{pt} typically deviates from unity and the deviation can sometimes be large, with the largest deviations found for the semiarid WG watershed. Extrapolating this result suggests that sparse network observations cannot generally be assumed to offer a well-calibrated representation of (the unknown) satellite footprint-scale true soil moisture. Instead, natural inhomogeneity in soil texture, land cover, topography, and microclimate will all contribute to subfootprint-scale variability in α_{pt}.

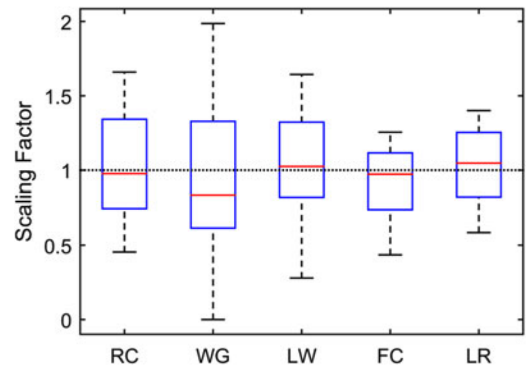

Fig. 5. Distribution of scaling factor (α_{pt} as in $X_{pt} = \alpha_{pt} \cdot X_{\mathrm{WASM}} + \beta + \varepsilon$) of point measurements (X_{pt}) and watershed average (WASM) at the five SMAP core validation sites shown in Fig. 1.

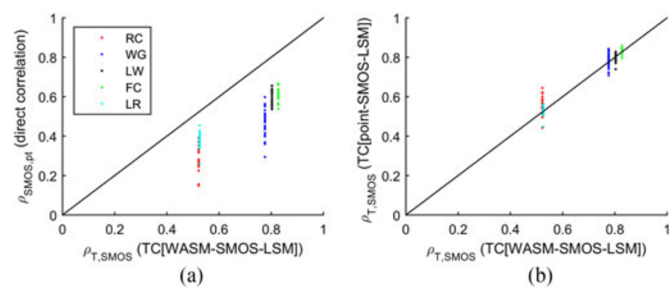

Fig. 6. (a) Direct correlation between anomalies of SMOS retrieval and point observations ($\rho_{SMOS,\mathrm{pt}}$) versus $\rho_{T,SMOS}$ derived via TC [WASM-SMOS-LSM]; (b) $\rho_{T,SMOS}$ derived via TC [point-SMOS-LSM] versus $\rho_{T,SMOS}$ derived via TC [WASM-SMOS-LSM].

As a result, the implicit assumption of $\alpha_{pt} = 1$ underlying the TC-based correction of RMSE does not generally hold. This, in turn, implies that the credible application of TC relies instead on the correction of alternative metrics which are insensitive to calibration, such as the correlation coefficient obtained via the ETC approach summarized in (14).

B. Verification of $\rho_{T,\mathrm{RS}}$ Within Core Sites

In contrast to RMSE, the satellite-truth correlation ($\rho_{T,\mathrm{RS}}$) can be acquired from the TC-based approach in (14) without need for any assumption regarding the absolute values of calibration constants in (1). Here, the evaluation of TC-based $\rho_{T,\mathrm{RS}}$ estimates over core sites provides a valuable verification for the eventual application of TC over sparse networks. TC-based estimates of $\rho_{T,\mathrm{RS}}$ are acquired from a collocated WASM-RS-LSM triplet (where RS represents either SMOS or ASCAT) [see Fig. 4(b)], which can be assumed to provide the best possible estimate of $\rho_{T,\mathrm{RS}}$ available at each core site. These reference values [plotted along the *x*-axis of Fig. 6(a) and (b)] are then compared to correlations calculated using *only a single measurement site* [plotted along the *y*-axis of Fig. 6(a) and (b)] to simulate typical data availability for the sparse network case.

Fig. 6 illustrates that biased estimates of $\rho_{T,\mathrm{RS}}$ are obtained when directly sampling the correlation coefficient between the anomaly time series of SMOS retrievals and a single measurement site [i.e., $\rho_{\mathrm{SMOS,pt}}$ in Fig. 6(a)]. That is, because of spatial representativeness error in point-scale soil moisture observations, $\rho_{\mathrm{SMOS,pt}}$ values are biased low relative to the TC-based reference $\rho_{T,\mathrm{RS}}$ values calculated using a WASM-RS-LSM triplet. In addition, spurious spread is introduced into $\rho_{T,\mathrm{RS}}$ estimates—reflecting site-to-site variations in footprint representativeness. However, when $\rho_{T,\mathrm{SMOS}}$ is instead estimated via TC by utilizing (14) and a point-RS-LSM triplet (as opposed to the WASM-RS-LSM triplet which serves as a reference), this bias and the spread are both significantly reduced and estimates at individual locations fall much closer to reference correlation values [see Fig. 6(b)].

Therefore, TC provides a viable means to effectively upscale the correlation metric calculated using single-point ground observations to accurately reflect benchmark correlation result obtained using a WASM time series acquired from a very dense array of ground-based soil moisture observations. As such, the verification shown in Fig. 6(b) implies that the statistical assumptions underlying the application of ETC (using a point-RS-LSM triplet) are generally valid and provides confidence for the application of ETC to SMAP soil moisture validation at sparse network sites.

C. Assessment of Sparse Network Sites

Analogous to its application in evaluating WASM of core validation sites (see e.g., Figs. 2 and 3), TC can also be utilized to determine the reliability of individual sparse site observations in terms of their spatial representativeness over satellite footprint scales. To this end, a retrospective sparse site assessment was carried out (utilizing *in situ*, SMOS and NRv3 data from January 12, 2010 to December 31, 2014) to determine the sparse network sites' reliability at the SMAP 36-km footprint scale. The correlation between point and footprint truth ($\rho_{T,\mathrm{pt}}$) is adopted as the primary metric that determines the fraction of footprint-scale soil moisture dynamics captured by point-scale observations at individual SCAN and CRN sites (see Fig. 7). Away from the core sites, no independent reference data are available to evaluate such estimates. However, TC-based estimates of $\rho_{T,\mathrm{pt}}$ are generally consistent, regardless of which remotely sensing product (SMOS or ASCAT) is utilized in the TC triple. This robustness provides some confidence that the error independence assumptions underlying the TC approach are respected. Note the relative closeness of average $\rho_{T,\mathrm{pt}}$ values obtained from SMOS-based and ASCAT-based triplets—at 0.67 $(\mathrm{median} = 0.70)$ and 0.61 $(\mathrm{median} = 0.65)$—respectively.

Based on Fig. 7, an arbitrary threshold of 0.70 [-] for $\rho_{T,\mathrm{pt}}$ is set to qualitatively classify the site reliability at 36-km spatial scale for the validation of SMAP L2SMP product. This threshold is equivalent to a signal-to-noise ratio of one [14], [36]. This reliability metric is sensitive to both the local performance of the ground-based sensor and the ability of the ground-based sampling point to represent a larger spatial area. That is, it reflects the joint impact of both instrumental and spatial representativeness errors in sparse ground-based observations.

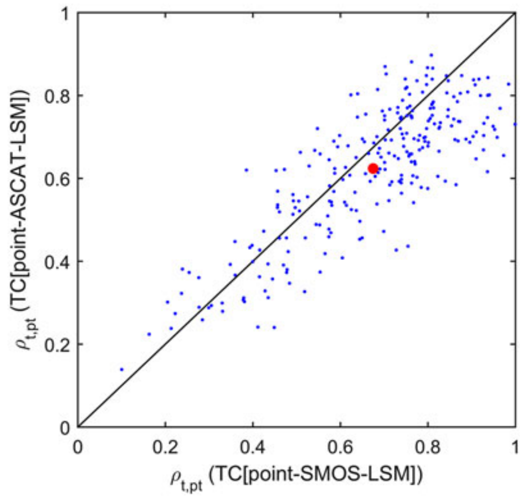

Fig. 7. TC-based estimates of $\rho_{T,pt}$ for CRN and SCAN sites obtained using point-SMOS-LSM (*x*-axis) and point-ASCAT-LSM (*y*-axis) triplets. Data points for individual sites are shown in blue and the mean value is shown in red.

Fig. 8. Distribution of $\rho_{T,pt}$ values obtained at CONUS SCAN and CRN sites. Locations where $\rho_{T,pt}$ values $\geq$ 0.70 are classified as "reliable" sites.

Based on TC [point-SMOS-LSM] analysis (note that SMOS and LSM are both re-sampled to the SMAP 36-km validation grid) using data from 2010 to 2014, a map of CONUS CRN and SCAN site $\rho_{T,\mathrm{pt}}$ metric is shown in Fig. 8. Examination of the site reliability versus land cover type (see Table II) suggests that sparse sites within pixels containing large water body or dense vegetation (i.e., forests) are generally less successful at capturing footprint-scale temporal variability than sites within lower biomass pixels. However, this result remains somewhat speculative as other factors like topography and soil texture also contribute to subfootprint-scale heterogeneity and upscaling error within point-scale observations. Additional research will be required to better link results in Fig. 8 to land surface conditions.

It should be noted that the filtering of "unreliable" sparse network sites is likely to result in the over-representation of relatively homogeneous pixels in the validation process, simply because footprint representativeness (i.e., "reliability") of sparse sites is naturally better in homogeneous pixels. This might then lead to an overestimation of the skill of the satellite

TABLE II
SUMMARY OF SCAN/CRN SITE RELIABILITY WITH RESPECT TO DOMINANT INTERNATIONAL GEOSPHERE-BIOSPHERE PROGRAMME LAND COVER TYPE

IGBP land cover	Reliable	Unreliable
Water	4	11
Evergreen Needleleaf Forest	3	4
Evergreen Broadleaf Forest	0	8
Deciduous Broadleaf Forest	6	4
Mixed Forests	11	10
Open Shrublands	11	20
Woody Savannas	14	7
Grasslands	45	49
Croplands	35	12
Urban and Built-Up	0	1
Cropland/Natural Vegetation Mosaic	29	8
Barren or Sparsely Vegetated	2	2

See Fig. 8 for a map of site reliability.

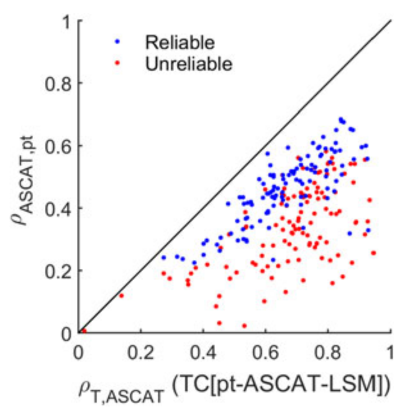

Fig. 9. Comparison of direct ASCAT-point correlation and TC-derived correlation between ASCAT and 36-km footprint truth. Site reliability matches that shown in Fig. 8, which was derived using SMOS (not ASCAT) soil moisture retrievals.

retrievals, which tend to perform better in areas lacking strong subfootprint-scale heterogeneity (note that the reliability metric is largely independent of the skill of the satellite retrievals used in the TC triplet). However, the classification of sparse site reliability is justified by the need to fairly evaluate satellite retrievals at sites where the validation data are reasonably representative of the footprint average condition.

D. Validation of Remote Sensing Retrievals at Sparse Site

Given the results presented in Figs. 6 and 7, TC is shown to be able to de-bias $\rho_{T,\mathrm{RS}}$ calculated using sparse site observations. Analogous to the eventual application to SMAP soil moisture validation, the TC-based correlation metrics for ASCAT ($\rho_{T,\mathrm{ASCAT}}$) retrievals during 2010–2014 are shown in Fig. 9. As seen in the core validation sites (see Fig. 6), estimates of $\rho_{T,\mathrm{RS}}$ via direct ASCAT-point correlations (i.e., $\rho_{\mathrm{ASCAT,pt}}$) are biased low relative to values of $\rho_{T,\mathrm{ASCAT}}$ obtained from TC applied to a point-ASCAT-LSM triplet. However, relatively smaller biases are found for sites classified as "reliable" (as determined from TC applied to a point-SMOS-LSM triplet). In other words, even in the absence of any TC-based correction, limiting the validation analysis to "reliable" sparse sites can provide less-biased estimates of $\rho_{T,\mathrm{RS}}$.

Note that the reliability classification of sites appears robust since it was based on SMOS and subsequently applied to ASCAT. Such robustness against variations in satellite products allows for the potential evaluation of SMAP retrievals using direct SMAP-point correlations sampled at reliable sparse sites which have been previously identified from a retrospective SMOS-based TC analysis. This is also potentially of great value during the early stage of calibration/validation activity when the satellite data record is too short to perform TC.

VI. TC APPLICATION TO SMAP SOIL MOISTURE SPARSE NETWORK VALIDATION

Results in Sections IV and V provide useful guidance for the eventual application of TC to enhance SMAP soil moisture validation using sparse networks. In particular, they suggest:

1) TC can be applied to reliably estimate the correlation metric between satellite retrievals and footprint truth using point measurements [see Fig. 6(b)]. On the other hand, using TC to correct for the point upscaling error in the RMSE-metric is potentially problematic (see discussion in Section II-B).
2) Using anomalies calculated from removal of 30-day moving average, consistent TC results are obtained from different combinations of datasets (see Figs. 2(a) and 3) and the obtained core site RMSE values agree well with results from previous field experiments. Therefore, this particular anomaly definition is preferable, although it eliminates sensitivity to slowly varying errors.
3) The simultaneous use of both active and passive satellite soil moisture products in a TC triplet does underestimate errors in the satellite products (see Fig. 4 and discussion in Section IV-B) which implies that active and passive microwave retrievals contain cross-correlated errors.

Based on these insights, a specific TC procedure for SMAP surface soil moisture assessment at a single site or a batch of sparse network sites is outlined below.

A. Retrospective Site Evaluation

The purpose of this procedure is to prepare sparse network data and ensure that its quality and availability are suitable for SMAP validation. The first step involves collecting, processing, and quality controlling (i.e., visual inspection) of historical soil moisture time series as well as relevant metadata. Next, the locations of the corresponding 36-km SMAP validation grid cells are defined for each sparse site, and historical satellite (e.g., SMOS) and LSM (e.g., NRv3) data (re-gridded to the 36-km SMAP grid) are extracted. Finally, the ETC approach in (14) is applied to a point-SMOS-NRv3 triplet of anomalies calculated from 30-day moving windows to determine site reliability at SMAP 36-km footprint scale based on the 0.70 threshold described in Section V-C.

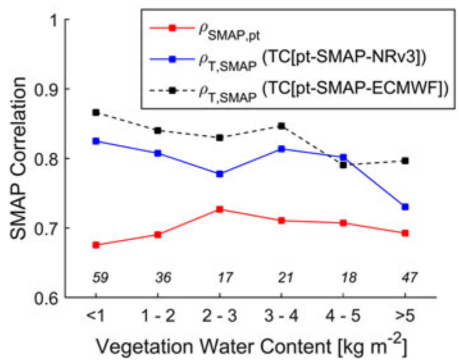

Fig. 10. Average anomaly correlation stratified by footprint vegetation water content between SMAP L2SMP (Mar. 31–Nov. 18, 2015) and 1) sparse point-scale observations (red); 2) 36-km footprint truth using a point-SMAP-NRv3 TC triplet (blue) and 3) same as 2) but using a point-SMAP-ECMWF TC triplet (black). Numbers of sites available within each VWC range are indicated above the *x*-axis.

B. Near-Real-Time SMAP L2SMP Validation

As new SMAP L2SMP retrievals become available, *in situ* and LSM data are extracted and matched-up with the retrievals, allowing a maximum of 2-h temporal offset. Anomaly time-series from 30-day moving windows are updated. Using a point-SMAP-LSM triplet, the TC-based correlation metric $\rho_{T,\mathrm{SMAP}}$ is then calculated using (14). Additional (non-TC-corrected) validation metrics such as RMSE, unbiased RMSE, bias, raw/anomaly correlation at each sparse site are also computed. Since sampling errors in TC estimates are expected to be large for short-term data sets, sparse network metrics are stratified by different conditions such as dominant land cover, vegetation water content, observed soil moisture range, and only averages of each stratification class are reported. Such averaging reduces the considerable sampling error in TC-based estimates resulting from short historical data records.

An example of one such preliminary assessment of the SMAP beta release L2SMP data is shown in Fig. 10 with a stratification based on vegetation water content (VWC)—an essential ancillary parameter for the SMAP baseline passive soil moisture retrieval algorithm [28]. The VWC estimates are available in the SMAP L2SMP data product and are derived from a climatology of the Normalized Vegetation Difference Index (NDVI), which was obtained from the Terra/MODIS MOD13A2 (Collection 5) product. The Level 1 SMAP accuracy goal (i.e., $0.04\,\mathrm{m}^3\cdot\mathrm{m}^{-3}$ RMSE after removal of the long-term mean bias) applies to land areas where VWC is no greater than $5\,\mathrm{kg}\cdot\mathrm{m}^{-2}$, which excludes most forest pixels. SMAP retrievals where VWC is greater than $5\,\mathrm{kg}\cdot\mathrm{m}^{-2}$ are flagged in the beta release; however, for diagnostic purposes we have included such data in this analysis. The L-band microwave signals penetrate better through less dense vegetation canopy, which should result in higher retrieval skill at low VWC conditions and *vice versa*. Results in Fig. 10 reflect averages of $\rho_{\mathrm{SMAP,pt}}$ and TC-based $\rho_{T,\mathrm{SMAP}}$ results acquired at individual CRN and SCAN sites and stratified by VWC. At each location, 30-day moving averages are first removed from each product, and the anomalies are subsequently binned according to the corresponding (daily) VWC values to calculate the correlation metrics.

Direct SMAP-*in situ* anomaly correlations ($\rho_{\mathrm{SMAP,pt}}$, in red) show a slightly decreasing trend as VWC increases above $2\,\mathrm{kg}\cdot\mathrm{m}^{-2}$ (see Fig. 10). However, in stark contrast to expectations, correlations in the VWC $\leq 2\,\mathrm{kg}\cdot\mathrm{m}^{-2}$ range are lower than those for the VWC $> 5\,\mathrm{kg}\cdot\mathrm{m}^{-2}$ case. The application of TC (i.e., $\rho_{T,\mathrm{SMAP}}$, in blue, using a point-SMAP-NRv3 triplet) produces a more reasonable (although still not completely monotonic) trend in correlation with increasing VWC. Therefore, TC-based correction of spatial representativeness errors produces correlation results that better reflect the expected relationship between vegetation canopy density and retrieval accuracy. In addition, as noted earlier, the application of TC results in a clear increase in correlation estimates relative to baseline $\rho_{\mathrm{SMAP,pt}}$ estimates which are spuriously degraded via the impact of spatial representativeness errors in the point-scale observations.

An area of potential concern for SMAP TC studies is that the GEOS-5 soil temperatures used in the L2SMP soil moisture retrieval algorithm are derived using a modeling system that overlaps significantly with the modeling system used to generate the NRv3 surface soil moisture product. In particular, GEOS-5 surface temperature fields are generated using more or less the same underlying LSM and the same GEOS-5 surface meteorological forcing as NRv3, except for the use of gauge-based precipitation observations in NRv3 (see Section III-D). This overlap opens up the possibility of some error cross-correlation in the SMAP and NRv3 soil moisture estimates utilized in our TC analysis. While these concerns are ameliorated by the fact that the GEOS-5 and NRv3 rainfall estimates are essentially independent, it is prudent to consider its potential impact on SMAP validation activities.

To directly examine this issue, NRv3 in the TC analysis for Fig. 10 was replaced by an alternative LSM soil moisture product—the 0.25° European Centre for Medium-Range Weather Forecast (ECMWF), which has been re-gridded to the SMAP EASE2 36-km grid. Due to the application of different modeling physics and unique land surface forcings, ECMWF-based soil moisture estimates should be relatively more independent with regard to GEOS-5 surface temperature-derived products. Nevertheless, ECMWF-based TC results (see Fig. 10, in black) present similar trends as the NRv3-based results with respect to VWC variations. However, slightly higher $\rho_{T,\mathrm{SMAP}}$ values obtained from the ECMWF-based triplet (relative to NRv3 results) suggests that small amounts of anticorrelation may persist between SMAP and NRv3 soil moisture errors. If left uncorrected, this could cause a slight underestimation of $\rho_{t,\mathrm{SMAP}}$ when applying TC using NRv3 soil moisture estimates. This potential issue will be monitored over the course of SMAP validation activities.

VII. Summary

In Section II, we reviewed the classic formulation of TC method and an upscaling strategy to obtain footprint-scale satellite product RMSE at point scale. A closer examination of the upscaling method demonstrates that TC can only solve for the impact of random representativeness errors in the point-scale data.

TC cannot correct RMSE estimates for the impact of systematic biases in sparse ground-based data. Since large additive [34], [35] and multiplicative biases (see Fig. 5) can occur in point-scale soil moisture observations (relative to a footprint-scale spatial average), it is not likely that standard TC approaches can ever fully correct RMSE-based evaluation metrics for the impact of point-to-footprint upscaling errors (as originally suggested by [12]). Fortunately, such biases do not impact correlation-based assessment of retrieval skill and the recent development of the ETC method [13] allows us to still obtain an unbiased estimation of the satellite-versus-truth correlation metric.

The robustness of the ETC-estimated correlation metric is tested and verified at five U.S. core validation sites (see Sections IV and V) in terms of the datasets and anomaly definitions used. The ETC approach provides a viable method for evaluating both the benchmark footprint-scale soil moisture values (i.e., WASM) derived from spatial aggregation of multiple observations within the core validation sites (see Fig. 3) and the reliability of point-scale sparse-site observations in representing footprint-scale soil moisture (see Figs. 7 and 8). More importantly, ETC provides a robust method for correcting estimates of correlation-based retrieval skill derived from only a single-point ground observation for the impact of point-to-footprint upscaling error (see Fig. 6).

The TC/ETC results presented here are based on soil moisture triplets derived from either: 1) ground-based observations, land surface modeling, and a single remote sensing product or 2) ground-based observations and two different remote sensing products. Due to the potential for introducing cross-correlated errors, the latter combination involving two satellite products (e.g., SMOS and ASCAT) should be used with caution (see Fig. 4). In addition, the robustness of TC results was maximized when applied to soil moisture anomalies defined as deviations from 30-day moving averages (see Fig. 2).

Based on the results presented in Sections IV and V, a procedure for retrospective sparse site evaluation and near-real-time SMAP validation is outlined in Section VI and an example of preliminary assessment of the SMAP Level 2 Passive Soil Moisture product (beta release) is presented in Fig. 10.

At the time of this writing, a total of six sparse networks consisting of over 400 ground observation locations across the globe have been included in the SMAP sparse network validation activities, and more networks are expected to join. Sparse network analysis has played an important supporting role in the preparation of SMAP L2SMP beta release [29] and the upcoming validated release. The diversity in land cover, soil, climate, and other properties represented by the sparse sites allows the examination of the influence of these factors. These results are currently being explored and may contribute to a better understanding of the performance SMAP under various surface conditions and facilitate ongoing soil moisture retrieval algorithm refinement.

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Fan Chen received the B.S. degree in physical geography from Peking University, Beijing, China, in 2001, and the Ph.D. degree in climatology from the University of North Carolina, Chapel Hill, NC, USA, in 2006.

Since 2008, she has been with Science Systems and Applications, Inc., and working as a Visiting Scientist at the Hydrology and Remote Sensing Laboratory, Agricultural Research Service of U.S. Department of Agriculture, Beltsville, Maryland, USA. Her research interests include methods of evaluating remotely sensed soil moisture retrievals and hydrologic modeling.

Wade T. Crow (M'03) received the Ph.D. degree in civil and environmental engineering from Princeton University, Princeton, NJ, USA, in 2001.

He is currently a Research Physical Scientist and Project Lead Scientist at the United States Department of Agriculture (USDA) Agricultural Research Service Hydrology and Remote Sensing Laboratory, Beltsville, MD. His research focuses on the development of hydrologic and agricultural applications for remote sensing data and the development of appropriate data assimilation approaches to facilitate this goal—with a special emphasis on techniques that fuse information from various disparate remote sensing sources. This work has led to extensive collaboration with operational USDA agencies involved in drought monitoring missions.

Dr. Crow has served (or currently serves) on the science teams for the NASA GPM, Hydros, SMAP, and AirMOSS missions, and was an editor for the *American Meteorological Society's Journal of Hydrometeorology.*

Andreas Colliander (S'04–A'06–M'07–SM'08) received the M.Sc. (Tech.), Lic.Sc. (Tech.), and D.Sc. (Tech.) degrees in electrical engineering from the Helsinki University of Technology (TKK; now Aalto University), Espoo, Finland, in 2002, 2005, and 2007, respectively.

He is currently a Research Scientist with the Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA. He is a member of the Science Algorithm Development Team for the Soil Moisture Active and Passive mission focusing on calibration and validation of the geophysical products.

Michael H. Cosh (M'02) received the Ph.D. degree in civil and environmental engineering from Cornell University, Ithaca, NY, USA, in 2002.

He is a Research Hydrologist with the U.S. Department of Agriculture, Agricultural Research Service, Hydrology and Remote Sensing Laboratory, Beltsville, MD, USA. His research interest includes the monitoring of soil moisture from both *in situ* resources and satellite products.

Dr. Cosh is serving as the Acting Research Leader for the Hydrology and Remote Sensing Laboratory, which includes 12 scientists working in areas of soil moisture remote sensing, evapotranspiration, and water quality. He has served as the Chairperson of both the Remote Sensing Technical Committee and the Large Scale Field Experiments Technical Committee for the American Geophysical Union.

Thomas J. Jackson (SM'96–F'02) received the Ph.D. degree in civil engineering from the University of Maryland, College Park, MD, USA, in 1976.

He is a Research Hydrologist with the U.S. Department of Agriculture, Agricultural Research Service, Hydrology and Remote Sensing Laboratory, Beltsville, MD, USA. His research interests include the application and development of remote sensing technology in hydrology and agriculture, primarily microwave measurement of soil moisture.

Dr. Jackson is or has been a member of the science and validation teams of the Aqua, ADEOS-II, Radarsat, Oceansat-1, Envisat, ALOS, SMOS, Aquarius, GCOM-W, and SMAP remote sensing satellites. He is a Fellow the Society of Photo-Optical Instrumentation Engineers, the American Meteorological Society, and the American Geophysical Union. In 2003, he received the William T. Pecora Award (NASA and Department of Interior) for outstanding contributions toward understanding the Earth by means of remote sensing and the AGU Hydrologic Sciences Award for outstanding contributions to the science of hydrology. He received the IEEE Geoscience and Remote Sensing Society Distinguished Achievement Award in 2011.

Rajat Bindlish (M'00–SM'05) received the B.S. degree in civil engineering from the Indian Institute of Technology, Bombay, India, in 1993, and the M.S. and Ph.D. degrees in civil engineering from The Pennsylvania State University, State College, PA, USA, in 1996 and 2000, respectively.

He is currently with Science Systems and Applications, Inc., working at the U. S. Department of Agriculture, Agricultural Research Service, Hydrology and Remote Sensing Laboratory, Beltsville, MD, USA. He is currently working on soil moisture estimation from microwave sensors and their subsequent application in land surface hydrology. His research interests involve the application of microwave remote sensing in hydrology.

Rolf H. Reichle received the M.S. degree ("Diplom") in physics from the University of Heidelberg, Heidelberg, Germany, in 1996, and the Ph.D. degree in environmental engineering from the Massachusetts Institute of Technology, Cambridge, MA, USA, in 2000.

He is currently a Research Physical Scientist with the Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, MD, USA. His research interests include land data assimilation, satellite-based remote sensing, and applications related to land-atmosphere interactions, weather prediction, and short-term climate forecasting.

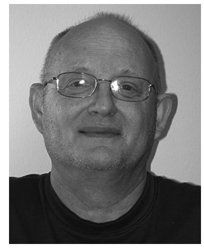
Steven K. Chan (M'01–SM'03) received the Ph.D. degree in electrical engineering from the University of Washington, Seattle, WA, USA, in 1998, specializing in electromagnetic wave propagation in random media.

He is currently a Scientist in hydrology at NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA, focusing on passive microwave soil moisture retrieval algorithm development. His work in remote sensing of soil moisture encompasses the NASA Aqua/AMSR-E (2002-2011), the JAXA GCOM-W/AMSR2 (2012-present), and more recently the NASA Soil Moisture Active Passive mission (2015-present).

David D. Bosch received the Ph.D. degree in hydrology from the University of Arizona, Tucson, AZ, USA, in 1990.

He is currently a Research Hydrologist with the Southeast Watershed Research Laboratory, Agricultural Research Service, Tifton, GA, USA. He joined the Agricultural Research Service, 1986. He leads a watershed research program investigating the impacts of land use on water balance and quality. His primary research interests include watershed and landscape scale hydrology; agricultural impacts on water quality; hydrologic and solute transport modeling of watershed processes; riparian buffer hydrology and solute transport; and developing new methods for assessing the impact of agricultural chemicals on ground and surface water supplies.

Dr. Bosch has been active in the validation of remotely sensed soil moisture products since 2000. He is a long-time member of the American Geophysical Union, the American Society of Agricultural and Biological Engineers, the American Society of Agronomy, and the Soil and Water Conservation Society.



Patrick J. Starks received the B.S. degree in physical geography from the University of Central Arkansas, Conway, AR, USA, in 1979, the M.A. degree in physical geography from the University of Nebraska-Omaha, Omaha, NE, USA, in 1984, and the Ph.D. degree in micrometeorology from the Department of Agronomy, University of Nebraska-Lincoln, Lincoln, NE, USA, in 1990.

From 1990 to 1992, he was a Postdoctoral Fellow in the Department of Atmospheric Science, University of Missouri-Columbia. Since 1992, he has been a Research Soil Scientist with the United States Department of Agriculture's Agricultural Research Service. He is currently with the U. S. Department of Agriculture, Agricultural Research Service, Grazinglands Research Laboratory, El Reno, OK, USA.

David C. Goodrich received the B.S. degree in civil and environmental engineering from the University of Wisconsin-Madison, Madison, WI, USA, in 1980, and received the Churchill Scholarship for a year of graduate study at Churchill College, Cambridge University, Cambridge, U.K. He also received the M.S. degree in civil and environmental engineering from the University of Wisconsin-Madison, Madison, WI, USA, in 1982 and the Ph.D. degree from the Department of Hydrology and Water Resources with emphasis in surface hydrologic modeling, University of Arizona, Tucson, AZ, USA, in 1990.

Since 1988, he has been a Research Hydraulic Engineer with the Southwest Watershed Research Center, U. S. Department of Agriculture, Agricultural Research Service, Tucson, AZ. Areas of research during his career have been directed to scaling issues in watershed rainfall–runoff response, identification of dominant hydrologic processes over a range of basin scales, climatic change impacts on semiarid hydrologic response, incorporation of remotely sensed data into hydrologic models, the functioning of semiarid riparian systems, nonmarket valuation of ecosystem services, flash-flood forecasting, and rapid post-fire watershed assessments.

Mark S. Seyfried received the Ph.D. degree from the University of Florida, Gainesville, FL, USA, in 1987.

He is a Soil Scientist with the U.S. Department of Agriculture, Agricultural Research Service, Northwest Watershed Research Center, Boise, ID, USA. His research interest includes measurement and simulation of soil water and temperature and how it is related to vegetation in under various climatic and soil conditions. He is currently investigating the effects of topography on the spatially integrated signal of soil water and temperature.

Dr. Seyfried is currently serving as the Lead Scientist for the hydrology research group in Boise and is a co-PI for the Reynolds Creek Critical Zone Observatory. He is a long-term member of the American Geophysical Union and Soil Science Society of America.